Deutsche Physikalische Gesellschaft DPG

Virtual 84th Annual Meeting of the DPG and DPG Meeting of the Condensed Matter Section (SKM)

with the Working Groups

Energy, Equal Opportunities, Information, Physics, Modern IT and Artificial Intelligence, Physics and Disarmament, Young DPG, Young Leaders in Physics

DPG SKM21

27 September – 1 October 2021

skm21.dpg-tagungen.de

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Content

Dear Participants,

On behalf of the German Physical Society (DPG), I would like to welcome you to the virtual 84. Annual Meeting of DPG and DPG-Tagung (DPG Meeting) of the Condensed Matter Section (SKM).

Due to the ongoing pandemic and the associated hygiene regulations, this meeting cannot yet take place in person, contrary to our hopes. Nevertheless, I am very pleased that our DPG Meeting will again offer an outstanding and exciting programme. This is all the more impressive as the organisation has taken place under difficult conditions.

This conference is of inestimable importance for scientific exchange in physics. But it is also an important contribution of the DPG as the world's largest physical society and communication platform to strengthen the acceptance and awareness of the importance of basic research, scientific thinking and facts, for the existence and future development of our society in politics and the public; and to do so with the special responsibility that those working in science, have a particularly high degree for shaping the whole of human life. The DPG has committed itself to this through its statutes, which is more urgently needed than ever to deal with the major challenges facing society; such as pandemics in particular, as well as climate change with its dramatic consequences for all life on our planet – as the Intergovernmental Panel on Climate Change (IPCC) report has once again warned.

I would like to express my great and heartfelt thanks to all those responsible for the success of this DPG Meeting. My special appreciation goes to the conference organisers, Prof. Erich Runge (Chair of the Condensed Matter Section, Fakultät für Mathematik und Naturwissenschaften, Technische Universität Ilmenau) and Prof. Dr. Norbert Esser (Local conference organisation, Institut für Festkörperphysik, TU Berlin and Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V., Material- u. Grenzflächenanalytik, Berlin), as well as the programme committee – consisting of the chairpersons of the divisions and working groups involved – for the outstanding programme of this conference. I would also like to thank the staff of the DPG Head Office for their support and supervision of all meetings.

I would also like to express my sincere thanks to the Wilhelm and Else Heraeus-Stiftung for again providing generous financial support to our young members.

I wish you all an exciting conference and many new insights.

Dr. Lutz Schröter
President
Deutsche Physikalische Gesellschaft e.V.

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Organisation

Organiser
Deutsche Physikalische Gesellschaft e. V.
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Email	dpg@dpg-physik.de
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Local Organiser
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Hardenbergstraße 36, 10623 Berlin and
Leibniz-Institut für Analytische Wissenschaften-ISAS-e.V.
Material- und Grenzflächenanalytik
Schwarzschildstraße 8, 12489 Berlin
EMail norbert.esser@isas.de

Scientific Organisation

Chair of the Condensed Matter Section (SKM)
Prof. Dr. Erich Runge
Fakultät für Mathematik und Naturwissenschaften
Technische Universität Ilmenau
Weimarer Straße 25, 98693 Ilmenau
Email erich.runge@tu-ilmenau.de

Chairs of the Participating Divisions of the DPG:

(BP)	Biological Physics	–	Prof. Dr. Gerhard Gompper (g.gompper@fz-juelich.de)
(CPP)	Chemical and Polymer Physics	–	Prof. Dr. Marcus Müller (mmueller@theorie.physik.uni-goettingen.de)
(DS)	Thin Films	–	Priv.-Doz. Dr. Patrick Vogt (patrick.vogt@hrz.tu-chemnitz.de)
(DY)	Dynamics and Statistical Physics	–	Prof. Dr. Markus Bär (markus.baer@ptb.de)
(HL)	Semiconductor Physics	–	Prof. Dr. Stephan Reitzenstein (stephan.reitzenstein@tu-berlin.de)
(KFM)	Crystalline Solids and their Microstructure	–	Prof. Dr. Stephan Krohns (stephan.krohns@physik.uni-augsburg.de)
(MA)	Magnetism	–	Prof. Dr. Heiko Wende (heiko.wende@uni-due.de)
(MM)	Metal and Material Physics	–	Prof. Dr. Gerhard Wilde (gwilde@uni-muenster.de)
(O)	Surface Science	–	Prof. Dr. Karsten Reuter (reuter@fhi-berlin.mpg.de)
(SOE)	Physics of Socio-economic Systems	–	Priv.-Doz. Dr. Jens C. Claussen (j.claussen@aston.ac.uk)
(TT)	Low Temperature Physics	–	Prof. Dr. Christian Enss (christian.enss@kip.uni-heidelberg.de
(VA)	Vacuum Science and Technology	–	Dr.-Ing. Thomas Giegerich (thomas.giegerich@kit.edu)

Chairs of the Participating Working Groups

(AGA)	Physics and Disarmament	–	Prof. Dr. Götz Neuneck (neuneck@me.com)
(AGI)	Information	–	Dr. Uwe Kahlert (kahlert@physik.rwth-aachen.de)
(AGyouLeaP)	young Leaders in Physics	–	Dr. Tobias Heindel (tobias.heindel@tu-berlin.de) J.Prof. Dr. Doris Reiter (doris.reiter@uni-muenster.de)
(AKC)	Equal Opportunities	–	OStR Agnes Sandner (akc@dpg-physik.de)
(AKE)	Energy	–	Dr. Karl-Friedrich Ziegahn (ziegahn@kit.edu)
(AKjDPG)	Young DPG	–	Dipl.-Phys. Philipp Jäger (philipp@pj4e.de)
(AKPIK)	Physics, Modern IT and Artificial Intelligence	–	Dr. Tim Ruhe (tim.ruhe@tu-dortmund.de)

Symposia

SYAM	–	Amorphous materials: structure, dynamics, properties
SYAN	–	Active nematics: From 2D to 3D
SYAW	–	Awards Symposium

SYAS – Attosecond and coherent spins: New frontiers
SYCE – Climate and energy: Challenges and options from a physics perspective
SYCL – Curvilinear condensed matter
SYCO – The Physics of CoViD Infections
SYCS – Multidimensional coherent spectroscopy of functional nanostructures
SYES – Spain as Guest of Honor
SYHN – Hybrid Nanomaterials: From Novel Physics and Multi-Scale Self-Organization to Functional Diversity on the Device Scale
SYMS – Novel phases and dynamical properties of magnetic skyrmions
SYNC – Advanced neuromorphic computing hardware: Towards efficient machine learning
SYNV – Potentials for NVs sensing magnetic phases, textures and excitations
SYPQ – The Rise of Photonic Quantum Technologies – Practical and Fundamental Aspects
SYQC – Facets of many-body quantum chaos
SYSD – SKM Dissertation Prize 2021
SYSM – Topological constraints in biological and synthetic soft matter
SYWH – Physics of van der Waals 2D heterostructures

Organisation of the online Exhibition of Scientific Instruments and Literature

DPG-Ausstellungs-, Kongreß- und Verwaltungsgesellschaft mbH
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Programme

The scientific programme consists of **1.254** contributions:

18	Plenary Talks
2	Evening Talks
9	Prize Talks
212	Invited Talks
14	Topical Talks
398	Contributions
597	Posters
4	Discussions

Acknowledgement

The Deutsche Physikalische Gesellschaft (DPG) wants to thank the following institutions for supporting the conference:

- Wilhelm and Else Heraeus-Stiftung, Hanau
- The Sponsors of the Conference
- DGM-Inventum GmbH
- and all staff who make the success of the conference possible.

Information for Participants

The virtuell conference will be held in the period 27 September – 1 October 2021.

Conference Location
Web-based Conference – Login information will be provided a few days before the event starts.

Conference Time Zone
Central European Summer Time (CEST), UTC+2.

Conference Website
https://skm21.dpg-tagungen.de/

Conference Platform Functionalities
To use all features of the digital conference, you need an up-to-date browser. The latest versions of Chrome, Firefox, Safari, and Edge with Blink engine are fully supported. JavaScript must be active. For video calls, permission to access your microphone and camera is required. Please note that firewalls of company or institute networks can also limit the functionality.
Immediately after logging in (with your credentials), you will be directed to the conference platform, which is the central access point on the web during the entire event. Here, all functionalities of the platform are available clearly and intuitively. In case of any technical issue please contact us at: +49 (0)69 75306 777.

In the header, you will find the main menu, which allows you to access the different areas of the conference – and to switch back and forth between them:

⇨ **Your Profile**
In the upper right corner of the screen, you will find access to your profile. All stored data concerning your person can be viewed here. Additionally, you are welcome to introduce yourself with a short description or a statement and mark your interests. Should you wish to network more closely with other participants, authors, or exhibitors during the conference, you can send them your virtual business card. Your e-mail address will also appear on this card.

⇨ **Schedule**
Here you will find an overview of the individual conference days and the respective contributions including short descriptions.

⇨ **Poster Hall**
View the submitted poster contributions and the corresponding abstracts and exchange ideas with the authors. During the poster sessions you will also have the opportunity to join a group video chat at each poster to exchange and discuss.

⇨ **Discussion Board**
Use the opportunity to exchange ideas with participants or start a thematic exchange via the „Create Thread“ button. Fill out the form and publish your contribution, which can now be commented on and discussed. A video chat room is linked to each contribution, where you can exchange ideas in small groups during the breaks, for example.

⇨ **Meet & Mingle**
Are you missing the real life coffee corner meetings at conferences? Then join our virtual breaks and meet colleagues in small or large groups!

⇨ **Directory**
Find other conference participants - also by areas of interest - and network via the contact request!

⇨ **Exhibition**
Within the area „Exhibition“ there will be an exhibition of scientific instruments of the conference sponsors during the entire time of the conference.

⇨ **Search**
If you want to find specific content and/or programme items, use the search function to find them very quickly. On the right side of the header, you will find your profile as well as a list of your contacts, and access to the chat function. The latter includes conversations already held with conference participants, but you can also start new conversations or individual video chats.

Electronic Programme Guide
Join the live stream or live zoom session to follow the current presentation.
Browse the programme for each day. By clicking on the individual contributions you will get additional information, such as the abstract. In addition to the basic information, you can ask the author a question about his or her contribution. This is publicly accessible. If you send a contact request to the participating authors, they can also exchange information bilaterally or arrange for an individual video chat. If you want to mark contributions in the run-up to or during the conference, you can highlight them with a „star". You will find the programme items marked in this way under „My Schedule".

Time Shift & On-Demand Content
If you have missed a presentation or want to listen to it again, you can still access the contributions up to 14 days after the event using your access data. The poster contributions and the networking opportunities with other conference participants will also be available to you until two weeks after the conference.

Conference Office
During the conference, you will find the conference office team in the Meet & Mingle area at the „Conference Office table". Opening hours are Mon-Thu, 8:30 am to 4:00 pm, Fri 8:30 am to 12:00 am. The team will be happy to answer any questions you may have about the conference.

Notice Board
All changes regarding the schedule of the conference will be updated currently. The information is identical to the programme updates of the scientific programme and is available at the scientific programme in other formats as well (ordered by publication date, filterable by conference part and as an rss-feed). Please use the form at *https://skm21.dpg-tagungen.de/programm/notice-board-form* to submit amendments, cancellations, etc.

Wilhelm and Else Heraeus Communication Programme
Within this programme, the active participation by young DPG members – from Germany and abroad – at the virtual DPG Meetings is financially supported.
For the virtual DPG-Meetings, the conference fee (and exclusively the "early bird rate") is subsidised at 100% (*submission of an application was open until 30 August 2021. Subsequent applications are not possible*). After the conference, your participation in the conference will be checked on the basis of the login data and the funding will be finally confirmed or rejected if no participation took place. Payment will be made – after prior notification by e-mail – by the end of October 2021 at the latest by bank transfer to the account you specified in your application.

The Deutsche Physikalische Gesellschaft thanks the Wilhelm and Else Heraeus-Stiftung for the generous financial support of young academic talents. We hope that young physicists will continue to seize the offered opportunity for active scientific communication at scientific conferences. A total of about 35,000 young academics were supported by this programme so far.

Information for Speakers
All speakers are invited to use our offer for a test session one week before the conference starts. The necessary information for the test session about day, time and login information will be sent out by email to the speakers. We would like to ask you to consider the following points for your presentation:

- Please use the same equipment with which you successfully completed your technical check to avoid technical problems during your presentation.
- Please be in the Zoom session of the virtual room where you will give your presentation at least 10 minutes before the session starts.
- Please sign in at Zoom with your full name so that the technical support can identify you as a speaker and give you the rights to share your screen, microphone and camera in Zoom.
- Please make sure that you respect your presentation time!

Information for Poster Presentations
The interactive poster sessions combine the classic contributed talks and posters in an attractive digital form. In addition to the posters, which are accessible throughout the whole conference, it is also possible to present the core messages of the poster in a short 3 minute video abstract, which can also be accessed on-demand.

We would like to ask you to consider the following points when creating your posters and videos:

- Please create your poster as a JPG/PNG file in portrait format (DIN A0; 84.10 cm wide and 118.90 cm high). The file must not exceed a maximum size of 25 MB.
- Please create your 3 minute video abstract in MP4 format. The file must not exceed a maximum size of 150 MB.

- The above criteria are based on the technical requirements of the conference platform used. Therefore, different formats are not possible unfortunately.

Presenting authors are requested to be available to answer questions and discuss via group video chat during the entire poster session at their poster.

Recording of Posters and Presentations
The posters, video abstracts, and the presentations will be available during and until 14 days (via the time-shift function) after the conference for all registered conference participants and are deleted after that. The DPG does not offer the presentations for public download.

Social Events

Evening Lectures

Public Evening Lecture (in German language)
Monday, 27 September, at 18:30, Room: PEL (and via Live-Stream on YouTube):
Prof. Dr. Robert Schlögl, Fritz Haber Institute of the Max Planck Society, Berlin, will speak about
„Die Rolle des Wasserstoffs im Energiesystem“.

Max-von-Laue-Lecture (in English language)
Thursday, 30 September, at 18:30, Room: MVL (and via Live-Stream on YouTube):
Prof. Steve Fetter, University of Maryland, College Park, USA, will speak about:
“What physicists can do to improve international security?”

The Evening Lectures are open to all conference participants and interested public. The lectures will be broadcasted live via the DPG YouTube channel https://www.youtube.com/watch?v=8PFYVW_MLpc. Registration is not necessary.

Annual General Meetings of the DPG Divisions and Working Groups

Division / Working Group		Date	Time	Location
(BP)	Biological Physics	Thur, Sept 30	18:00 - 19:00	MVBP
(CPP)	Chemical and Polymer Physics	Thur, Sept 30	17:30 - 18:30	MVCPP
(DS)	Thin Films	Thur, Sept 30	18:00 - 19:00	MVDS
(DY)	Dynamics and Statistical Physics	Thur, Sept 30	18:00 - 19:00	MVDY
(HL)	Semiconductor Physics	Thur, Sept 30	18:00 - 19:00	MVHL
(KFM)	Crystalline Solids and their Microstructures	Wed, Sept 29	13:00 - 13:30	MVKFM
(MA)	Magnetism	Thur, Sept 30	17:30 - 18:30	MVMA
(MM)	Metal and Material Physics	Wed, Sept 29	18:00 - 19:00	MVMM
(SOE)	Physics of Socio-economic Systems	Wed, Sept 29	18:00 - 19:00	MVSOE
(TT)	Low Temperature Physics	Thur, Sept 30	18:00 - 19:30	MVTT
(VA)	Vacuum Science and Technology	Mon, Sept 27	14:00 - 15:00	MVVA
(AGA)	Physics and Disarmament	Thur, Sept 30	17:00 - 18:00	MVAGA
(AGI)	Information	Wed, Sept 29	16:30 - 18:00	MVAGI

Award Presentation of the SKM Dissertation Prize
Five selected finalists will give their presentations at the SKM Dissertation Prize 2021 (SYSD) symposium. The Award Presentation will take place on Wednesday, 29 September at 16:10 in the Audimax 1.

Industry afternoon „Science meets Industry“
On Wednesday, 29 September 2021, at 13:30, Room: H1, the industry afternoon „Science meets Industry“ (SMI) will take place, in which the main sponsors of the conference will present their company, products and their use in research in the form of a short lecture (12 min. + 3 min. discussion). The schedule is as follows:

13:30 – 13:45	**SPECS Surface Nano Analysis GmbH** *„Collaboration of Science and Industry: Developments towards Novel and Revolutionary Analytical Approaches“*
13:50 – 14:05	**Hamamatsu Photonics Deutschland GmbH** *„Hamamatsu Photonics – ein „Hidden Champion“ der Optoelektronik“*
14:10 – 14:25	**Class 5 Photonics GmbH** *„Basics and concepts of optical parametric chirped-pulse amplification (OPCPA)“*

14:30 – 14:45	**Zurich Instruments AG** *„Boost your signal detection – while keeping the setup simple“*
14:50 – 15:05	**Bluefors Oy** *„Next steps in Cryogenics“*

All conference participants are kindly invited to the lectures.

Exhibition of the Sponsors & „Meet-your-exhibitor“
During the entire conference there will be an exhibition of scientific instruments of the conference sponsors, were the companies will present their latest products (see the detailed list at the end of this booklet). The exhibition will take place under the area „Exhibition“ of the conference platform.

In addition to the product presentation, you will also have the opportunity to meet a respective company representative at a „Meet-your-exhibitor“ table in a casual and informal atmosphere. Use the time to tentatively find out about the latest products and make new industry contacts.

In the „Meet & Mingle“ area of the conference platform you will find the „Meet-your-exhibitor“ tables at the following times:

Monday, 27 Sep 2021

13:00 – 13:30	iseg Spezialelektronik GmbH
13:00 – 13:30	Quantum Design GmbH
13:00 – 13:30	SAES Getters SpA, Italy
13:00 – 13:30	Incienta Technologie GmbH

Tuesday, 28 Sep 2021

12:00 – 13:30	Deutsche Forschungsgemeinschaft (DFG)
13:00 – 13:30	Cryogenic LTD., United Kingdom
13:00 – 13:30	Techn. Universität München (FRM II)
13:00 – 13:30	Menlo Systems GmbH

Wednesday, 29 Sept 2021

12:00 – 13:30	Deutsche Forschungsgemeinschaft (DFG)
13:00 – 13:30	Cryovac GmbH & Co. KG
13:00 – 13:30	Pfeiffer Vacuum GmbH
13:00 – 13:30	Onnes Technologies B.V., The Netherlands

Thursday, 30 Sept 2021

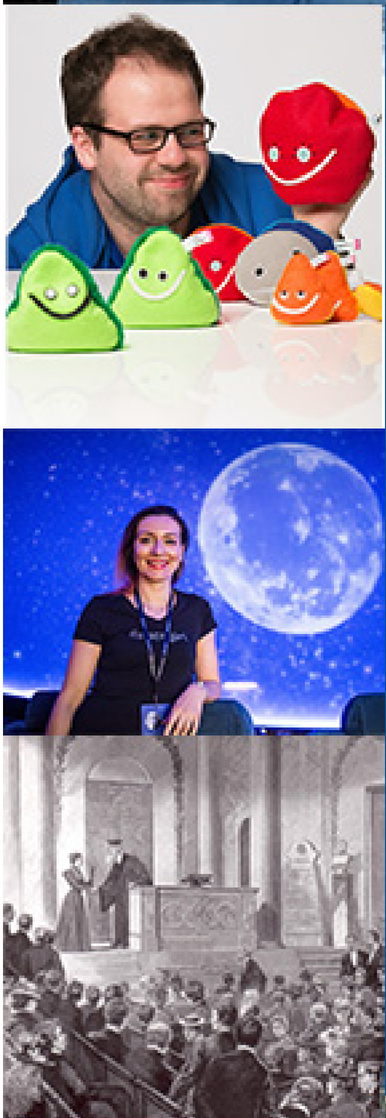
12:00 – 13:30	Deutsche Forschungsgemeinschaft (DFG)
13:00 – 13:30	Cryoandmore Budzylek GbR
13:00 – 13:30	Agilent Technologies Sales & Services GmbH & Co.KG

Friday, 1 Oct 2021

13:00 – 13:30	HTS-110, New Zealand
13:00 – 13:30	CreaTec Fischer & Co. GmbH
13:00 – 13:30	Oxford University Press, United Kingdom

All conference participants are welcome to attend the exhibition as well as the „Meet-your-exhibitor“ tables of the sponsors.

„Who inspires you?“
Since the anniversary year 2020 the DPG presents inspiring personalities on Instagram (@dpgphysik) and at www.175inspirierende.dpg-physik.de. Submit online suggestions for the 175 Inspirers: 175inspirierende@dpg-physik.de .

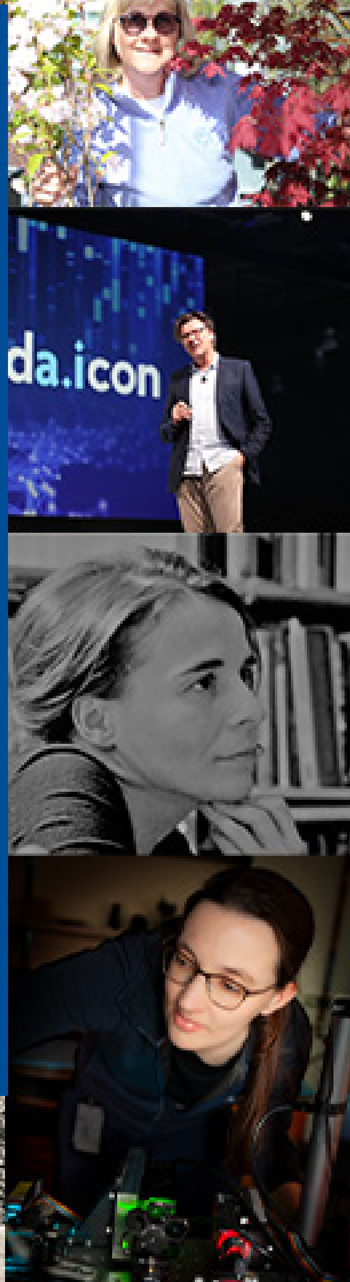


Sie gestalten Wissenschaft, gründen Unternehmen, prägen Gesellschaft, schaffen Kunst: Treffen Sie **175 Inspirierende** Physiker:innen auf dem DPG-Instagram- oder Facebook-Kanal und unter

www.175inspirierende.dpg-physik.de

Wer fehlt noch in diesem Kreis? Schlagen Sie Inspirierende vor!

175 Jahre
Deutsche Physikalische Gesellschaft



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Synopsis of the Daily Programme

Monday, September 27, 2021

			Plenary Talks
09:00	Audimax 1	PV I	Inference and Mitigation of COVID-19 •Viola Priesemann
09:00	Audimax 2	PV II	Quantum thermodynamics – superconducting circuit approach •Jukka Pekola
16:30	Audimax 1	PV III	Complex networks with complex nodes •Raissa D'Souza
16:30	Audimax 2	PV IV	Functional Three Dimensional Mesostructures as Bioelectronic Interfaces •John Rogers

SYSD

			Invited Talks
10:00	Audimax 2	SYSD 1.1	Avoided quasiparticle decay from strong quantum interactions •Ruben Verresen, Roderich Moessner, Frank Pollmann
10:25	Audimax 2	SYSD 1.2	Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications •Juliane Borchert
10:55	Audimax 2	SYSD 1.3	Attosecond-fast electron dynamics in graphene and graphene-based interfaces •Christian Heide
11:20	Audimax 2	SYSD 1.4	The thermodynamics of stochastic systems with time delay •Sarah A.M. Loos
11:50	Audimax 2	SYSD 1.5	First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM •Benjamin Zingsem
			Session
10:00	Audimax 2	SYSD 1	Presentations of the Finalists for the 2021 SKM Dissertation Prize

SYCO

			Invited Talks
13:30	Audimax 1	SYCO 1.1	A Tethered Ligand Assay to Probe SARS-CoV-2:ACE2 Interactions Magnus Bauer, Sophia Gruber, Adina Hausch, Lukas Milles, Thomas Nicolaus, Leonard Schendel, Pilar Lopez Navajas, Erik Procko, Daniel Lietha, Rafael Bernadi, Hermann Gaub, •Jan Lipfert
14:00	Audimax 1	SYCO 1.2	From molecular simulations towards antiviral therapeutics against COVID-19 •Rebecca Wade
14:45	Audimax 1	SYCO 1.3	The physical phenotype of blood cells is altered in COVID-19 Markéta Kubánková, Martin Kräter, Bettina Hohberger, •Jochen Guck
15:15	Audimax 1	SYCO 1.4	Extended lifetime of respiratory droplets in a turbulent vapor puff and its implications on airborne disease transmission •Detlef Lohse, Kai Leong Chong, Chong Shen Ng, Naoki Hori, Morgan Li, Rui Yang, Roberto Verzicco
15:45	Audimax 1	SYCO 1.5	Beyond the demographic vaccine distribution: Where, when and to whom should vaccines be provided first? •Benno Liebchen, Jens Grauer, Fabian Schwarzendahl, Hartmut Löwen
			Session
13:30	Audimax 1	SYCO 1	The Physics of CoViD Infections

Monday, September 27, 2021

SYNV

			Invited Talks
13:30	Audimax 2	SYNV 1.1	Harnessing Nitrogen Vacancy Centers in Diamond for Next-Generation Quantum Science and Technology •Chunhui Du
14:00	Audimax 2	SYNV 1.2	Nanoscale imaging of spin textures with single spins in diamond •Patrick Maletinsky
14:30	Audimax 2	SYNV 1.3	Spin-based microscopy of 2D magnetic systems •Jörg Wrachtrup
15:15	Audimax 2	SYNV 1.4	Exploring antiferromagnetic order at the nanoscale with a single spin microscope •Vincent Jacques
15:45	Audimax 2	SYNV 1.5	Nanoscale magnetic resonance spectroscopy with NV-diamond quantum sensors •Dominik Bucher
			Session
13:30	Audimax 2	SYNV 1	Potentials for NVs sensing magnetic phases, textures and excitations

SYSM

			Invited Talks
10:00	Audimax 1	SYSM 1.1	Interphase Chromatin Undergoes a Local Sol-Gel Transition Upon Cell Differentiation •Alexandra Zidovska
10:30	Audimax 1	SYSM 1.2	Topological Tuning of DNA Mobility in Entangled Solutions of Supercoiled Plasmids •Jan Smrek, Jonathan Garamella, Rae Robertson-Anderson, Davide Michieletto
11:15	Audimax 1	SYSM 1.3	Dynamics of macromolecular networks under topological and environmental constraints: some outstanding challenges •Dimitris Vlassopoulos
11:45	Audimax 1	SYSM 1.4	Supercoiling in a Protein Increases its Stability •Joanna Sulkowska, Szymon Niewieczerzał
12:15	Audimax 1	SYSM 1.5	Topology for soft matter photonics •Igor Musevic
			Session
10:00	Audimax 1	SYSM 1	Topological constraints in biological and synthetic soft matter

BP

			Invited Talks
10:00	H1	BP 1.1	Physics-Informed Deep Learning for Characterizing Perturbed Cell Growth •Robert Endres, Henry Cavanagh, Rob Lind, Andreas Mosbach, Gabriel Scalliet
11:30	H1	BP 2.1	PINCH-1 promotes migration in extracellular matrices and influences the mechano-phenotype •Claudia Tanja Mierke
			Sessions
10:00	H1	BP 1	Statistical physics of biological systems
11:30	H1	BP 2	Cytoskeleton

CPP

			Invited Talks
13:30	H1	CPP 2.1	On the permeability of dense polymer membranes •Joachim Dzubiella

Monday, September 27, 2021

CPP

13:30	H3	CPP 3.1	Emulsion Templating: Unexpected Morphology of Monodisperse Macroporous Polystyrene •Cosima Stubenrauch, Lukas Koch, Sophia Botsch, Wiebke Drenckhan
14:30	H3	CPP 3.4	Structural Transitions of Molecules on Surfaces •Angelika Kühnle

Sessions

11:15	H3	CPP 1	2D materials and their heterostructures
13:30	H1	CPP 2	Hydrogels and Microgels
13:30	H3	CPP 3	Polymer Physics

DS

Sessions

10:00	H3	DS 1	Thin Film Properties
11:15	H3	DS 2	2D materials and their heterostructures
13:30	H4	DS 3	2D semiconductors and van der Waals heterostructures I

DY

Session

10:00	H1	DY 1	Statistical physics of biological systems

HL

Invited Talks

10:00	H4	HL 1.1	Phonon Screening of Excitons in Halide Perovskites and Beyond •Marina Filip
10:30	H4	HL 1.2	Anharmonic semiconductors – Lessons Learned from Halide perovskites •Omer Yaffe
11:00	H4	HL 1.3	Exciton structure symmetry analysis for quantum-well layered halide perovskites and charge-energy transfer in presence of π-conjugated organic chromophores •Claudio Quarti
11:45	H4	HL 1.4	Solid state ionics of hybrid halide perovskites: equilibrium situation and light effects •Alessandro Senocrate, Gee Yeong Kim, Tae-Youl Yang, Giuliano Gregori, Michael Grätzel, Joachim Maier
12:15	H4	HL 1.5	Unifying Ultrafast Polarization Responses of Lead Halide Perovskites via Two-Dimensional Optical Kerr Effect •Sebastian F. Maehrlein
13:30	H4	HL 5.1	The role of chalcogen vacancies for atomic defect emission in MoS_2 Elmar Mitterreiter, Bruno Schuler, Daniel Hernangómez-Pérez, Julian Klein, Jonathan Finley, Sivan Refaely-Abramson, Alexander Holleitner, Alexander Weber-Bargioni, •Christoph Kastl

Sessions

10:00	H4	HL 1	Focus Session: When theory meets experiment: Hybrid halide perovskites for applications beyond solar
10:00	H7	HL 2	Focus Session: Exotic Charge Density Wave States of Matter: Correlations and Topology
10:00	P	HL 3	Poster Session I
11:15	H3	HL 4	2D materials and their heterostructures
13:30	H4	HL 5	2D semiconductors and van der Waals heterostructures I
13:30	H5	HL 6	Focus Session: Magnon Polarons – Magnon-Phonon Coupling and Spin Transport

Monday, September 27, 2021

MA

			Invited Talks
10:00	H5	MA 1.1	Utilizing Vacuum States above Surfaces for Imaging and Manipulation of Atomic-Scale Magnetism •Anika Schlenhoff
13:30	H5	MA 2.1	Magnon-polarons in magnetic insulators •Benedetta Flebus
14:00	H5	MA 2.2	Spin-phonon coupling in non-local spin transport through magnetic insulators •Rembert Duine
14:30	H5	MA 2.3	Double accumulation and anisotropic transport of magneto-elastic bosons in yttrium iron garnet films •Alexander A. Serga
15:15	H5	MA 2.5	Magnon polarons and the low-temperature spin-Seebeck effect •Piet Brouwer, Rico Schmidt
15:45	H5	MA 2.6	Magnon-Polarons in different flavors: (anti)ferromagnetic to topological •Akashdeep Kamra
16:15	H5	MA 2.7	Magnon polarons in antiferromagnetic insulator Cr2O3 •Jing Shi
			Sessions
10:00	H5	MA 1	Surface Magnetism (joint session MA/O)
13:30	H5	MA 2	Focus Session: Magnon Polarons – Magnon-Phonon Coupling and Spin Transport
13:30	P	MA 3	Posters Magnetism I

MM

			Invited Talks
10:00	H8	MM 1.1	Using mobile interfaces to rapidly move atoms and create sharp chemical boundaries in Fe-C-Mn alloys •Sybrand van der Zwaag
15:15	H2	MM 4.1	Investigation of the early stage of reactive interdiffusion in the Cu-Al system by in-situ transmission electron microscopy Florent Moisy, •Xavier Sauvage, Eric Hug
			Sessions
10:00	H8	MM 1	Topical Session Interface-Dominated Phenomena – Moving Interfaces
11:15	H8	MM 2	Topical Session Interface-Dominated Phemomena – Moving Interfaces / Functional Properties
13:30	H2	MM 3	Topical Session Interface-Dominated Phenomena – Defect Structures and Mechanical Properties
15:15	H2	MM 4	Topical Session Interface-Dominated Phenomena – Diffusion

TT

			Invited Talks
11:45	H7	TT 2.4	Electronic instabilities of kagomé metals and density waves in the AV_3Sb_5 materials •Leon Balents
14:45	H7	TT 4.4	2D Magnetism and Its Efficient Control •Cheng Gong
			Sessions
10:00	H6	TT 1	Focus Session: Disordered and Granular Superconductors: Fundamentals and Applications in Quantum Technology I
10:00	H7	TT 2	Focus Session: Exotic Charge Density Wave States of Matter: Correlations and Topology

Monday, September 27, 2021

TT

13:30	H6	TT 3	Focus Session: Entanglement as a Probe for Correlated Quantum Matter
13:30	H7	TT 4	Focus Session: Correlated van-der-Waals Magnets
13:30	P	TT 5	Poster Session: Superconductivity

VA

Invited Talks

10:00	H2	VA 1.1	Deterministic and stochastic numerical approaches in Rarefied Gas Dynamics •Stylianos Varoutis, Christos Tantos
10:30	H2	VA 1.2	Deterministic modeling of neutral gas flows of tokamak nuclear fusion devices •Christos Tantos, Stylianos Varoutis
11:00	H2	VA 1.3	Stochastic Simulation of Mercury Diffusion Pumps Using Direct Simulation Monte Carlo •Tim Teichmann, Christian Day, Thomas Giegerich
11:45	H2	VA 2.1	IFMIF-DONES gas flow modelling using Test Particle Monte-Carlo Simulations •Volker Hauer
12:15	H2	VA 2.2	Current design status and outgassing considerations for the vacuum system of the Einstein Telescope •Katharina Battes, Christian Day, Stefan Hanke

Sessions

10:00	H2	VA 1	Rarefied gas flows and novel approaches for particle simulation
11:45	H2	VA 2	Vacuum technology: New developments and applications
14:00	MVVA	VA 3	Annual General Meeting of the Vacuum Science and Technology Division

AKC

Invited Talk, Discussion

15:15	H1	AKC 1.1	Gender and Diversity Studies as a Tool to Overcome Social Inequalities in Physics •Helene Götschel
15:45	H1	AKC 1.2	Diversity in Physics? •Andrea B. Bossmann, Franziska Kaiser, Helene Götschel

Session

15:15	H1	AKC 1	Diversity in Physics

AKE

Invited Talks

13:30	H8	AKE 1.1	Elektrische Energiespeicherung mit Flüssigmetallen und Salzschmelzen •Tom Weier, Gerrit M. Horstmann, Steffen Landgraf, Michael Nimtz, Paolo Personnettaz, Frank Stefani, Norbert Weber
14:00	H8	AKE 1.2	Hydrogen and e-fuels – energy systems, technology, and projects •Alexander Tremel
14:30	H8	AKE 2.1	NOx und andere luftverunreinigende Stoffe in der Außenluft und in Innenräumen: Ursachen und Wirkung •Tunga Salthammer
15:15	H8	AKE 2.2	Highly Efficient Monolithic Tandem Devices with Perovskite Top Cells •Steve Albrecht
15:45	H8	AKE 2.3	Limits to wind energy: From the physical basis to practical implications •Axel Kleidon

Sessions

13:30	H8	AKE 1	Thermische und chemische Energiespeicher
14:30	H8	AKE 2	Technologien für die Energiewende und ihre Implikationen I

Monday, September 27, 2021

			Meet-your-exhibitor
13:00	Meet&Mingle		iseg Spezialelektronik GmbH
13:00	Meet&Mingle		Quantum Design GmbH
13:00	Meet&Mingle		SAES Getters SpA
13:00	Meet&Mingle		Incienta Technologies GmbH

			Public Evening Lecture
18:30	PEL	PV V	Die Rolle des Wasserstoffs im Energiesystem •Robert Schlögl

Tuesday, September 28, 2021

Plenary Talks

09:00	Audimax 1	PV VI	Correlated electrons with knots •Silke Bühler-Paschen
09:00	Audimax 2	PV VII	Cuprous oxide: the ultimate material for studying excitons? •Manfred Bayer
16:30	Audimax 1	PV VIII	The Structural Origins of Wood Cell Wall Toughness •Cynthia Volkert, Mona-Christin Maaß, Salimeh Saleh, Holger Militz
16:30	Audimax 2	PV IX	Microscopic polarization and magnetization fields: Towards a 'post modern' theory •John Sipe

SYAM

Invited Talks

13:30	Audimax 1	SYAM 1.1	Glassy dynamics of vitrimers •Liesbeth Janssen
14:00	Audimax 1	SYAM 1.2	Liquid-Liquid Phase Transition in Thin Vapor-Deposited Glass Films •Zahra Fakhraai
14:30	Audimax 1	SYAM 1.3	Connection between structural properties and atomic motion in ultraviscous metallic liquids close to the dynamical arrest •Beatrice Ruta, Nico Neuber, Isabella Gallino, Ralf Busch
15:15	Audimax 1	SYAM 1.4	Signatures of the spatial extent of plastic events in the yielding transition in amorphous solids •Celine Ruscher, Daniel Korchinski, Joerg Rottler
15:45	Audimax 1	SYAM 1.5	Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment •Olfa D'Angelo, W. Till Kranz

Session

13:30	Audimax 1	SYAM 1	Amorphous materials: structure, dynamics, properties

SYCS

Invited Talks

10:00	Audimax 1	SYCS 1.1	Multidimensional coherent spectroscopy of perovskite nanocrystals •Steven Cundiff, Albert Liu, Diogo Almeida, Gabriel Nagamine, Lazaro Padilha
10:30	Audimax 1	SYCS 1.2	Coherent multidimensional techniques for the characterization of nanomaterials •Elisabetta Collini
11:00	Audimax 1	SYCS 1.3	Exciton Dynamics revealed by Multidimensional Coherent Spectroscopies applied to Light-Harvesting Systems •Thomas L.C. Jansen
11:45	Audimax 1	SYCS 1.4	Revealing couplings with action-based 2D microscopy •Tobias Brixner
12:15	Audimax 1	SYCS 1.5	Low-frequency phonons affect charge carrier dynamics in hybrid perovskites •Mischa Bonn

Session

10:00	Audimax 1	SYCS 1	Symposium: Multidimensional coherent spectroscopy of functional nanostructures

SYMS

Invited Talks

10:00	Audimax 2	SYMS 1.1	Imaging skyrmions in synthetic antiferromagnets by single spin relaxometry •Aurore Finco

Tuesday, September 28, 2021

SYMS

10:30	Audimax 2	SYMS 1.2	Microwave spectroscopy of the skyrmionic states in a chiral magnetic insulator •Aisha Aqeel, Jan Sahliger, Takuya Taniguchi, Stefan Maendl, Denis Mettus, Helmuth Berger, Andreas Bauer, Markus Garst, Christian Pfleiderer, Christian H. Back
11:15	Audimax 2	SYMS 1.3	Archimedean Screw in Driven Chiral Magnets •Nina del Ser
11:45	Audimax 2	SYMS 1.4	Frustration-driven magnetic fluctuations as the origin of the low-temperature skyrmion phase in $Co_7Zn_7Mn_6$ •Jonathan White, Victor Ukleev, Kosuke Karube, Peter Derlet, Chennan Wang, Hubertus Luetkens, Daisuke Morikawa, Akiko Kikkawa, Lucile Mangin-Thro, Andrew Wildes, Yuichi Yamasaki, Yuichi Yokoyama, Le Yu, Cinthia Piamonteze, Nicolas Jaouen, Yusuke Tokunaga, Henrik Rønnow, Taka-hisa Arima, Yoshinori Tokura, Jonathan White
12:15	Audimax 2	SYMS 1.5	Magnetic Skyrmions as Topological Multi-Media Influencers •Sebastián A. Díaz
			Session
10:00	Audimax 2	SYMS 1	Novel phases and dynamical properties of magnetic skyrmions

SYQC

			Invited Talks
13:30	Audimax 2	SYQC 1.1	Holographic interpretation of SYK quantum chaos •Alexander Altland
14:00	Audimax 2	SYQC 1.2	Non-Fermi liquids and the lattice •Sean Hartnoll
14:30	Audimax 2	SYQC 1.3	Dual-unitary circuits: non-equilibrium dynamics and spectral statistics •Bruno Bertini
15:15	Audimax 2	SYQC 1.4	Post-Ehrenfest many-body quantum interferences in ultracold atoms •Steven Tomsovic
15:45	Audimax 2	SYQC 1.5	Dynamics in unitary and non-unitary quantum circuits •Vedika Khemani
			Session
13:30	Audimax 2	SYQC 1	Facets of many-body quantum chaos

CPP

			Invited Talks
10:00	H3	CPP 4.1	Adaptable amphiphilic co-networks: structure and properties in relation with multi-quantum NMR •Michael Lang, Reinhard Scholz, Lucas Löser, Carolin Bunk, Frank Böhme, Kay Saalwächter
10:30	H3	CPP 4.2	Adaptive networks through supramolecular interactions •Ilja Voets
11:45	H3	CPP 4.5	Tunable self-assembled hydrogels from block copolymers with thermoresponsive and pH-responsive blocks •Christine M. Papadakis, Florian A. Jung, Constantinos Tsitsilianis
			Sessions
10:00	H3	CPP 4	Focus: The Physics of Adaptive Polymer Networks
17:30	P	CPP 5	Poster Session I
17:30	P	CPP 6	Poster Session II

Tuesday, September 28, 2021

DS

Topical Talks

13:30	H3	DS 5.1	Single crystal diamond grown by CVD: state of the art, current challenges and applications •Jean-Charles Arnault, Samuel Saada, Victor Ralchenko
14:00	H3	DS 5.2	Tuning Semiconductor Mode-Locked Laser Frequency Combs by Gain and Cavity Design Stefan Meinecke, •Kathy Lüdge
14:30	H3	DS 5.3	Monolayer-thick GaN/AlN heterostructures for UVB & UVC ranges: technology, design and properties Valentin Jmerik, Alexey Toropov, Valery Davydov, •Sergey Ivanov
15:15	H3	DS 5.4	Optical and vibrational properties of layered 2D materials •Janina Maultzsch
15:45	H3	DS 5.5	Organic/inorganic low dimensional material systems: Fundamental aspects and device applications •Emil List-Kratochvil

Sessions

10:00	P	DS 4	Poster
13:30	H3	DS 5	Focus Session: Highlights of Materials Science and Applied Physics I

DY

Invited Talk

10:00	H6	DY 2.1	Local Versus Global Two-Photon Interference in Quantum Networks •Sonja Barkhofen, Thomas Nitsche, Syamsundar De, Evan Meyer-Scott, Johannes Tiedau, Jan Sperling, Aurél Gábris, Igor Jex, Christine Silberhorn

Sessions

10:00	H6	DY 2	Quantum Chaos
17:30	P	DY 3	Poster Sesssion I: Quantum Chaos and Many-Body Quantum Dynamics
17:30	P	DY 4	Poster Session II: Nonlinear Dynamics, Simulations and Machine Learning
17:30	P	DY 5	Poster Session III: Statistical Physics, Complex Fluids and Soft Matter

HL

Invited Talks

10:00	H4	HL 7.1	Ultrafast Spin-Lasers Natalie Jung, Markus Lindemann, Tobias Pusch, Rainer Michalzik, Martin R. Hofmann, •Nils C. Gerhardt
13:30	H4	HL 11.1	Modulation Doping in High-Mobility Alkaline-Earth Stannates •Bharat Jalan
14:00	H4	HL 11.2	Ultrathin oxides on InGaN nanowires: Hybrid nanostructure photoelectrodes and optical analysis of chemical processes P. Neuderth, J. Schörmann, M. Coll, M. de la Mata, J. Arbiol, R. Marschall, •M. Eickhoff
14:30	H4	HL 11.3	Doping and charge compensation mechanisms in semiconducting oxides •Andreas Klein
15:00	H4	HL 11.4	Oxide Memristors for edge computing and secure electronics •Heidemarie Schmidt
15:30	H4	HL 11.5	Integration of 33°Y-$LiNbO_3$ films with high-frequency BAW resonators Sondes Boujnah, Mihaela Ivan, Vincent Astié, Samuel Margueron, Mario Constanza, Jean-Manuel Decams, •Ausrine Bartasyte

Sessions

10:00	H4	HL 7	Semiconductor Lasers
10:00	P	HL 8	Poster Session II
11:45	H4	HL 9	Nitride: Preparation, Charakterization and Devices

Tuesday, September 28, 2021

HL

13:30	H3	HL 10	Focus Session: Highlights of Materials Science and Applied Physics I
13:30	H4	HL 11	Focus Session: Functional Metal Oxides for Novel Applications and Devices
13:30	H5	HL 12	Focus Session: Spin-Charge Interconversion
13:30	P	HL 13	Poster Session III

KFM

Invited Talks

10:00	H2	KFM 1.1	Effect of humidity on the ferroelectric domain wall dynamics in BaTiO3 thin films Irena Spasojevic, Albert Verdaguer, Gustau Catalan, •Neus Domingo
11:30	H2	KFM 1.5	Magnetic avalanche of non-oxide conductive domain walls •Somnath Ghara, Korbinian Geirhos, Lukas Kuerten, Peter Lunkenheimer, Vladimir Tsurkan, Manfred Fiebig, István Kézsmárki
14:15	H2	KFM 4.1	Single crystal diamond growth by chemical vapor deposition for high-end applications: Recent trends and state of the art •Matthias Schreck, Theodor Grünwald
14:45	H2	KFM 4.2	Development of diamond based kinetic inductance detectors •Francesco Mazzocchi, Dirk Strauss, Theo Scherer

Sessions

10:00	H2	KFM 1	Focus Session I: Ferroics – Domains and Domain Walls
11:15	H5	KFM 2	Materials for Energy Storage
13:30	H2	KFM 3	Focus Session II: Ferroics – Domains and Domain Walls
14:15	H2	KFM 4	Focus Session III: Diamond
16:00	P	KFM 5	Poster Session KFM

MA

Invited Talks

10:00	H5	MA 4.1	2D Magnetic materials •Alberto Morpurgo
13:30	H5	MA 6.1	Spin-charge interconversion with oxide 2-dimensional electron gases •Manuel Bibes
14:00	H5	MA 6.2	Spin-to-charge current conversion for logic devices •Felix Casanova
14:30	H5	MA 6.3	Electrical and thermal generation of spin currents by magnetic graphene •B.J van Wees, T.S. Ghiasi, A.A. Kaverzin, D.K. de Wal, A.H. Dismukes, Bart Wees
15:15	H5	MA 6.4	Ferroelectric switching of spin-to-charge conversion in GeTe •Christian Rinaldi
15:45	H5	MA 6.5	Theory of spin and orbital Edelstein effects in a topological oxide two-dimensional electron gas •Annika Johansson, Börge Göbel, Jürgen Henk, Manuel Bibes, Ingrid Mertig
16:15	H5	MA 6.6	Nonlinear magnetoresistance and Hall effect from spin-momentum locking •Giovanni Vignale

Sessions

10:00	H5	MA 4	Spin-Dependent 2D Phenomena
10:00	P	MA 5	Posters Magnetism II
13:30	H5	MA 6	Focus Session: Spin-Charge Interconversion

MM

Session

10:00	P	MM 5	Topical Session Interface Dominated Phenomena – Poster

Tuesday, September 28, 2021

TT

			Invited Talk
10:00	H7	TT 6.1	Spin Triplet Superconductivity within Superconductors as Determined by FMR Spin pumping •Lesley Cohen
			Sessions
10:00	H7	TT 6	Focus Session: Emerging Phenomena in Superconducting Low Dimensional Hybrid Systems I
13:30	H6	TT 7	Focus Session: Disordered and Granular Superconductors: Fundamentals and Applications in Quantum Technology II
13:30	H7	TT 8	Focus Session: Emerging Phenomena in Superconducting Low Dimensional Hybrid Systems II
13:30	P	TT 9	Poster Session: Correlated Electrons

AKC

			Discussion
12:00	H5	AKC 2.1	The time after: How COVID-19 crisis redefined the R&I leadership •Jeanne Rubner, Burghilde Wieneke-Toutaoui, Kees Van der Beek, Sara Pirrone, Sunny Xin Wang
			Session
12:00	H5	AKC 2	The time after: How COVID-19 crisis redefined the R&I leadership

AKE

			Invited Talks
10:00	H8	AKE 3.1	Zur Energiewende: Zweispeicher-Modell und Pumpspeicherkraftwerke im aufgelassenen Tagebauloch •Gerhard Luther, Horst Schmidt-Böcking
10:30	H8	AKE 3.2	Bioenergy: Chances and Pitfalls •Katja Bühler
11:15	H8	AKE 3.3	Import options for chemical energy carriers from renewable sources to Germany •Johannes Hampp, Michael Düren, Tom Brown
11:45	H8	AKE 3.4	Geothermal Energy: Risks and benefits of utilizing hot fluids from the deep underground •Hannes Hofmann, Simona Regenspurg, Ernst Huenges
12:15	H8	AKE 3.5	Einsatz bildgebender Messverfahren und numerischer Modellierungswerkzeuge für die Verbesserung der Energieeffizienz industrieller Mehrphasenprozesse •Uwe Hampel
13:30	H8	AKE 4.1	Nukleare Entsorgung im Kontext der internationalen Nutzung der Kernenergie •Thorsten Stumpf
14:00	H8	AKE 4.2	Nuclear fusion on the way to ITER and beyond •Thomas Pütterich, the ASDEX Upgrade Team
14:30	H8	AKE 4.3	Hochbelastbare Materialien für die Kernfusion: Entwicklungen und Perspektiven •Christian Linsmeier
			Sessions
10:00	H8	AKE 3	Technologien für die Energiewende und ihre Implikationen II
13:30	H8	AKE 4	Herausforderungen bei nuklearen Energietechnologien

Tuesday, September 28, 2021

AKPIK

			Sessions
11:15	H1	AKPIK 1	RDM I: NFDI consortia
13:30	H1	AKPIK 2	RDM II: Perspectives in Research Data Management

AGI

			Invited Talks, Topical Talk
11:15	H1	AGI 1.1	Challenges in data preservation in high energy physics •Ulrich Schwickerath
11:45	H1	AGI 1.2	The PUNCH4NFDI Consortium in the NFDI •Thomas Schörner
12:05	H1	AGI 1.3	DAPHNE4NFDI – Daten aus Photonen und Neutronenexperimenten Anton Barty, Bridget Murphy, Astrid Schneidewind, Wiebe Lohstroh, •Christian Gutt
12:25	H1	AGI 1.4	FAIRmat – Making Materials Data Findable and AI Ready Claudia Draxl, •FAIRmat team
13:30	H1	AGI 2.1	NFDI4Phys research data management for the next decades •Hans-Günther Döbereiner
14:00	H1	AGI 2.2	Semantic Research Data Management in the National Research Data Initiative (NFDI) •Sören Auer
14:30	H1	AGI 2.3	NFDI, EOSC, Gaia-X: Three Data Clouds – One Goal? •Klaus Tochtermann
15:30	H1	AGI 2.4	Research Data Management and Higher Education in Physics •Janice Bode, Philipp Jaeger
16:00	H1	AGI 2.5	Discussion •Philipp Jäger, Uwe Kahlert, Tim Ruhe
			Sessions
11:15	H1	AGI 1	RDM I: NFDI consortia
13:30	H1	AGI 2	RDM II: Perspectives in Research Data Management

		Meet-your-exhibitor
12:00	Meet&Mingle	Deutsche Forschungsgemeinschaft (DFG)
13:00	Meet&Mingle	Cryogenic LTD
13:00	Meet&Mingle	Techn. Universität München (FRM II)
13:00	Meet&Mingle	Menlo Systems GmbH

Wednesday, September 29, 2021

			Plenary Talks
09:00	Audimax 1	PV X	Revealing the topological nature of transport at mesoscopic scales with quantum interferences •Helene Bouchiat, A. Bernard, A. Murani, B. Dassonneville, A. Kasumov, M. Ferrier, R. Deblock, S. Guéron
09:00	Audimax 2	PV XI	Quantum choreography to the beat of light •Rupert Huber

SYAW

			Prize Talks
13:30	Audimax 1	SYAW 1.1	Organic semiconductors – materials for today and tomorrow •Anna Köhler (Laureate of the Max-Born-Prize 2020)
14:00	Audimax 1	SYAW 1.2	PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors •Grzegorz Karczewski (Laureate of the Smoluchowski-E.-Warburg-Prize 2021)
14:40	Audimax 1	SYAW 1.3	Fingerprints of correlation in electronic spectra of materials •Lucia Reining (Laureate of the Gentner-Kastler-Prize 2020)
15:10	Audimax 1	SYAW 1.4	Artificial Spin Ice: From Correlations to Computation •Naëmi Leo (Laureate of the Hertha-Sponer-Prize 2021)
15:40	Audimax 1	SYAW 1.5	From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices •Andreas K. Hüttel (Laureate of the Walter-Schottky-Prize 2021)
16:10	Audimax 1		**Presentation of the Dissertation Prize 2021 to the winner**
16:20	Audimax 1	SYAW 1.6	Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain •Zhe Wang (Laureate of the Walter-Schottky-Prize 2020)
16:50	Audimax 1	SYAW 1.7	Imaging the effect of electron transfer at the atomic scale •Laerte Patera (Laureate of the Gustav-Hertz-Prize 2020)
			Session
13:30	Audimax 1	SYAW 1	Prize Talks

SYCL

			Invited Talks
10:00	Audimax 2	SYCL 1.1	Curvature Effects and Topological Defects in Chiral Condensed and Soft Matter •Avadh Saxena
10:30	Audimax 2	SYCL 1.2	Topology and Transport in nanostructures with curved geometries •Carmine Ortix
11:15	Audimax 2	SYCL 2.1	Superconductors and nanomagnets evolve into 3D •Oleksandr Dobrovolskiy
11:45	Audimax 2	SYCL 2.2	Properties of domain walls and skyrmions in curved ferromagnets •Volodymyr Kravchuk
12:15	Audimax 2	SYCL 2.3	X-ray three-dimensional magnetic imaging •Valerio Scagnoli
			Sessions
10:00	Audimax 2	SYCL 1	Curvilinear condensed matter 1
11:15	Audimax 2	SYCL 2	Curvilinear condensed matter 2

Wednesday, September 29, 2021

SYES

			Invited Talks
13:30	Audimax 2	SYES 1.1	DFMC-GEFES •Julia Herrero-Albillos
13:40	Audimax 2	SYES 1.2	Towards Phononic Circuits based on Optomechanics •Clivia M. Sotomayor Torres
14:10	Audimax 2	SYES 1.3	Adding magnetic functionalities to epitaxial graphene •Rodolfo Miranda
14:45	Audimax 2	SYES 1.4	Bringing nanophotonics to the atomic scale •Javier Aizpurua
15:15	Audimax 2	SYES 1.5	Hydrodynamics of collective cell migration in epithelial tissues •Jaume Casademunt
15:45	Audimax 2	SYES 1.6	Understanding the physical variables driving mechanosensing •Pere Roca-Cusachs
			Session
13:30	Audimax 2	SYES 1	Spain as Guest of Honor

SYNC

			Invited Talks
10:00	Audimax 1	SYNC 1.1	Equilibrium Propagation: a Road for Physics-Based Learning •Damien Querlioz
10:30	Audimax 1	SYNC 1.2	Machine Learning and Neuromorphic Computing: Why Physics and Complex Systems are Indispensable •Ingo Fischer
11:00	Audimax 1	SYNC 1.3	Photonic Tensor Core Processor and Photonic Memristor for Machine Intelligence •Volker Sorger
11:45	Audimax 1	SYNC 1.4	Material learning with disordered dopant networks •Wilfred van der Wiel
12:15	Audimax 1	SYNC 1.5	In-memory computing with non-volatile analog devices for machine learning applications •John Paul Strachan
			Session
10:00	Audimax 1	SYNC 1	Symposium: Advanced neuromorphic computing hardware: Towards efficient machine learning

CPP

			Invited Talks
10:00	H3	CPP 7.1	Chemically Fueled Out-Of-Equilibrium Self-Assemblies and Autonomous Material Systems •Andreas Walther
11:15	H3	CPP 7.4	The quest for robust superhydrophobic surfaces •Robin Ras
			Sessions
10:00	H3	CPP 7	Soft Matter
17:30	P	CPP 8	Poster Session III

DY

			Invited Talks
13:30	H6	DY 9.1	Nanofriction in Ion Coulomb Systems •Tanja Mehlstäubler

Wednesday, September 29, 2021

DY

15:00	H6	DY 10.1	Effect of fibrosis on propagation on non-linear waves and onset of arrhythmias in cardiac tissue •Alexander Panfilov, Timur Nezlobinsky, Farhad Pashakhanloo
16:00	H6	DY 10.4	Chaos and nonlinear dynamics in the heart: Experiments and simulations of arrhythmias and defibrillation •Flavio fenton
			Sessions
10:00	H3	DY 6	Soft Matter
10:00	H6	DY 7	Focus Session: Facets of Many-Body Quantum Chaos (organised by Markus Heyl and Klaus Richter)
11:15	H7	DY 8	Quantum Computing
13:30	H6	DY 9	Many-Body Quantum Dynamics I
15:00	H6	DY 10	Focus session: Nonlinear Dynamics of the Heart I (organized by Markus Bär, Stefan Luther and Ulrich Parlitz)

HL

			Invited Talk
10:00	H4	HL 14.1	Quantum Interference of Identical Photons from Remote Quantum Dots •Giang N. Nguyen, Liang Zhai, Clemens Spinnler, Julian Ritzmann, Matthias C. Löbl, Andreas D. Wieck, Arne Ludwig, Alisa Javadi, Richard J. Warburton
			Session
10:00	H4	HL 14	Materials and devices for quantum technology

KFM

			Sessions
10:00	H5	KFM 6	Skyrmions I
10:00	H1	KFM 7	Dielectric, Elastic and Electromechanical Properties
10:45	H1	KFM 8	Crystal Structure / Real Structure / Microstructure
12:00	H1	KFM 9	Instrumentation and Methods
13:00	MVKFM	KFM 10	Annual General Meeting of the Crystalline Solids and their Microstructure Division

MA

			Invited Talks
10:00	H5	MA 7.1	Anatomy of skyrmion-defect interactions and their impact on detection protocols •Samir Lounis
13:30	H5	MA 10.1	Topological spin crystals stabilized by itinerant frustration •Yukitoshi Motome
14:00	H5	MA 10.2	Formation of spin-hedgehog lattices and giant topological transport properties in chiral magnets •Naoya Kanazawa
14:30	H5	MA 10.3	Topological-chiral magnetic interactions driven by emergent orbital magnetism •Sergii Grytsiuk, Jan-Philipp Hanke, Markus Hoffmann, Juba Bouaziz, Olena Gomonay, Gustav Bihlmayer, Samir Lounis, Yuriy Mokrousov, Stefan Blügel
15:15	H5	MA 10.4	Complex spin structures in thin transition metals films and their oxides •Matthias Bode
			Sessions
10:00	H5	MA 7	Skyrmions I
10:00	H2	MA 8	INNOMAG e.V. Dissertationspreis / Ph.D. Thesis Prize (2020)
12:30	H2	MA 9	INNOMAG e.V. Diploma/Master Prize (2021)

Wednesday, September 29, 2021

MA

13:30	H5	MA 10	Focus Session: Higher-Order Magnetic Interactions – Implications in 2D and 3D Magnetism I
13:30	P	MA 11	Posters Magnetism III
14:30	H2	MA 12	INNOMAG e.V. Dissertationspreis / Ph.D. Thesis Prize (2021)

MM

Invited Talks

10:00	H8	MM 6.1	CALPHAD-informed density-based grain boundary thermodynamics •Reza Darvishi Kamachali, Lei Wang, Linlin Li, Anna Manzoni, Birgit Skrotzki, Gregory Thompson
11:15	H8	MM 7.1	Computational methods for grain boundary segregation in metallic alloys •Lorenz Romaner, Daniel Scheiber, Vsevolod Razumovskiy, Oleg Peil, Christoph Dösinger, Alexander Reichmann

Sessions

10:00	H8	MM 6	Topical Session Interface-Dominated Phenomena – Thermodynamics
11:15	H8	MM 7	Topical Session Interface-Dominated Phenomena – Segregation and Embrittlement
18:00	MVMM	MM 8	Annual General Meeting of the Metal and Material Physics Division

SOE

Prize Talks

15:00	YSA	SOE 1.1	Quantifying science and art •Roberta Sinatra (Laureate of the Young Scientist Award 2020)
15:45	YSA	SOE 1.2	Multilayer modeling and analysis of complex socio-economic systems •Manlio De Domenico (Laureate of the Young Scientist Award 2020)

Sessions

15:00	YSA	SOE 1	Young Scientist Award for Socio-and Econophysics
17:00	P	SOE 2	Poster
18:00	MVSOE	SOE 3	Annual General Meeting of the Physics of Socio-economic Systems Division

TT

Sessions

10:00	H4	TT 10	Materials and devices for quantum technology
10:00	H6	TT 11	Focus Session: Facets of Many-Body Quantum Chaos (organised by Markus Heyl and Klaus Richter)
10:00	H7	TT 12	New Experimental Techniques
11:15	H7	TT 13	Quantum Computing
13:30	H6	TT 14	Many-Body Quantum Dynamics I

AGI

Session

16:30	MVAGI	AGI 3	Annual General Meeting of the Working Group on Information

SMI

Session

13:30	H1	SMI 1	Science meets industry

Meet-your-exhibitor

12:00	Meet&Mingle		Deutsche Forschungsgemeinschaft (DFG)
13:00	Meet&Mingle		Cryovac GmbH & Co. KG
13:00	Meet&Mingle		Pfeiffer Vacuum GmbH
13:00	Meet&Mingle		Onnes Technologies B.V.

Thursday, September 30, 2021

			Plenary Talks
09:00	Audimax 1	PV XII	Quantum networks – from dreams to reality •Jian-Wei Pan
09:00	Audimax 2	PV XIII	Status and Perspectives of Concentrating Solar Power Technologies •Robert Pitz-Paal
16:30	Audimax 1	PV XIV	Wanderings at the Crossroad between Nonlinear Dynamics and Systems Biology •Alain Karma
16:30	Audimax 2	PV XV	Cavity Magnonics •Can-Ming Hu

SYAS

			Invited Talks
10:00	Audimax 2	SYAS 1.1	Ultrafast Coherent Spin-Lattice Interactions in Iron Films •Steven Johnson
10:30	Audimax 2	SYAS 1.2	Ultrafast spin, charge and nuclear dynamics: ab-initio description •Sangeeta Sharma, John Kay Dewhurst
11:15	Audimax 2	SYAS 1.3	Light-wave driven Spin Dynamics •Martin Schultze, Markus Münzenberg, Sangeeta Sharma
11:45	Audimax 2	SYAS 1.4	All-coherent subcycle switching of spins by THz near fields •Christoph Lange, Stefan Schlauderer, Sebastian Baierl, Thomas Ebnet, Christoph Schmid, Darren Valovcin, Anatoly Zvezdin, Alexey Kimel, Rostislav Mikhaylovskiy, Rupert Huber
12:15	Audimax 2	SYAS 1.5	Ultrafast optically-induced spin transfer in ferromagnetic alloys •Stefan Mathias
			Session
10:00	Audimax 2	SYAS 1	Attosecond and Coherent Spins: New Frontiers

SYCE

			Invited Talks
13:30	Audimax 1	SYCE 1.1	The challenge of anthropogenic climate change – Earth system analysis can guide climate mitigation policy •Matthias Hofmann
14:00	Audimax 1	SYCE 1.2	Towards a carbon-free energy system: Expectations from R&D in renewable energy technologies •Bernd Rech, Rutger Schlatmann
14:30	Audimax 1	SYCE 1.3	Decarbonizing the Heating Sector – Challenges and Solutions •Florian Weiser
15:15	Audimax 1	SYCE 1.4	A carbon-free Energy System in 2050: Modelling the Energy Transition •Christoph Kost, Philip Sterchele, Hans-Martin Henning
15:45	Audimax 1	SYCE 1.5	The transition of the electricity system to 100% renewable energy: agent-based modeling of investment decisions under climate policies •Kristian Lindgren
			Session
13:30	Audimax 1	SYCE 1	Climate and energy: Challenges and options from a physics perspective

SYHN

			Invited Talks
10:00	Audimax 1	SYHN 1.1	Scaling behavior of stiffness and strength of hierarchical network nanomaterials •Shan Shi

Thursday, September 30, 2021

SYHN

10:30	Audimax 1	SYHN 1.2	Functional and programmable DNA nanotechnology •Laura Na Liu
11:15	Audimax 1	SYHN 1.3	Multivalent nanoparticles for targeted binding •Stefano Angioletti-Uberti
11:45	Audimax 1	SYHN 1.4	Programming Nanoscale Self-Assembly •Oleg Gang
12:15	Audimax 1	SYHN 1.5	Achieving Global Tunability via Local Programming of a Structure's Composition •Jochen Mueller
			Session
10:00	Audimax 1	SYHN 1	Hybrid Nanomaterials: From Novel Physics and Multi-Scale Self-Organization to Functional Diversity on the Device Scale

SYWH

			Invited Talks
13:30	Audimax 2	SYWH 1.1	Spin interactions in van der Waals topological materials and magnets •Saroj Dash
14:00	Audimax 2	SYWH 1.2	Exciton optics, dynamics and transport in atomically thin materials •Ermin Malic, Samuel Brem, Raul Perea-Causin, Daniel Erkensten, Roberto Rosati
14:30	Audimax 2	SYWH 1.3	Correlated Electrons in van der Waals Superlattices: Control and Understanding •Tim Wehling
15:15	Audimax 2	SYWH 1.4	Exciton manipulation and transport in 2D semiconductor heterostructures •Andras Kis
15:45	Audimax 2	SYWH 1.5	Chern Insulators, van Hove singularities and Topological Flat-bands in Magic-angle Twisted Bilayer Graphene* •Eva Andrei, Shuang Wu, Zhenyuan Zhang
			Session
13:30	Audimax 2	SYWH 1	Symposium: Physics of van der Waals 2D heterostructures

BP

			Invited Talks
10:00	H1	BP 3.1	SARS-CoV-2 induced membrane remodeling in infected cells revealed by in celullo cryo-ET Steffen Klein, Liv Zimmermann, Sophie Winter, Mirko Cortese, Moritz Wachsmuth-Melm, Christopher Neufeldt, Berati Cerikan, Megan Stanifer, Steeve Boulant, Ralf Bartenschlager, •Petr Chlanda
13:30	H6	BP 6.1	How do lipids and proteins diffuse in cell membranes, and what do the diffusion experiments actually measure? •Ilpo Vattulainen
15:00	H6	BP 7.1	Shaping embryos through controlled tissue phase transitions •Otger Campàs
			Sessions
10:00	H1	BP 3	Protein Structure and Dynamics
11:15	P	BP 4	Posters Biological Physics
11:45	H2	BP 5	Active Matter
13:30	H6	BP 6	Membranes and Vesicles
15:00	H6	BP 7	Cell Mechanics, Cell Adhesion and Migration, Multicellular Systems
18:00	MVBP	BP 8	Annual General Meeting of the Biological Physics Division

Thursday, September 30, 2021

CPP

			Invited Talk
13:30	H3	CPP 10.1	Nanophotonic structures by inkjet printing Yidenekachew J. Donie, Qiaoshuang Zhang, Guillaume Gomard, •Uli Lemmer
			Sessions
11:45	H2	CPP 9	Active Matter
13:30	H3	CPP 10	Organic Electronics and Photovoltaics, Electrical and Optical Properties
15:15	H5	CPP 11	Thin Oxides and Organic Thin Films
17:30	MVCPP	CPP 12	Annual General Meeting of the Chemical and Polymer Physics Division

DS

			Topical Talks
13:30	H1	DS 6.1	Exceptional Topology of Non-Hermitian Systems: from Theoretical Foundations to Novel Quantum Sensors •Jan Carl Budich
14:00	H1	DS 6.2	In situ fabrication of (Bi,Sb)-based topological insulator – superconductor hybrid devices •Peter Schüffelgen
14:30	H1	DS 6.3	Atomic monolayers as two-dimensional topological insulators •Ralph Claessen
15:15	H1	DS 6.4	Topological Insulator Lasers •Mordechai Segev
15:45	H1	DS 6.5	TBA •Morais Smith
			Sessions
13:30	H1	DS 6	Focus Session: Topological Phenomena in Synthetic Matter
15:15	H5	DS 7	Thin Oxides and Organic Thin Films
18:00	MVDS	DS 8	Annual General Meeting of the Thin Films Division

DY

			Invited Talks
13:30	H2	DY 13.1	Multi-scale modeling of dyadic structure-function relation in ventricular cardiac myocytes •Martin Falcke, Filippo G. Cosi, Wolfgang Giese, Wilhelm Neubert, Stefan Luther, Nagaiah Chmakuri, Ulrich Parlitz
14:45	H2	DY 13.4	Cardiac repolarization dynamics and arrhythmias in healthy and diseased hearts •Esther Pueyo
15:45	H2	DY 13.7	Dynamics of paroxysmal tachycardias •Gil Bub
			Sessions
10:00	H2	DY 11	Many-Body Quantum Dynamics II
11:45	H2	DY 12	Active Matter
13:30	H2	DY 13	Focus session: Nonlinear Dynamics of the Heart II (organized by Markus Bär, Stefan Luther and Ulrich Parlitz)
18:00	MVDY	DY 14	Annual General Meeting of the Dynamics and Statistical Physics Division

HL

			Invited Talks
10:00	H4	HL 15.1	Quasi-instantaneous switch-off of deep-strong light-matter coupling •Christoph Lange, Joshua Mornhinweg, Maike Halbhuber, Viola Zeller, Cristiano Ciuti, Dominique Bougeard, Rupert Huber

Thursday, September 30, 2021

HL

10:30	H4	HL 15.2	Lithium niobate nonlinear nanophotonics •Frank Setzpfandt
11:00	H4	HL 15.3	Quadratic nanomaterials for integrated photonic devices •Rachel Grange
11:45	H4	HL 15.4	Topological plasmonics: Ultrafast vector movies of plasmonic skyrmions on the nanoscale •Harald Giessen, Pascal Dreher, David Janoschka, Frank Meyer zu Heringdorf, Tim Davis, Bettina Frank
12:15	H4	HL 15.5	Supercontinuum second-harmonic generation spectroscopy of 2D semiconductors •Steffen Michaelis de Vasconcellos
13:30	H4	HL 18.1	Telecom wavelength quantum dot-based single-photon sources for quantum technologies •Anna Musial

Sessions

10:00	H4	HL 15	Focus Session: Tailored Nonlinear Photonics
11:15	H1	HL 16	Semiconductors: Optical, Transport and Ultrafast Properties
13:30	H1	HL 17	Focus Session: Topological Phenomena in Synthetic Matter
13:30	H4	HL 18	Quantum Dots and Wires
13:30	P	HL 19	Poster Session IV
18:00	MVHL	HL 20	Annual General Meeting of the Semiconductor Physics Division

KFM

Session

13:30	H3	KFM 11	Organic Electronics and Photovoltaics, Electrical and Optical Properties

MA

Invited Talks

10:00	H5	MA 13.1	Magnetism and superconductivity: new physics one atom at a time •Alexander Balatsky
10:45	H5	MA 13.3	Magnetic adatom chains on superconducting $NbSe_2$ Eva Liebhaber, Lisa M. Rütten, Gael Reecht, Jacob F. Steiner, Sebastian Rohlf, Kai Rossnagel, Felix von Oppen, •Katharina J. Franke
11:30	H5	MA 13.5	Yu-Shiba-Rusinov states and ordering of magnetic Impurities near the boundary •Jelena Klinovaja
12:15	H5	MA 13.7	Resonance from antiferromagnetic spin fluctuations for spin-triplet superconductivity in UTe2 •Pengcheng Dai
13:30	H5	MA 14.1	The role of itinerant electrons and higher order magnetic interactions among fluctuating local moments in metallic magnets •Julie Staunton

Sessions

10:00	H5	MA 13	PhD Focus Session: Symposium on Strange Bedfellows – Magnetism Meets Superconductivity" (joint session MA/AKjDPG)
13:30	H5	MA 14	Focus Session: Higher-Order Magnetic Interactions – Implications in 2D and 3D Magnetism II
13:30	P	MA 15	Posters Magnetism IV
17:30	MVMA	MA 16	Annual General Meeting of the Magnetism Division

Thursday, September 30, 2021

SOE

			Topical Talks
10:00	H3	SOE 4.1	Felix Auerbach and Zipf's Law for Cities •Diego Rybski, Antonio Ciccone
10:30	H3	SOE 4.2	Envy-induced class separation in societies of competing agents •Claudius Gros
			Sessions
10:00	H3	SOE 4	Dynamics and Scaling of Cities and Societies
11:15	H3	SOE 5	Financial Systems
11:45	H3	SOE 6	Dynamics of Social and Adaptive Networks I

TT

			Invited Talk
13:30	H7	TT 21.1	A new class of charge density wave superconductors in the topological kagome metals AV_3Sb_5 (A=K, Rb, Cs) •Stephen Wilson
			Sessions
10:00	H2	TT 15	Many-Body Quantum Dynamics II
10:00	H5	TT 16	PhD Focus Session: Symposium on Strange Bedfellows – Magnetism Meets Superconductivity" (joint session MA/AKjDPG)
10:00	H6	TT 17	Charge Density Wave Materials
10:00	H7	TT 18	Frustrated Magnets
11:15	H6	TT 19	Unconventional Superconductors
13:30	H4	TT 20	Quantum Dots and Wires
13:30	H7	TT 21	Focus Session: Topological Kagome Metals
13:30	P	TT 22	Poster Session: Disordered and Granular Superconductors: Fundamentals and Applications in Quantum Technology
13:30	P	TT 23	Poster Session: Emerging Phenomena in Superconducting Low Dimensional Hybrid Systems
13:30	P	TT 24	Poster Session: Transport
13:30	P	TT 25	Poster Session: Topology
18:00	MVTT	TT 26	Annual General Meeting of the Low Temperature Physics Division

AKPIK

			Session
13:30	P	AKPIK 3	AKPIK Postersession

AGA

			Invited Talks
11:15	H8	AGA 2.1	TPNW Verification: Domains, Boundary Conditions, Priorities & Problems •Thomas E. Shea
12:00	H8	AGA 2.2	International Partnership for Nuclear Disarmament Verification: Current Status and Future Prospects •Irmgard Niemeyer, Gerald Kirchner, Götz Neuneck
13:30	H8	AGA 3.1	Denuclearization of the Korean Peninsula •Tariq Rauf
14:15	H8	AGA 3.2	The DPRK's SLBMs and SRBMs – A Brief Update on North Korea's Missile Activities •Markus Schiller
15:15	H8	AGA 3.3	One Size does not Fit All: Greatly Different Mandates for Denuclearizing Nuclear States •Robert Kelley
16:00	H8	AGA 4.1	The Space Debris Challenge and ESA's Space Safety Programme •Holger Krag

Thursday, September 30, 2021

AGA

Sessions

10:00	H8	AGA 1	Disarmament Verification I
11:15	H8	AGA 2	Disarmament Verification II
13:30	H8	AGA 3	North Korea: Denuclearization
16:00	H8	AGA 4	Space Security
17:00	MVAGA	AGA 5	Annual General Meeting of the Working Group on Physics and Disarmament

Meet-your-exhibitor

12:00	Meet&Mingle		Deutsche Forschungsgemeinschaft (DFG)
13:00	Meet&Mingle		Cryoandmore Budzylek GbR
13:00	Meet&Mingle		Agilent Technologies Sales & Services GmbH

Evening Lecture

18:30	MVL	PV XVI	Max von Laue Lecture: What physicists can do to improve international security? •Steve Fetter

Friday, October 1, 2021

			Plenary Talks
09:00	Audimax 1	PV XVII	Superconductivity near room temperature •Mikhail Eremets
09:00	Audimax 2	PV XVIII	Machine Learning meets Quantum Physics •Klaus-Robert Müller
15:15	Audimax 1	PV XIX	Scalable semiconductor quantum and classical photonic systems •Jelena Vuckovic
15:15	Audimax 2	PV XX	From Self-Assembled Soft Matter to Mesostructured Quantum Materials •Ulrich Wiesner

SYAN

			Invited Talks
10:00	Audimax 1	SYAN 1.1	Corrugated patterns made from an active nematic sheet •Anis Senoussi, Shunichi Kashida, Raphaël Voituriez, Jean-Christophe Galas, Ananyo Maitra, Estevez-Torres André
10:30	Audimax 1	SYAN 1.2	Wrinkling instability in 3D active nematics •Isabella Guido
11:15	Audimax 1	SYAN 1.3	Three-dimensional active nematic defects and their energetics •Miha Ravnik
11:45	Audimax 1	SYAN 1.4	Liquid-crystal organization of liver tissue •Benjamin M Friedrich, Hernan Morales-Navarrete, Andre Scholich, Hidenori Nonaka, Fabian Segovia Miranda, Steffen Lange, Jens Karschau, Yannis Kalaidzidis, Frank Jülicher, Marino Zerial
12:15	Audimax 1	SYAN 1.5	Machine learning active nematic hydrodynamics •Vincenzo Vitelli
			Session
10:00	Audimax 1	SYAN 1	Active nematics: From 2D to 3D

SYPQ

			Invited Talks
10:00	Audimax 2	SYPQ 1.1	Quantum dots operating at telecom wavelengths for photonic quantum technology •Simone Luca Portalupi
10:30	Audimax 2	SYPQ 1.2	Photonic graph states for quantum communication and quantum computing •Stefanie Barz
11:00	Audimax 2	SYPQ 1.3	Rare-earth ion doped solids at sub-Kelvins: practical and fundamental aspects •Pavel Bushev
11:45	Audimax 2	SYPQ 1.4	Quantum Light and Strongly Correlated Electronic States in a Moiré Heterostructure •Brian Gerardot
12:15	Audimax 2	SYPQ 1.5	Quantum communication in fibers and free-space •Rupert Ursin
			Session
10:00	Audimax 2	SYPQ 1	Symposium: The Rise of Photonic Quantum Technologies – Practical and Fundamental Aspects

BP

			Session
11:15	H2	BP 9	Machine Learning in Dynamical Systems and Statistical Physics

Friday, October 1, 2021

CPP

			Invited Talks
10:00	H3	CPP 13.1	Electron-lattice relaxation effects in halide perovskites •David A. Egger
11:45	H3	CPP 13.6	Light-actuated colloidal nano- and microparticles •Cornelia Denz, Matthias Rueschenbaum, Valeria Bobkova, Julian Jeggle, Raphael Wittkowski
13:30	H3	CPP 15.1	Data-driven protein design and simulation •Andrew Ferguson
			Sessions
10:00	H3	CPP 13	Molecular Electronics, Hybrid and Perovskite Photovoltaics
10:00	H2	CPP 14	Condensed-Matter Simulations augmented by Advanced Statistical Methodologies
13:30	H3	CPP 15	Theory and Simulation

DS

			Sessions
10:00	H1	DS 9	Focus Session: Highlights of Materials Science and Applied Physics II
11:15	H1	DS 10	Focus Session: Highlights of Materials Science and Applied Physics III
13:30	H4	DS 11	2D semiconductors and van der Waals heterostructures II

DY

			Invited Talks
13:30	ESS	DY 18.1	Network-Induced Multistability Through Lossy Coupling •Jürgen Kurths
14:00	ESS	DY 18.2	Control of synchronization in two-layer power grids •Simona Olmi, Carl Totz, Eckehard Schöll
15:00	ESS	DY 18.3	Relay and complete synchronization of chimeras and solitary states in heterogeneous networks of chaotic maps Elena Rybalova, Eckehard Schöll, •Galina Strelkova
15:30	ESS	DY 18.4	A bridge between the fractal geometry of the Mandelbrot set and partially synchronized dynamics of chimera states. •Ralph G Andrejzak
			Sessions
10:00	H2	DY 15	Condensed-Matter Simulations augmented by Advanced Statistical Methodologies
11:15	H2	DY 16	Machine Learning in Dynamical Systems and Statistical Physics
13:30	H3	DY 17	Theory and Simulation
13:30	ESS	DY 18	Symposium: Synchronization Patterns in Complex Dynamical Networks (organized by Jakub Sawicki, Sabine Klapp, Markus Bär and Jens Christian Claussen)
13:30	H6	DY 19	Transport

HL

			Invited Talks, Discussion
10:00	H4	HL 22.1	Two-dimensional gain materials for new nanolaser concepts •Christopher Gies
10:30	H4	HL 22.2	Room-temperature polariton lattices for quantum simulation •Stephane Kena-Cohen
11:00	H4	HL 22.3	Topological nanocavity lasers and topological high-power lasers •Yasutomo Ota, Yasuhiko Arakawa, Satoshi Iwamoto

Friday, October 1, 2021

HL

11:45	H4	HL 22.4	Topological Insulator Lasers •Miguel A. Bandres, Steffen Wittek, Gal Harari, Mordechai Segev, Demetrios N. Christodoulides, Mercedeh Khajavikhan
12:15	H4	HL 22.5	When polariton condensates have dissipations or have no excitons •Hui Deng
13:30	Audimax 2	HL 24.1	Panel Discussion on Quantum Technologies •Tobias Heindel, Doris Reiter

Sessions

10:00	H1	HL 21	Focus Session: Highlights of Materials Science and Applied Physics II
10:00	H4	HL 22	Focus Session: Emerging Semiconductor Laser Concepts
11:15	H1	HL 23	Focus Session: Highlights of Materials Science and Applied Physics III
13:30	Audimax 2	HL 24	Quo Vadis Quantum Technologies? About Promises, Prospects, and Challenges
13:30	H4	HL 25	2D semiconductors and van der Waals heterostructures II

KFM

Sessions

10:00	H5	KFM 12	Skyrmions II
10:00	H7	KFM 13	Topological Insulators and Semimetals

MA

Invited Talks, Discussion

10:00	H5	MA 17.1	Emergent electromagnetic response of nanometer-sized spin textures •Max Hirschberger, Takashi Kurumaji, Leonie Spitz
13:30	H5	MA 19.1	"Neuromorphic Computing": A Productive Contradiction in Terms •Herbert Jaeger
14:00	H5	MA 19.2	Neuromorphic computing with radiofrequency spintronic devices •Alice Mizrahi, Nathan Leroux, Danijela Markovic, Dedalo Sanz Hernandez, Juan Trastoy, Paolo Bortolotti, Leandro Martins, Alex Jenkins, Ricardo Ferreira, Julie Grollier
14:40	H5	MA 19.3	Data Storage and Processing in the Cognitive Era •Giovanni Cherubini
15:10	H5	MA 19.4	Brain-inspired approaches and ultrafast magnetism for Green ICT •Theo Rasing
15:50	H5	MA 19.5	Panel discussion PhD Focus Session •Tobias Hula, Mauricio Bejarano, Luis Flacke

Sessions

10:00	H5	MA 17	Skyrmions II
10:00	P	MA 18	Posters Magnetism V
13:30	H5	MA 19	PhD Focus Session: Symposium on "Magnetism - A Potential Platform for Big Data?" (joint session MA/O/AKjDPG)

SOE

Topical Talk

10:00	H6	SOE 7.1	Why Ergodicity Breaking from Climate Change matters in Ecosystems? •Jan Nagler

Sessions

10:00	H6	SOE 7	Socio-economic models of climate change impact
11:15	H6	SOE 8	Dynamics of Social and Adaptive Networks II
13:30	ESS	SOE 9	Symposium: Synchronization Patterns in Complex Dynamical Networks (organized by Jakub Sawicki, Sabine Klapp, Markus Bär and Jens Christian Claussen)

Friday, October 1, 2021

TT

Sessions

10:00	H7	TT 27	Topological Insulators and Semimetals
13:30	H6	TT 28	Transport
13:30	H7	TT 29	Topological Superconductors

AGA

Sessions

10:00	H8	AGA 6	Non-Proliferation and Nuclear Verification
11:15	H8	AGA 7	Nuclear Archeology
12:30	H8	AGA 8	Preventive Arms Control

Meet-your-exhibitor

13:00	Meet&Mingle	HTS-110
13:00	Meet&Mingle	CreaTec Fischer & Co. GmbH
13:00	Meet&Mingle	Oxford University Press

Plenary and Evening Talks

Plenary Talk PV I Mon 9:00 Audimax 1

Inference and Mitigation of COVID-19 — •Viola Priesemann — MPI for Dynamics and Selforganization, Göttingen

How can we infer the spread of SARS-CoV-2 in a population, and how can we derive effective mitigation measures? How do non-pharmaceutical interventions, the vaccination progress and the emergence of new variants impact the viral spread? We recapitulate the basic principles of spreading dynamics, and highlight their implications for collective dynamics. On this basis, we investigate different COVID-19 mitigation strategies. In particular, we demonstrate a tipping point for the test-trace-isolate system, which incurs (transient) supra-exponential growth. We then show how the pace of lifting restrictions is determined by the progress of vaccination, and finally investigate the emergence of novel variants. With this work, we contribute to the basic understanding of spreading dynamics in populations, and provide approaches, which may guide mitigation policies.

Plenary Talk PV II Mon 9:00 Audimax 2

Quantum thermodynamics - superconducting circuit approach — •Jukka Pekola — QTF Centre of Excellence, Aalto University, Helsinki, Finland

I start by introducing ideas and principles of how to realize thermodynamic phenomena and devices in circuits composed of superconducting elements, including qubits, combined with heat baths formed of on-chip electronic reservoirs. This way we have demonstrated quantum limited heat transport by microwave photons [1,2], quantum heat valves [3] and rectifiers [4] and ultrasensitive calorimetric detectors [5]. Towards the end of the talk I present progress in realizing quantum heat engines and refrigerators based on thermodynamic cycles [6], and results on ultimate energy resolution of nanocalorimeters [5,7,8].

[1] M. Meschke, W. Guichard, and J. P. Pekola, Nature 444, 187 (2006). [2] A.V. Timofeev, M. Helle, M. Meschke, M. Möttönen, and J.P. Pekola, Phys. Rev. Lett. 102, 200801 (2009). [3] A. Ronzani, B. Karimi, J. Senior, Y.-C. Chang, J. T. Peltonen, C. Chen, and J. P. Pekola, Nat. Phys. 14, 991 (2018). [4] J. Senior, A. Gubaydullin, B. Karimi, J. T. Peltonen, J. Ankerhold, and J. P. Pekola, Comm. Phys. 3, 40 (2020). [5] B. Karimi, F. Brange, P. Samuelsson, and J. P. Pekola, Nat. Commun. 11, 367 (2020). [6] B. Karimi and J. P. Pekola, Phys. Rev. B 94, 184503 (2016). [7] Bayan Karimi, Jukka P. Pekola, Phys. Rev. Lett. 124, 170601 (2020). [8] B. Karimi, D. Nikolic, T. Tuukkanen, J. T. Peltonen, W. Belzig, and J. P. Pekola, Phys. Rev. Appl. 13, 054001 (2020).

Plenary Talk PV III Mon 16:30 Audimax 1

Complex networks with complex nodes — •Raissa D'Souza — University of California, Davis CA, USA

Real world networks – from brain networks to social networks to critical infrastructure networks – are composed of nodes with nonlinear behaviors coupled together via non-trivial network structures. Approaches from statistical physics study how behaviors arise in collections of simple elements connected together in complex structures such as modular or scale-free networks. They provide understanding about massive networks, revealing implications that network structure can have on network function and resilience. In contrast, approaches from dynamical systems and control theory typically study small systems of nonlinear nodes connected together in simple networks. This talk presents recent work bridging the gap of complex networks with complex nodes. First is considering nonlinear phase-amplitude oscillators coupled together by simple ring networks and how the interplay of nodal dynamics and coupling structure gives rise to emergent long-range order. Next is increasing the structural complexity from dyadic networks to hypergraphs to capture higher-order interactions and study cluster synchronization. The focus will then turn to social networks, starting from modeling humans as nodes with underlying attributes coupled in complete graphs, and moving on to real-world multiplex social networks in macaque monkey societies. We reveal the tensions between the forces of homophily and social balance, and show how the competition between rewarding talent and rewarding social reputation can cause cascading rank rearrangements in established social hierarchies.

Plenary Talk PV IV Mon 16:30 Audimax 2

Functional Three Dimensional Mesostructures as Bioelectronic Interfaces — •John Rogers — Northwestern University, Evanston, USA

Complex, three dimensional (3D) assemblies of micro/nanomaterials form naturally in biological systems, where they provide sophisticated function in even the most basic forms of life. In spite of their broad potential utility in man-made devices, design options for analogous abiotic 3D mesostructures are severely constrained by the comparatively primitive capabilities that are available with established techniques for materials growth, assembly and 3D printing. This talk summarizes progress on strategies that rely on geometric transformation of preformed 2D functional micro/nanostructures into 3D architectures by controlled processes of actively induced compressive buckling. The emphasis is on the foundational materials and mechanics principles, computational approaches that enable inverse designs, and examples of applications in areas ranging from thermoelectrics to microelectromechanical systems to biologically inspired open mesoscale microfluidic/electronic networks as functional interfaces to 3D cell cultures, including spheroids, organoids, assembloids and mini-brains.

Evening Talk PV V Mon 18:30 PEL

Die Rolle des Wasserstoffs im Energiesystem — •Robert Schlögl — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Deutschland

Wasserstoff ist die einzige Möglichkeit erneuerbare Energien global auszutauschen und damit den Bedarf an erneuerbarer Energie mit den Erzeugungsmöglichkeiten der Sonne zu verbinden. Eine zügige Umsetzung der Energiewende setzt nun voraus, dass wir die technischen und organisatorischen Hindernisse überwinden um zu einem globalen Markt für erneuerbare Energie zu gelangen. Der Beitrag adressiert einige technische Herausforderungen und beschreibt die politischen Maßnahmen zur Einführung einer Wasserstoffwirtschaft.

Plenary Talk PV VI Tue 9:00 Audimax 1

Correlated electrons with knots — •Silke Bühler-Paschen — TU Wien, Vienna, Austria

Strongly correlated quantum materials are fertile ground for new physics and offer numerous opportunities for discovery. To explore how the landscape of correlated quantum phases is enriched in the presence of nontrivial electronic topology, characterized by topological knots (or nodes) in momentum space, represents a new frontier. After a general discussion of this background, I will present our recent results on a Weyl semimetal driven by strong correlations, and highlight its giant topological responses as well as the ease to achieve genuine topology control. I will close by discussing the prospect of finding further correlation-driven topological phases and their potential for quantum applications.

Plenary Talk PV VII Tue 9:00 Audimax 2

Cuprous oxide: the ultimate material for studying excitons? — •Manfred Bayer — Experimentelle Physik, TU Dortmund

Excitons determine the optical properties of semiconductors. They are currently attracting intense renewed interest due to their large binding energies in novel materials such as transition metal dichalkogenides. Excitons are typically described by the hydrogen model. The highest observed principal quantum number n has been five or less in almost any semiconductor. The only exception is cuprous oxide, Cu_2O, in which excitons were demonstrated for the first time in 1952. Recently, the combination of high resolution laser spectroscopy and high crystal quality allowed the extension of the exciton series up to n=28, showing also the exceptional position of cuprous oxide for studying exciton physics. This contribution discusses the status achieved in the assessment of excitons in Cu_2O: (i) About 60 quantum number combinations (n, orbital angular momentum L), defining different shells, have been observed spectroscopically, also by applying electric or magnetic fields. (ii) Not only the optically active states that are allowed in different orders of light-matter coupling, but also the optically forbidden states could be detected up to $n = 6$. (iii) In the fine structure of the excitons pronounced deviations from the hydrogen model are found, which arise from breaking of the rotational into discrete symmetries in the crystal. (iv) Due to the large size of excitons with high principal quantum numbers, pronounced interaction effects with other excitons are observed. A consequence is the Rydberg blockade, where the presence of one exciton blocks excitation of another one in its surrounding.

Plenary Talk PV VIII Tue 16:30 Audimax 1

The Structural Origins of Wood Cell Wall Toughness — •Cynthia Volkert[1], Mona-Christin Maass[1], Salimeh Saleh[1], and Holger Militz[2] — [1]Institute of Materials Physics, University of Göttingen, Göttingen, Germany — [2]Wood Biology and Wood Products, University of Göttingen, Göttingen, Germany

Properties that are determined by structure - rather than by composition - are the basis of synthetic architected and meta-materials and of almost all natural materials. One remarkable example is wood. Despite being composed of only polymers, its hierarchical structure leads to specific strengths and stiffnesses that compete with those of high-performance engineering alloys.

The study presented here relates cellulose microfibril arrangements to splitting fracture toughness in pine wood cell walls using in-situ electron microscopy and reveals a previously unknown toughening mechanism [1]. The splitting cracks propagate along the direction of the microfibrils, and are steered to and trapped at highly tough interfaces, where the microfibrils change direction. This previously unexplained arrangement of the microfibrils can now be understood as a natural adaptation of living wood to enhance its toughness.

The microfibril structure can be mimicked to provide a powerful, new tactic for designing tough engineering composites by arranging fibers and layers to introduce tough interfaces that attract and trap delamination cracks. Perspectives for the application of this tactic to several technological problems will be discussed.

[1] M.-C. Maaß et al. Adv. Mater. 2020, 32, 1907693

Plenary Talk PV IX Tue 16:30 Audimax 2

Microscopic polarization and magnetization fields: Towards a 'post modern' theory — •John Sipe — Department of Physics, University of Toronto, 60 St. George St., Toronto, ON M5S 1A7 Canada

The response of solids to incident electromagnetic fields is often heuristically formulated in terms of macroscopic polarization and magnetization fields. The 'modern theory of polarization,' and its extension to magnetization, gives this a new level of rigour for time independent and uniform applied fields. We review the philosophy and main results of this strategy, and report on a new approach based on introducing microscopic polarization and magnetization fields. This 'post-modern' strategy can be used to address the response to electromagnetic fields varying arbitrarily in space and time. We connect it to earlier work on atoms and molecules, identifying important similarities and differences.

Plenary Talk PV X Wed 9:00 Audimax 1

Revealing the topological nature of transport at mesoscopic scales with quantum interferences — •Helene Bouchiat, A. Bernard, A. Murani, B. Dassonneville, A. Kasumov, M. Ferrier, R. Deblock, and S. Guéron — Laboratoire de Physique des Solides, University Paris Saclay, 91405 Orsay, France

A mesoscopic conductor is characterized by its size smaller than the phase coherence length of electronic wave-functions (typically one micrometer at low temperature). Mesoscopic electronic transport depends strongly on the nature of interferences between these wave functions determined by the scattering disorder potential which tends to localize electronic states at low dimension. Moreover, these interferences can be modulated by a magnetic flux through the Aharonov-Bohm effect giving rise to orbital persistent currents in ring geometries. These interferences also determine the Josephson supercurrent of a mesoscopic normal conductor when connected to superconducting electrodes. We show that these basic fundamental properties of mesoscopic quantum interferences can be used to reveal the existence and the physical location of 1d protected states in topological insulators. This method is illustrated in the case of crystalline bismuth nanowires which were found to belong to a class of newly discovered higher order topological insulators with helical ballistic hinge states coexisting with trivial bulk and surface diffusive states. In particular we discuss SQUID like periodic magnetic oscillations observed in Bi based Josephson junctions.

Plenary Talk PV XI Wed 9:00 Audimax 2

Quantum choreography to the beat of light — •Rupert Huber — Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany

Lightwave electronics has pushed the control of condensed matter to unprecedented time scales. By harnessing the carrier wave of intense light as an alternating voltage, electrons can be driven faster than a cycle of light, opening a fascinating quantum world full of promise for future quantum technologies.

We will discuss prominent examples of lightwave-driven dynamics in solids, ranging from dynamical Bloch oscillations to lightwave valleytronics and super-resolution all-optical band structure reconstruction. In topological insulators, ballistic and quasi-relativistic electron motion leads to a new quality of non-integer high-harmonic generation, unveiling the Berry curvature of the surface state. Moreover, we combine lightwave electronics with low-temperature scanning tunneling microscopy to take atom-scale slow-motion movies of an individual vibrating molecule. Lightwaves inside the tunnelling junction can even serve as femtosecond atomic forces to choreograph a coherent structural motion of a single-molecule switch. This concept offers a radically new way of directly watching and controlling key elementary dynamics in nature and steer (bio)chemical reactions or ultrafast phase transitions, on their intrinsic spatio-temporal scales.

Plenary Talk PV XII Thu 9:00 Audimax 1

Quantum networks - from dreams to reality — •Jian-Wei Pan — University of Science and Technology of China, 96 Jinzhai Road, Hefei 230026, China

Photons, the fast flying qubits which can be controlled with high precision using linear optics and have weak interaction with environment, are the natural candidate for quantum communications. By developing a quantum science satellite Micius and exploiting the negligible decoherence and photon loss in the out space, practically secure quantum cryptography, entanglement distribution, and quantum teleportation have been achieved over thousand kilometer scale, laying the foundation for future global quantum internet. Surprisingly, despite the extremely weak optical nonlinearity at single-photon level, an effective interaction between independent indistinguishable photons can be effectively induced by a multi-photon interferometry, which allowed the first creation of multi-particle entanglement and test of Einstein's local realism in the most extreme way. By developing high-performance quantum light sources, the multi-photon interference has been scaled up to implement boson sampling with up to 76 photons out of a 100-mode interferometer, which yields a Hilbert state space dimension of 10^30 and a rate that is 10^14 faster than using the state-of-the-art simulation strategy on supercomputers.

Plenary Talk PV XIII Thu 9:00 Audimax 2

Status and Perspectives of Concentrating Solar Power Technologies — •Robert Pitz-Paal — DLR, Institut für Solarforschung, Cologne, Germany

In CSP technology concentrating collectors are used to generate high temperature heat that drives a conventional power cycle. As heat can be stored simpler and cheaper than electricity the concept is very suitable to provide electricity according to the demand in particular covering the load peak after sunset typical in many Sunbelt countries. CSP electricity costs have dropped approx. by half since the beginning of the commercial implementation phase in 2007 along with the implementation of 6,2 GW of CSP plants worldwide. They range today from 12 €cents/kWh down to 6 €cents/kwh depending on size of the power plant, solar resource and financing conditions. Further cost reduction is driven by mass production effects but also through technical innovations that lead to higher system efficiencies, resulting in more electricity output per sqm of concentrator surface. The talk will provide background information on the current market and cost situation. It will highlight new technology concepts and report on the progress of research projects that target to increase system efficiency through higher operation temperature in the heat transfer fluid of the system.

Plenary Talk PV XIV Thu 16:30 Audimax 1

Wanderings at the Crossroad between Nonlinear Dynamics and Systems Biology — •Alain Karma — Northeastern University, Boston, USA

Insights into biological systems have been historically obtained by two very different approaches. Nonlinear dynamics has primarily focused on understanding the temporal behavior of specific sub-systems at a single level of biological organization using mathematical models, often represented by a set of differential equations with fixed parameters such as those describing gene regulatory circuits, metabolic networks, or intra- and inter-cellular signaling and communication pathways. While this approach can shed light on the behavior of specific sub-systems, it does not generally describe the coupling between different levels of biological organizations, which severely limits its scope. Systems biology, in contrast, attempts to understand biological systems globally by using high-throughput technologies and bioinformatics to probe the interaction of large ensembles of genes, proteins, and small molecules acting across different levels of biological organization. This approach has proven useful to identify genes and signaling pathways underlying diseases but does not predict how living organisms maintain their function and adapt to changing environments. This talk will describe recent progress to combine those two approaches to understand the dynamical coupling between different levels of biological organizations in the context of cardiac excitable dynamics. The results provide a fundamental basis for personalized therapies of heart rhythm disorders and other human diseases.

Plenary Talk PV XV Thu 16:30 Audimax 2

Cavity Magnonics — •Can-Ming Hu — University of Manitoba, Winnipeg, Canada

Cavity Magnonics (also known as Cavity Spintronics and Spin Cavitronics) is an emerging field that studies the light-matter interactions involving cavity photons and magnons [1-3]. Via the quantum physics of spin-photon entanglement on the one hand, and classical electrodynamic coupling on the other, magnon-photon coupling connects some of the most exciting modern physics, such as quantum information and quantum optics, with one of the oldest science on the earth, the magnetism.

This talk aims to introduce this frontier to the general audience of condensed matter physics. Starting with the intuitive example of coupled harmonic oscillators, I will explain the concepts of coherent and dissipative coupling, based on which two streams of research will be presented: (i) The development of diverse quantum transducers utilizing coherent coupling. (ii) The study of dissipative coupling governed by a non-Hermitian Hamiltonian, which leads to intriguing effects such as level attraction, nonreciprocal microwave transmission, exceptional points, and bound state in continuum. Students who are looking for frontier research opportunities are encouraged to attend.

[1] C.-M. Hu, Phys. in Canada, 72, No. 2, 76 (2016); arXiv: 1508.01966 (2015).
[2] D. Lachance-Quirion, et al., Appl. Phys. Express 12, 070101 (2019).
[3] Babak Zare Rameshti, et al., arXiv: 2106.09312 (2021).

Evening Talk PV XVI Thu 18:30 MVL

Max von Laue Lecture: What physicists can do to improve international security? — •Steve Fetter — University of Maryland, College Park, USA

After developing nuclear weapons, physicists were at the forefront in alerting policymakers and the public to the dangers of nuclear war. National academies, non-governmental organizations, and individual scientists helped conceive and promote arms control concepts and develop verification technologies which formed the foundation for treaties that enhanced international security and stability. That foundation is now crumbling, as treaties are discarded and a new generation of nuclear weapon systems is under development. Moreover, new security challenges are arising from emerging technologies, including quantum sensors and computing; artificial intelligence, machine learning, and robotics; cybersecurity; small satellites; and gene synthesis and editing. The physics community can play an important role in educating policymakers and the public about these risks and how they can be reduced.

Plenary Talk PV XVII Fri 9:00 Audimax 1

Superconductivity near room temperature — •Mikhail Eremets — Max-Planck-Institut fur Chemie (Otto-Hahn-Institut) Hahn-Meitner Weg 1 55128 Mainz Germany

Superconductivity at ambient conditions is one of the most challenging and long-standing problems in condensed-matter physics. Recently, superconductivity at 203 K was discovered in H3S at high pressure (Drozdov,Eremets et al. 2015), breaking archaic paradigms on conventional superconductivity. In the last years, many other superconductors were discovered and Tc of 250 K (Drozdov, Kong et al. 2019, Somayazulu, Ahart et al. 2019, Flores-Livas, L et al. 2020) was reached in a superhydride LaH10. Even higher critical temperatures were predicted theoretically (Sun, Lv et al. 2019). These record-breaking superconductors model atomic metallic hydrogen where high-temperature superconductivity was predicted 50 years ago (Ashcroft 1968, Ashcroft 2004). In this respect, I will show the most recent efforts on seeking the superconducting phase of pure hydrogen (Eremets, Drozdov et al. 2019). The progress towards room temperature superconductivity at moderate and ambient pressure is likely to be related to light-elements materials with strong covalent bonding.

Plenary Talk PV XVIII Fri 9:00 Audimax 2

Machine Learning meets Quantum Physics — •Klaus-Robert Müller — TU Berlin, Germany, Korea University, Seoul, Korea and MPII, Saarbrücken, Germany

The talk will first briefly introduce machine learning (ML) concepts, before applying them in Quantum chemistry and materials. This will include kernel-based learning methods and deep neural networks. A particular focus will lie on the challenge of interpreting nonlinear machine learning models. In other words, given that we have an excellent predictor of quantum chemical properties, how can we gain an understanding of the physics or chemistry that this learning machine has implemented? I will show selected examples of ML applied for predicting properties of small molecules and also for materials.

Plenary Talk PV XIX Fri 15:15 Audimax 1

Scalable semiconductor quantum and classical photonic systems — •Jelena Vuckovic — Stanford University

Classical and quantum photonics with superior properties can be implemented in a variety of photonic materials (silicon, diamond, silicon carbide) by combining state of the art optimization and machine learning techniques (photonics inverse design) with new fabrication approaches.

Plenary Talk PV XX Fri 15:15 Audimax 2

From Self-Assembled Soft Matter to Mesostructured Quantum Materials — •Ulrich Wiesner — Cornell University, Ithaca, NY 14853, US

Block copolymer (BCP) self-assembly (SA), a hallmark of soft condensed matter physics, continues to attract substantial academic and industrial interest. The dependence of SA structures and length scales on macromolecular characteristics like block fractions and molar mass allows for exquisite control over mesoscale lattice symmetry and parameters uncommon to the atomic lattice scale. This talk will provide an overview of polymer solution-based approaches that have been developed in recent years to translate this structure control to electronic materials, from energy conversion and storage devices all the way to quantum materials. Emphasis will be on fundamental understanding of structure formation principles, that can be generalized to a host of material classes from all-organic materials to carbons, oxides, semiconductors and metals all the way to superconductors, and resulting structure-property correlations. These solution-based SA approaches enable systematic studies of the influence of mesostructure on materials properties, resulting in what is often referred to as metamaterials. Mesostructured superconductors, in particular, are a fertile recent area for exploration of the impact of mesoscale order and porosity on the properties of correlated electron systems leading to quantum metamaterials. First examples will be discussed suggesting a fruitful convergence of soft matter self-assembly with condensed matter physics.

Symposium SKM Dissertation Prize 2021 (SYSD)

jointly organized by
the divisions of the Condensed Matter Section (SKM)

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The divisions belonging to the Condensed Matter Section (SKM) of the DPG annually awards the SKM Dissertation Prize. The prize acknowledges outstanding research during the PhD work in the research areas of SKM completed between 1 October 2018 bis 30 September 2020, and its excellent oral presentation. Based on nominations, a jury formed by the chairpersons of all SKM divisions has selected five finalists for the award to present their work in this symposium. The winner will be selected after the symposium and publicly announced Wednesday, September 29th, in the afternoon during the Awards Symposium (SYAW).

Overview of Invited Talks and Sessions

(Lecture hall Audimax 2)

Invited Talks

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Sessions

SYSD 1.1–1.5	Mon	10:00–12:15	Audimax 2	**Presentations of the Finalists for the 2021 SKM Dissertation Prize**

Sessions

SYSD 1: Presentations of the Finalists for the 2021 SKM Dissertation Prize

The divisions belonging to the Condensed Matter Section (SKM) of the DPG award annually the SKM Dissertation Prize. The prize acknowledges outstanding research during the PhD work in the research areas of SKM completed between 1 October 2018 bis 30 September 2020, and its excellent oral presentation. Based on nominations a jury formed by the chairpersons of all SKM divisions has selected five finalists for the award to present their work in this symposium. The winner will be selected after the symposium and publicly announced Wednesday, September 29th, in the afternoon during the ceremonial session.

Time: Monday 10:00–12:15 Location: Audimax 2

Invited Talk SYSD 1.1 Mon 10:00 Audimax 2
Avoided quasiparticle decay from strong quantum interactions — •Ruben Verresen[1,2,3], Roderich Moessner[2], and Frank Pollmann[3] — [1]Harvard University, Cambridge, USA — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [3]Technische Universität München, Munich, Germany
The emergent phenomenon of quasiparticles is key to understanding the properties of quantum states of matter. Known to be long lived at the lowest energies, quasiparticles are expected to become unstable when encountering the inevitable continuum of many-particle excited states at high energies, where decay is kinematically allowed. In this talk, I will show that although this expectation is correct for weak interactions, quasiparticles are generically stabilized by strong interactions pushing them out of the continuum. This general mechanism of avoided decay is straightforwardly illustrated in an exactly solvable model. Moreover, we develop a state-of-the-art numerical tool based on tensor networks which allows us to observe avoided decay in the spin-1/2 triangular-lattice Heisenberg antiferromagnet (TLHAF). This is surprising given the expectation of magnon decay in this paradigmatic frustrated magnet. Turning to existing experimental data, we identify the detailed phenomenology of avoided decay in the TLHAF material $Ba_3CoSb_2O_9$ and even in liquid helium. This mechanism provides a new window into quantum matter in the strongly interacting regime. Moreover, our numerical algorithm gives access to spectral functions for general 2D quantum magnets, providing a direct link between theory and experimental inelastic neutron scattering data.

Invited Talk SYSD 1.2 Mon 10:25 Audimax 2
Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications — •Juliane Borchert — Cavendish Laboratory, University of Cambridge — AMOLF Institut, Amsterdam — Clarendon Laboratory, University of Oxford
Perovskite materials are a highly promising material class for the realisation of the next generation of thin, lightweight, bendable solar cells. Here I focus on co-evaporation of perovskites which is a versatile method to deposit thin films. Co-evaporated films are exceptionally smooth and uniform and, due to the additive nature of the technique, can be deposited onto solvent-sensitive substrates. This is crucial for the fabrication of flexible substrates or when building a multilayer stack for tandem solar cells. In my dissertation research, I realised the first reported co-evaporation of formamidinium lead triiodide ($FAPbI_3$) solar cells which achieved high efficiencies. Subsequently, I studied the impact of impurities on the co-evaporation of methylammonium lead triiodide ($MAPbI_3$) and gained crucial insights to improve the process control and reproducibility of the co-evaporation of perovskite thin films. Finally, the experience and knowledge gained from these two studies were combined to fabricate co-evaporated patterned $FAPbI_3$ thin films for applications in semi-transparent solar cells and micro-lasers. These results are important contributions towards the deeper understanding of organic-inorganic halide perovskites and their properties as well as towards the development of stable, efficient, large-scale perovskites solar cells.

5-Minute Break

Invited Talk SYSD 1.3 Mon 10:55 Audimax 2
Attosecond-fast electron dynamics in graphene and graphene-based interfaces — •Christian Heide — Friedrich-Alexander Universität Erlangen-Nürnberg, 91058 Erlangen
Graphene, a two-dimensional material, is an ideal material to coherently drive electrons in a conducting material using strong light fields. In the band structure, when the electron is driven near the Dirac point - the point where the conduction and valence bands touch - the wave function of the electron can split into a superposition of the two band states. After half an optical cycle of about 1.3 femtoseconds (1 fs = 10^{-15}s), these parts of the wave function meet again and interfere, producing a current flow within one femtosecond. Its amplitude and phase are not only sensitive to the waveform of the laser field, but also to the band structure and its topology, which makes this process interesting for ultrafast electronics and the study of solid-state properties.

Furthermore, graphene attached to a semiconductor forms a functional Schottky junction. We have shown that charge transfer across the interface occurs within 0.3 fs - the fastest known charge transfer between two solids. The reason for the short charge transfer time is the combination of the materials used: the atomically thin graphene with excited electrons directly at the interface and the extended semiconductor, which is ideally suited to receive the excited electrons.

Both results, the coherent control of electrons in an electrical conductor and the attosecond-fast charge transfer, are important steps towards light-field driven electronics, i.e. another direct link between photonics and electronics.

Invited Talk SYSD 1.4 Mon 11:20 Audimax 2
The thermodynamics of stochastic systems with time delay — •Sarah A.M. Loos — ICTP, International Centre for Theoretical Physics, Strada Costiera, 11, 34151 Trieste TS, Italien
Recently, the field of stochastic thermodynamics has greatly advanced our understanding of biological, physical, and artificial microscopic systems, which fluctuate strongly due to thermal noise and often operate far from thermal equilibrium. Far less is known, however, when, in addition to noise, time-delayed forces act on the system, which may originate from feedback loops or may stem from communication delays between individual living or artificial-intelligent components. In this talk, I discuss technical challenges and uncover unexpected physical phenomena that arise from time delays. For example, an external time-delayed force may cool a stochastic system[1], in sharp contrast to non-delayed forces that always heat it up. When reversed in time, the history-dependence of a delay process transforms into a dependence on its own future, entailing acausality; which has nontrivial consequences for the thermodynamic arrow of time. In particular, the total entropy production is composed not only of the usual contributions of heat release and Shannon entropy change, but also of an information-theoretic term[2]. We discuss this information-term and show relations between time-delayed stochastic process and the famous Maxwell demon thought experiment.

[1] Loos, Klapp, Sci.Rep. 9,11 (2019). Loos, Hermann, Klapp, Entropy 23, 696 (2021). [2] Loos, Klapp, NJP 22, 123051 (2020).

5-Minute Break

Invited Talk SYSD 1.5 Mon 11:50 Audimax 2
First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM — •Benjamin Zingsem — Uni Duisburg
Spin-wave spectroscopy methods, such as electron-spin-resonance (ESR), and ferromagnetic resonance (FMR), are vital tools for materials characterization and chemical monitoring. Magnetic data storage, such as MRAM and hard-disk drives, but also magnetic materials for efficient and sustainable energy conversion in magnetic motors and turbines hinge on the precise knowledge of magnetic material parameters. These parameters can be extracted with the highest accuracy using FMR. On the other hand, ESR can determine the spin states of unpaired electrons in chemical compounds and during catalytic reactions, providing fundamental insight into the electron configuration. Together with momentum-sensitive techniques, such as Brillouin light scattering, both techniques are also central to spintronics experiments and the design of spintronic and magnonic devices. Here, we demonstrate a new technique to spatially resolve spin-resonances on the single nanometer scale with the potential for atomic resolution by transmission electron microscopy (TEM). The precessional torque of a spin excitation is coupled to a highly coherent electron beam, which reveals localized resonant spin excitations in transmission electron microscopy. This technique can be applied in-situ and in-operando on its own and together with conventional spectroscopy methods. As a model system, we present first results of magnonic networks comprising ferromagnetic nanoparticles and observe the spatial distributions of various spin-resonance modes.

Awards Symposium (SYAW)

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Overview of Prize Talks and Sessions

(Lecture hall Audimax 1)

Prize Talks

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Sessions

SYAW 1.1–1.7	Wed	13:30–17:20	Audimax 1	**Prize Talks**

Sessions

SYAW 1: Prize Talks

Time: Wednesday 13:30–17:20 Location: Audimax 1

Prize Talk SYAW 1.1 Wed 13:30 Audimax 1
Organic semiconductors - materials for today and tomorrow — •Anna Köhler — Universität Bayreuth, 95448 Bayreuth — Laureate of the Max-Born-Prize 2020
Even though organic semiconductors are a firm part of our daily life, e.g. as displays in mobile phones and as photoconductors in every photocopier, many aspects of their semiconducting nature are still scientifically challenging. To allow for future, advanced applications, such as flexible solar cells, bioelectronic sensors or coated electrotextiles, we need a deeper appreciation of their optoelectronic properties. In this talk I want to introduce what makes up the optical and electronic properties of this class of semiconductors, what determines how they work, and how do they differ from inorganic semiconductors. I will focus on particular how quantum size effects impact on (i) the binding energy of excitons and how this can be overcome for solar cell applications, and (ii) the magnitude of the exchange energy between singlet and triplet states and illustrate approaches to employ this for display applications.

Prize Talk SYAW 1.2 Wed 14:00 Audimax 1
PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors — •Grzegorz Karczewski — Institute of Physics, Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warszawa, Poland — Laureate of the Smoluchowski-Warburg-Prize 2021
The presentation will be devoted to describe the morphological, optical and transport properties of a PbTe/CdTe nanocomposite. Such a nanocomposite is fabricated by depositing alternating multiple PbTe and CdTe thin films by molecular beam epitaxy (MBE). PbTe and CdTe are immiscible. The immiscibility is due to the different crystal structures in which the two materials crystallize (PbTe in the rock salt and CdTe in the zinc blende structure). The observed topological transitions leading to material separation in the PbTe/CdTe system can be treated as an analogue of the spinodal decomposition of an immiscible solution in the solid state and thus can be qualitatively described by the Cahn-Hillard model.
Resistors made of the PbTe/CdTe nanocomposite exhibit pronounced sensitivity to infrared radiation at room temperature. Possible mechanisms causing the relatively high performance of PbTe/CdTe detectors are the decrease in electron concentration in the conductive PbTe layers due to the capture of mobile electrons by the dangling bonds present at the PbTe/CdTe interfaces and the effective suppression of Auger recombination in nanostructures made of narrow and wide band gap semiconductors.

10-Minute Break

Prize Talk SYAW 1.3 Wed 14:40 Audimax 1
Fingerprints of correlation in electronic spectra of materials — •Lucia Reining — LSI, CNRS/CEA/Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau,France — European Theoretical Spectroscopy Facility — Laureate of the Gentner-Kastler-Prize 2020
Many properties of materials are determined by electronic excitations, which can be observed in spectroscopic experiments, such as absorption or photoemission. However, electronic spectra of a real many-body system are often very different from what an independent-particle picture would suggest. How can theory understand, and how can calculations predict, the wealth of unexpected phenomena that may take place ? Density functional theory and many-body perturbation theory based on Green's functions are powerful approaches to face this problem, and indeed, ab initio calculations often yield reliable band structures. However, electronic excitation spectra contain much more: they may exhibit lifetime broadening, an incoherent background or distinct satellite structures. These features are pure correlation effects that cannot be captured by any independent-particle picture, and they are at the forefront of the capabilities of current first principles approaches. In this talk we will present recent progress in the theoretical description and analysis of correlation effects such as satellites in photoemission and inelastic x-ray scattering spectra, using density functionals [1], Green's functions [2], and close collaboration with experiment, and we will discuss new challenges.
[1] e.g., M. Panholzer, M. Gatti, and L. Reining, Phys. Rev. Lett. 120, 166402 (2018). [2] e.g., J.S. Zhou, et al., J. Chem. Phys. 143, 184109 (2015); PNAS 117, 28596 (2020).

Prize Talk SYAW 1.4 Wed 15:10 Audimax 1
Artificial Spin Ice: From Correlations to Computation — •Naëmi Leo — CIC nanoGUNE BRTA, Donostia - San Sebastián, Spain — Laureate of the Hertha-Sponer-Prize 2021
Collective ordering phenomena in magnetic materials can lead to the emergence of surprising material properties, especially when spin-spin interactions are competing. Artificial spin ices, which are arrays of magnetostatically-coupled single-domain nanomagnets, have become a testbed to study emergent correlations and phase transitions in tailored two-dimensional lattices. In recent years, further functionalities of such magnetic metamaterials have been explored, based on their field-driven reconfigurability and thermally-driven relaxation behaviour. These could open up the potential for novel low-powered computation schemes.
In this talk, I will give a brief introduction into the field of artificial spin ices. Then I will discuss observation of ordering phenomena in extended lattices as well as recent developments to manipulate the relaxation kinetics via light-controlled plasmonic heating in small-scale circuits for nanomagnetic computation.

Prize Talk SYAW 1.5 Wed 15:40 Audimax 1
From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices — •Andreas K. Hüttel — Institute for Exp. and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — Laureate of the Walter-Schottky-Prize 2021
Single wall carbon nanotubes are in many respects an outstanding model system. From transport spectroscopy, ferromagnet/superconductor-nanotube hybrid devices, and nano-electromechanics all the way to microwave optomechanics, the work of my group here covers by now a wide range of topics. I intend to present both a brief introduction and a select number of recent highlights, with an outlook towards our future research plans.

10-Minute Break

Prize Talk SYAW 1.6 Wed 16:20 Audimax 1
Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain — •Zhe Wang — Department of Physics, TU Dortmund University, Dortmund, Germany — Laureate of the Walter-Schottky-Prize 2020
One-dimensional (1D) spin chains are text-book examples for illustrating basic concepts, such as phase transition and spin dynamics. Apart from magnon excitations with an integer quantum number, excitations with fractional quantumnumber (e.g. spinons with S = 1/2) and complex magnon bound states (i.e. Bethe strings) are usually introduced also in the context of spin-chain models. As being exactly solvable, the 1D models provide understanding of the basic concepts in the exact sense, thus it is also a subject of a constant stream of theoretical studies. However, an experimental study of the exotic magnetic excitations is far from straightforward. This is because a proper material realization of the 1D models is scarce, and the magnetic excitations need to be disentangled from other degrees offreedom and at the same time, detectable by available experimental techniques. Recently, these difficulties are overcome in our experimental studies of the spin-1/2 antiferromagnetic Heisenberg-Ising chain compounds SrCo2V2O8 and BaCo2V2O8. I will present our terahertz spectroscopic investigations of quantum spin dynamics in these compounds as a function of temperature and in high magnetic fields. We have been able to identify the long sought-after many-body string excitations, the excitations of confined spinons, as well as magnons, which are characteristic for the different phases connected by magnetic field-induced quantum phase transitions in the 1D spin-1/2 Heisenberg-Ising antiferromagnet.

Prize Talk SYAW 1.7 Wed 16:50 Audimax 1
Imaging the effect of electron transfer at the atomic scale — •Laerte Patera — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — Laureate of the Gustav-Hertz-Prize 2020
Electron transfer plays a crucial role in many chemical processes, from photosynthesis to combustion and corrosion. However, the way in which redox reactions affect individual molecules and, in particular, their electronic structure, remains largely unclear. Unveiling these fundamental aspects requires the development of experimental tools allowing the observation of electron transfer down to the single molecule level. Here, we demonstrate the capability of performing tunnelling experiments on non-conductive substrates to map the orbital structure of isolated molecules upon electron transfer. By driving a change in the redox state of a molecule synchronized with the oscillating tip of an Atomic Force Microscope, previously inaccessible electronic transitions are resolved in space and energy [1]. Our results unveil the effects of electron transfer and polaron formation on the single-orbital scale, opening the door to the investigation of redox reactions and charging-related phenomena with sub-ångström resolution.
[1] L. L. Patera, F. Queck, P. Scheuerer and J. Repp, Nature 566, 245-248 (2019).

Symposium Amorphous materials: structure, dynamics, properties (SYAM)

jointly organised by
the Chemical and Polymer Physics Division (CPP),
the Dynamics and Statistical Physics Division (DY), and
the Metal and Material Physics Division (MM)

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A wide variety of materials are not in a crystalline state but rather resemble a frozen liquid, in which constituent particles lack long range spatial order. This class of materials includes “hard” glassy metals and polymers, but also “soft” glasses such as suspensions, emulsions, foams, colloidal and granular assemblies. Although these systems differ widely in their length, time, and energy scales, many of their dynamical and rheological properties are universal owing to their disordered nature. These systems are endowed with a hierarchy of relaxation times that are key to understanding their response to external driving. While the yielding transition in the limit of slow athermal driving has hallmarks of critical behavior typical for a dynamical phase transition, new (thermal) effects come into play when glasses are operated closer to their glass transition temperature. This symposium invites experimental, theoretical, and computational explorations of all facets of glassy behavior in amorphous materials. This includes in particular approaches to characterize and predict the slowing down of the dynamics (vitrification) at the glass transition in the bulk and under confinement, the ensuing nonequilibrium relaxation dynamics in the glassy state, and studies of the structural, thermal and mechanical properties of such materials.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 1)

Invited Talks

SYAM 1.1	Tue	13:30–14:00	Audimax 1	**Glassy dynamics of vitrimers** — •Liesbeth Janssen
SYAM 1.2	Tue	14:00–14:30	Audimax 1	**Liquid-Liquid Phase Transition in Thin Vapor-Deposited Glass Films** — •Zahra Fakhraai
SYAM 1.3	Tue	14:30–15:00	Audimax 1	**Connection between structural properties and atomic motion in ultraviscous metallic liquids close to the dynamical arrest** — •Beatrice Ruta, Nico Neuber, Isabella Gallino, Ralf Busch
SYAM 1.4	Tue	15:15–15:45	Audimax 1	**Signatures of the spatial extent of plastic events in the yielding transition in amorphous solids** — •Celine Ruscher, Daniel Korchinski, Joerg Rottler
SYAM 1.5	Tue	15:45–16:15	Audimax 1	**Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment** — •Olfa D’Angelo, W. Till Kranz

Sessions

SYAM 1.1–1.5	Tue	13:30–16:15	Audimax 1	**Amorphous materials: structure, dynamics, properties**

Sessions

– Invited Talks –

SYAM 1: Amorphous materials: structure, dynamics, properties

Time: Tuesday 13:30–16:15 Location: Audimax 1

Invited Talk SYAM 1.1 Tue 13:30 Audimax 1

Glassy dynamics of vitrimers — •Liesbeth Janssen — Eindhoven University of Technology, The Netherlands

Vitrimers are a promising new type of polymer glasses that combine the recyclability of thermoplastics with the high mechanical performance of thermosets. At the heart of their exceptional material properties lies highly unusual glass-forming behavior. In this talk I will discuss how we can model and understand this behavior, using coarse-grained simulations and first-principles-based theory [1].

[1] S. Ciarella, R.A. Biezemans, L.M.C. Janssen, Understanding, predicting, and tuning the fragility of vitrimeric polymers, Proc. Natl. Acad. Sci. USA 116, 25013 (2019).

Invited Talk SYAM 1.2 Tue 14:00 Audimax 1

Liquid-Liquid Phase Transition in Thin Vapor-Deposited Glass Films — •Zahra Fakhraai — Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104

Physical vapor deposition can produce glasses with near-equilibrium properties at low temperatures. This phenomenon is enabled by the enhanced mobility at the surface region, which enables access low-energy states in the energy landscape that are otherwise kinetically inaccessible. In thin films (For TPD molecule, h~20-50 nm), where surface mobility is further enhanced, we observe a liquid-liquid phase transition to a high-density supercooled liquid (HD-SCL) phase. The HD-SCL is formed when vapor deposition is performed below the phase transition temperature (T_LL). Above T_LL films of the same thickness follow the supercooled liquid (SCL) state. Films deposited in the HD-SCL state have densities that exceed even the crystal density. The kinetic stability of these films, measured using solvent vapor-annealing, also shows a sharp change at T_LL, further confirming the liquid-liquid phase transition phenomenon. The HD-SCL is only energetically favored in the thin film regime and rapidly transforms to the ordinary SCL or glass upon further deposition (h > 60 nm). This rapid transition is a sign that the specific boundary conditions of thin films can enable the observation of phases that are otherwise unstable in bulk glasses. We discuss how this phenomenon may be related to the observation of low Tg in liquid-quenched thin films of molecular and polymeric glasses and how it may more generally elucidate the nature of phase transitions in glasses.

Invited Talk SYAM 1.3 Tue 14:30 Audimax 1

Connection between structural properties and atomic motion in ultraviscous metallic liquids close to the dynamical arrest — •Beatrice Ruta[1], Nico Neuber[2], Isabella Gallino[2], and Ralf Busch[2] — [1]Univ Lyon 1, CNRS, Institut Lumière Matière, Villeurbanne, France — [2]Chair of Metallic Materials, Saarland University, Saarbrücken, Germany

Glass-formers are considered as archetypes of complex systems and the glass transition keeps fascinating scientists since decades. Although the impressive works done in the last year, still little is known on the mechanism of atomic motion governing the dynamics in ultra-viscous liquids close to the dynamical arrest, due to the difficulty to prove the slow collective particle motion of glass formers.

Thanks to the use of intense coherent X-ray beams available in third generation synchrotrons, we have performed the first experimental investigations of the temperature and wavelength dependence of the atomic motion in supercooled alloys close to the glass transition [1-3]. We find that the dynamics is strongly influenced by the underlying structure which can lead to peculiar oscillations of the microscopic relaxation time in correspondence to structural features [3]. This behavior is accompanied by dramatic changes in the shape of the intermediate scattering functions and suggests the presence of large dynamical heterogeneities at the mesoscopic scale.

[1] S. Hechler et al. Phys. Rev. Mat., 2, 085603, 2018
[2] B. Ruta et al. Phys. Rev. Lett. 125, 055701 2020
[3] N. Neuber et al. In preparation

15 min. break

Invited Talk SYAM 1.4 Tue 15:15 Audimax 1

Signatures of the spatial extent of plastic events in the yielding transition in amorphous solids — •Celine Ruscher[1,2], Daniel Korchinski[2], and Joerg Rottler[2] — [1]Institut Charles Sadron, Strasbourg, France — [2]Stewart Blusson Quantum Matter Institute, The University of British Columbia, Vancouver, Canada

Amorphous solids are yield stress materials whose flow consists of periods of elastic loading interrupted by rapid stress drops, or avalanches, coming from microscopic rearrangements known as shear transformations (STs). From the microscopic point of view, the density of STs, or density of local residual stresses, $P(x)$, governs the statistical properties of global collective failure events at the yielding transition.

Using atomistic simulations, we reveal the evolution of $P(x)$ upon deformation. A pseudogap form $P(x) \sim x^{\theta}$ is observed in the freshly quenched state and in the early stages of deformation. After a few percent strain, however, $P(x)$ starts to develop a system size dependent plateau in the small x limit. To explain the origin of the plateau we consider a mesoscopic elastoplastic approach. Our results show how the spatial extent of avalanches in the stationary regime has a profound effect on the distribution of local residual stresses x. While the entrance into the plateau is set by the lower cutoff of the mechanical noise produced by individual STs, the departure from the usually assumed power-law pseudogap form comes from stress fluctuations induced by collective avalanches.

Invited Talk SYAM 1.5 Tue 15:45 Audimax 1

Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment — •Olfa D'Angelo[1] and W. Till Kranz[2] — [1]Inst. Materialphysik im Weltraum, DLR-Köln — [2]Inst. Theoretische Physik, Uni. Köln

The variety in granular materials' behaviour makes them fascinating materials, but also difficult to encompass into a globalised theory. Recently, Kranz et al. described granular fluids close to the glass transition using mode coupling theory, and extended this theory towards the non-linear rheology of granular fluids submitted to finite shear rates [1]. This approach allows to embrace in a single theoretical framework the variety of rheological responses observed in dense granular fluids, as it predicts and delineates rheological regimes comprising Newtonian, shear thinning, and shear thickening (Bagnoldian).

We provide the first experimental validation of this theory [2], through flow curves spanning six orders of magnitude in shear rate, over a wide range of packing fractions. As we uncover the predicted rheological regimes in an air-fluidised granular bed of glass beads, we explore the areas of uncertainties in comparing our careful measurements to the theory. Experimental results and theory compare very favourably; besides the predicted regimes, experiments reveal an additional regime at high Peclet number, where Bagnold scaling is lost.

[1] W.T. Kranz, F. Frahsa, A. Zippelius, M. Fuchs, and M. Sperl, Phys. Rev. Fluids **5**, 024305 (2020).
[2] O. D'Angelo, A. Shetty, M. Sperl, and W.T. Kranz, in preparation (2021).

Symposium Active nematics: From 2D to 3D (SYAN)

jointly organised by
the Biological Physics Division (BP),
the Chemical and Polymer Physics Division (CPP), and
the Dynamics and Statistical Physics Division (DY)

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Active nematics are one of the most studied manifestations of active matter with main examples being mixtures of cytoskeletal filaments and motor proteins, but also force-generating, deforming and reorienting cells in living tissue. While the vast majority of active nematics have been studied in 2D systems, recently several advances towards 3D active nematics were made. Examples are systems that undergo multiple transitions from 3D space-filling to a compressed sheet, active filaments embedded in a passive liquid crystal and organoids in the case of tissue. The symposium will feature the experimental and theoretical challenges in the transition from 2D to 3D active nematic systems and its implications.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 1)

Invited Talks

SYAN 1.1	Fri	10:00–10:30	Audimax 1	**Corrugated patterns made from an active nematic sheet** — •Anis Senoussi, Shunichi Kashida, Raphaël Voituriez, Jean-Christophe Galas, Ananyo Maitra, Estevez-Torres André
SYAN 1.2	Fri	10:30–11:00	Audimax 1	**Wrinkling instability in 3D active nematics** — •Isabella Guido
SYAN 1.3	Fri	11:15–11:45	Audimax 1	**Three-dimensional active nematic defects and their energetics** — •Miha Ravnik
SYAN 1.4	Fri	11:45–12:15	Audimax 1	**Liquid-crystal organization of liver tissue** — •Benjamin M Friedrich, Hernan Morales-Navarrete, Andre Scholich, Hidenori Nonaka, Fabian Segovia Miranda, Steffen Lange, Jens Karschau, Yannis Kalaidzidis, Frank Jülicher, Marino Zerial
SYAN 1.5	Fri	12:15–12:45	Audimax 1	**Machine learning active nematic hydrodynamics** — •Vincenzo Vitelli

Sessions

SYAN 1.1–1.5	Fri	10:00–12:45	Audimax 1	**Active nematics: From 2D to 3D**

Sessions

– Invited Talks –

SYAN 1: Active nematics: From 2D to 3D

Time: Friday 10:00–12:45 Location: Audimax 1

Invited Talk SYAN 1.1 Fri 10:00 Audimax 1

Corrugated patterns made from an active nematic sheet — •Anis Senoussi[1], Shunichi Kashida[3], Raphaël Voituriez[2], Jean-Christophe Galas[2], Ananyo Maitra[2], and Estevez-Torres André[2] — [1]ESPCI, Paris, France — [2]Sorbonne Université, Paris, France — [3]xFOREST Therapeutics, Kyoto, Japan

To what extent can we engineer matter that shapes itself? To investigate this question, we study a 3D solution of multimeric kinesin motors and microtubule filaments. In addition to previously described patterns such as asters and chaotic flows, we report that such a solution can spontaneously form a 2D free-standing nematic active sheet that actively buckles out of plane into a centimeter-sized periodic corrugated sheet in the presence of a depletant. This pattern is stable at low activity and is transient - ultimately breaking into chaotic flows - at higher activities. We demonstrate that the wavelength and dynamics of the corrugations are controlled by the motor concentration and the depletant concentration, in good agreement with a hydrodynamic theory of active fluids. Our results underline the importance of both passive and active forces in shaping active matter and provide some insights on how active fluids can be sculpted into a static material through an active mechanism.

Invited Talk SYAN 1.2 Fri 10:30 Audimax 1

Wrinkling instability in 3D active nematics — •Isabella Guido — Max Planck Institute for Dynamics and Self-organization

Networks of biopolymers and motor proteins are useful model systems for the understanding of emergent behaviours of active matter. In this study we investigate how this active filamentous structures promote nonequilibrium processes induced by active stress at the microscale. By combining passive processes that produce entropic forces and extensile and contractile forces exerted by motors we show that the system exhibits a nematic organization characterised by long-range orientational order. The evolution of the system over time is particularly interesting and unique. We observe 3D to 2D transition by contracting into a sheet, expansion in the direction perpendicular to the contraction, 3D wrinkling pattern formation, and finally, explosion into a spatio-temporal disordered state. Finally, we examine the influence of external stimuli such as confinement, crowding agent and filament length on the properties of the different development phases of the system.

15. min break

Invited Talk SYAN 1.3 Fri 11:15 Audimax 1

Three-dimensional active nematic defects and their energetics — •Miha Ravnik — Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia — Josef Stefan Institute, Ljubljana, Slovenia

Active nematic fluids regularly exhibit topological defects, undergoing distinct dynamics which is determined by the coupling between the orientational order and the material flow. The type of defects and their role naturally depend on the dimensionality of the system, but importantly also on the geometry, confinement, flow, driving, and activity. Here, we present structures of topological defects in active nematic complex fluids, forming umbilic defects, singular loops, point defects, and disclinations. Specifically, we show defect profiles and dynamics in a three-dimensional active nematic droplet, also highlighting the role of different surface coupling regimes. Further, we demonstrate the dynamics of general singular defect loops in three-dimensional active nematics, which we show is strongly affected by the local twisting of the nematic director close to the singular defect cores. Finally, we discuss the energetics *energy dissipation and production- in active nematics as affected by topological defects.

Invited Talk SYAN 1.4 Fri 11:45 Audimax 1

Liquid-crystal organization of liver tissue — •Benjamin M Friedrich[1,2], Hernan Morales-Navarrete[3], Andre Scholich[4], Hidenori Nonaka[3], Fabian Segovia Miranda[3], Steffen Lange[2,5], Jens Karschau[2], Yannis Kalaidzidis[3], Frank Jülicher[4], and Marino Zerial[3] — [1]Physics of Life, TU Dresden, Germany — [2]cfaed, TU Dresden, Germany — [3]MPI CBG, Dresden, Germany — [4]MPI PKS, Dresden, Germany — [5]HTW, Dresden, Germany

Tissue function requires specific spatial organization of different cell types, yet should be flexible to allow for cell division and growth. Liquid-crystal order can serve this purpose. We present a general framework to quantify liquid-crystal order in 3D tissues and apply it to high-resolution imaging of mouse liver. We show that nematic cell polarity axes of hepatocytes (the main cell type in the liver) follow long-range liquid-crystal order. These tissue-level patterns of cell polarity are co-aligned with a structural anisotropy of two transport networks, blood-transporting sinusoids and bile-transporting canaliculi that intertwine the tissue. Silencing communication from hepatocytes to sinusoids via Integrin-β1 knockdown disrupted both liquid-crystal order of hepatocytes and organization of the sinusoidal network, suggesting that bi-directional communication between hepatocytes and sinusoids orchestrates tissue architecture. Using a network generation algorithm, we computationally explore the resilience of anisotropic sinusoidal networks to local damage, thus addressing the link between form and function in a complex tissue with biaxial liquid-crystal order.

Invited Talk SYAN 1.5 Fri 12:15 Audimax 1

Machine learning active nematic hydrodynamics — •Vincenzo Vitelli — James Franck Institute and Department of physics, University of Chicago

Hydrodynamic theories effectively describe many-body systems out of equilibrium in terms of a few macroscopic parameters. However, such parameters are difficult to determine from microscopic information. Seldom is this challenge more apparent than in active matter, where the hydrodynamic parameters are in fact fields that encode the distribution of energy-injecting microscopic components. In this talk, I will use active nematics to demonstrate that neural networks can map out the spatiotemporal variation of multiple hydrodynamic parameters and forecast the chaotic dynamics of these systems. We analyze biofilament/molecular-motor experiments with microtubule/kinesin and actin/myosin complexes as computer vision problems. Our algorithms can determine how activity and elastic moduli change as a function of space and time, as well as adenosine triphosphate (ATP) or motor concentration both in 2D and 3D. The only input needed is the orientation of the biofilaments and not the coupled velocity field which is harder to access in experiments. We can also forecast the evolution of these chaotic many-body systems solely from image sequences of their past using a combination of autoencoders and recurrent neural networks with residual architecture. In realistic experimental setups for which the initial conditions are not perfectly known, our physics-inspired machine-learning algorithms can surpass deterministic simulations.

Symposium Attosecond and coherent spins: New frontiers (SYAS)

jointly organised by
the Magnetism Division (MA),
the Surface Science Division (O),
the Low Temperature Division (TT),
the Thin Films Division (DS), and
the Semiconductor Physics Division (HL)

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Overview of Invited Talks and Sessions

(Lecture hall Audimax 2)

Invited Talks

SYAS 1.1	Thu	10:00–10:30	Audimax 2	**Ultrafast Coherent Spin-Lattice Interactions in Iron Films** — •Steven Johnson
SYAS 1.2	Thu	10:30–11:00	Audimax 2	**Ultrafast spin, charge and nuclear dynamics: ab-initio description** — •Sangeeta Sharma, John Kay Dewhurst
SYAS 1.3	Thu	11:15–11:45	Audimax 2	**Light-wave driven Spin Dynamics** — •Martin Schultze, Markus Münzenberg, Sangeeta Sharma
SYAS 1.4	Thu	11:45–12:15	Audimax 2	**All-coherent subcycle switching of spins by THz near fields** — •Christoph Lange, Stefan Schlauderer, Sebastian Baierl, Thomas Ebnet, Christoph Schmid, Darren Valovcin, Anatoly Zvezdin, Alexey Kimel, Rostislav Mikhaylovskiy, Rupert Huber
SYAS 1.5	Thu	12:15–12:45	Audimax 2	**Ultrafast optically-induced spin transfer in ferromagnetic alloys** — •Stefan Mathias

Sessions

SYAS 1.1–1.5	Thu	10:00–12:45	Audimax 2	**Attosecond and Coherent Spins: New Frontiers**

Sessions

– Invited Talks –

SYAS 1: Attosecond and Coherent Spins: New Frontiers

Ultrafast magnetism, attosecond lasers and methods using x-ray pulses to explore structural dynamics are reaching new limits. This session is dedicated to new developments and recent major recent milestones, from hard x-ray bunches to attosecond pulses, breaking new frontiers and time records, towards the observation to study coherent spin processes. This phenomenon is originating from coherent charge transfer, driven by a few cycle laser pulse, and is relevant for all materials and interfaces, from semiconductors, metals to molecules. Examples for these systems will be demonstrated.

Time: Thursday 10:00–12:45 Location: Audimax 2

Invited Talk SYAS 1.1 Thu 10:00 Audimax 2

Ultrafast Coherent Spin-Lattice Interactions in Iron Films — •Steven Johnson — Institute for Quantum Electronic, Eidgenossische Technische Hochschule, Zürich, Swiitzerland — SwissFEL, Paul Scherrer Institut, Villigen, Switzerland

The interaction of spins in a ferromagnet with the underlying lattice during the process of ultrafast demagentization has for some time been shrouded in mystery, and is intimately connected to the fundamental question of exactly how angular momentum is conserved in such processes. The original Einstein de Haas experiment of the early 20th century showed dramatically that the angular momentum of the electron spins responsible for ferromagnetism is the same angular momentum that we know well from classical mechanics. In this talk I explore how the Einstein de Haas effect can manifest in the time domain on ultrafast time scales in response to ultrafast demagnetization of a 3d ferromagnet. In a thin film geometry, the transfer of angular momentum to the lattice is accomplished by a transient mechanical torque that launches a small but measurable transverse displacement wave into the film. I also describe an experiment using ultrafast x-ray diffraction performed at the LCLS free electron laser that observed these dynamics. Based on this we make a first estimate of the magnitude and time scale of angular momentum transfer to the lattice in the first few hundred femtoseconds after ultrafast demagnetization. I also discuss future directions in this research to further investigate the underlying mechanisms.

Invited Talk SYAS 1.2 Thu 10:30 Audimax 2

Ultrafast spin, charge and nuclear dynamics: ab-initio description — •Sangeeta Sharma[1] and John Kay Dewhurst[2] — [1]Max Born Institute Berlin — [2]Max planck Institute Halle

Laser induced ultrafast dynamics is a burgeoning field of condensed matter physics promising the ultimate short time control of light over matter. From the outset of research into femtomagnetism, the field in which spins are manipulated by light on femtosecond or faster time scales, several questions have arisen and remain highly debated: How does the light interact with spin moments? How is the angular momentum conserved between the nuclei, spin, and angular momentum degrees of freedom during this interaction? What causes the ultrafast optical switching of magnetic structures from anti-ferromagnetic to ferromagnetic and back again? What is the ultimate time limit on the speed of spin manipulation? What is the impact of nuclear dynamics on the light-spin interaction?

In my talk I will advocate a parameter free ab-initio approach to treating ultrafast light-matter interactions, and discuss how this approach has led both to new answers to these old questions but also to the uncovering of novel and hitherto unsuspected early time spin dynamics phenomena. In particular I will demonstrate OISTR (optical inter-site spin transfer)[1,2] to be one of the fastest means of spin manipulation via light with changes in magnetic structure occurring on attosecond time scales. I will also discuss the impact of nuclear dynamics on laser induced spin dynamics and demonstrate how selective phonon modes can be used to enhance the OISTR effect.

15 min. break

Invited Talk SYAS 1.3 Thu 11:15 Audimax 2

Light-wave driven Spin Dynamics — •Martin Schultze[1], Markus Münzenberg[2], and Sangeeta Sharma[3] — [1]Institut für Experimentalphysik, TU Graz, Austria — [2]Ernst-Moritz-Arndt-Universität, Greifswald — [3]Max-Born-Institut, Berlin

In electronics, functionality is achieved by switching between electronic states of matter by applying external electric or magnetic fields. Strong couplings inbetween charge carriers and to the crystal lattice conspire to randomize energies and momenta extremely fast and efficiently, leaving no room for any sort of coherence.

However, the prospects of coherent control protocols as demonstrated in isolated atomic systems are alluring and contemporary ultrafast laser sources might be a new ingredient to overcome this entrapment. This talk will discuss two experiments demonstrating that single cycle optical fields at optical frequencies allow manipulating electronic and spin degrees of freedom in solid state systems at optical clock rates faster than de-coherence. Ultrafast bidirectional energy transfer between a light-field and the band-structure of silica proves the early times reversibility of electronic excitations and holds promise of novel ultrafast, coherent optoelectronic applications.

As a corollary of this ultrafast coherent modification of the electronic system, in suitably chosen herterostructures also the spin system can be manipulated coherently. Optically induced spin transfer is demonstrated as a route to the direct, all-optical manipulation of macroscopic magnetic moments on previously inaccessible attosecond timescales.

Invited Talk SYAS 1.4 Thu 11:45 Audimax 2

All-coherent subcycle switching of spins by THz near fields — •Christoph Lange[1], Stefan Schlauderer[2], Sebastian Baierl[2], Thomas Ebnet[2], Christoph Schmid[2], Darren Valovcin[3], Anatoly Zvezdin[4], Alexey Kimel[5], Rostislav Mikhaylovskiy[6], and Rupert Huber[2] — [1]Department of Physics, TU Dortmund University, 44227 Dortmund, Germany — [2]Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [3]Department of Physics, University of California at Santa Barbara, Santa Barbara, California 93106, USA — [4]P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow 119991, Russia. — [5]Radboud University, Institute for Molecules and Materials, Nijmegen 6525 AJ, The Netherlands. — [6]Department of Physics, Lancaster University, Bailrigg, Lancaster LA1 1YW, UK.

As state-of-the-art electronics encounters ultimate limits, novel concepts for harnessing coherent charge and spin dynamics are being sought after. Here, we perform subcycle control of solid-state spins by exploiting a novel electric-dipole mediated mechanism to induce unprecedentedly large spin oscillations in the antiferromagnet TmFeO3. Strong, single-cycle THz pulses are enhanced by a custom metallic antenna fabricated on top of a bulk TmFeO3 sample, where the antenna's atomically strong near fields change the magnetic anisotropy on a subcycle scale. The resulting spin dynamics include a characteristic phase flip, an asymmetric splitting of the magnon resonance, and a long-lived offset of the polarization rotation, representing a novel fingerprint of all-coherent spin switching with minimal energy dissipation.

Invited Talk SYAS 1.5 Thu 12:15 Audimax 2

Ultrafast optically-induced spin transfer in ferromagnetic alloys — •Stefan Mathias — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The idea of using light to manipulate electronic and spin excitations in materials on their fundamental time and length scales requires new approaches in experiment and theory, to observe and understand these excitations. The ultimate speed limit for all-optical manipulation requires control schemes for which the electronic or magnetic sub-systems of the materials are directly manipulated on the timescale of the laser excitation pulse. In our work, we provide experimental evidence of such a direct, ultrafast optically-induced spin transfer between two magnetic subsystems in an alloy of Fe and Ni [1] and various Heusler compounds [2].

[1] Hofherr et al., Ultrafast optically induced spin transfer in ferromagnetic alloys, Science Adv. 6, eaay8717 (2020) [2] Steil et al., Efficiency of ultrafast optically induced spin transfer in Heusler compounds, Physical Review Research 2, 023199 (2020)

Symposium Climate and energy: Challenges and options from a physics perspective (SYCE)

jointly organised by
the Physics of Socio-economic Systems Division (SOE),
the Dynamics and Statistical Physics Division (DY), and
the Working Group on Energy (AKE)

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Climate change poses pressing challenges about its implications as well as about understanding complex systems, including the transition of our energy system to completely renewable supply, understanding boundary conditions and understanding climate function and impact. Physics essentially contributes to this issue because it underlies developing and improving renewable energy supply devices and plants and also adds a holistic perspective towards planning and operation of fully renewable energy systems as well as socio-economic systems as a whole. The Symposium on the energy transition, climate and its impact as well as human interactions with these processes brings together approaches from physics and the exact sciences to provide a platform for cross-disciplinary discussions. Specifically, we address the pivotal issue how to most effectively and quickly make the transition to renewable generation and distribution in the areas of heating, and mobility, both in the private and industrial sectors.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 1)

Invited Talks

SYCE 1.1	Thu	13:30–14:00	Audimax 1	**The challenge of anthropogenic climate change - Earth system analysis can guide climate mitigation policy** — •Matthias Hofmann
SYCE 1.2	Thu	14:00–14:30	Audimax 1	**Towards a carbon-free energy system: Expectations from R&D in renewable energy technologies** — •Bernd Rech, Rutger Schlatmann
SYCE 1.3	Thu	14:30–15:00	Audimax 1	**Decarbonizing the Heating Sector - Challenges and Solutions** — •Florian Weiser
SYCE 1.4	Thu	15:15–15:45	Audimax 1	**A carbon-free Energy System in 2050: Modelling the Energy Transition** — •Christoph Kost, Philip Sterchele, Hans-Martin Henning
SYCE 1.5	Thu	15:45–16:15	Audimax 1	**The transition of the electricity system to 100% renewable energy: agent-based modeling of investment decisions under climate policies** — •Kristian Lindgren

Sessions

SYCE 1.1–1.5	Thu	13:30–16:15	Audimax 1	**Climate and energy: Challenges and options from a physics perspective**

Sessions

– Invited Talks –

SYCE 1: Climate and energy: Challenges and options from a physics perspective

Time: Thursday 13:30–16:15 Location: Audimax 1

Invited Talk SYCE 1.1 Thu 13:30 Audimax 1

The challenge of anthropogenic climate change - Earth system analysis can guide climate mitigation policy — •Matthias Hofmann — Potsdam Institute for Climate Impact Research, Germany

Since the industrial revolution humanity exerts a steadily growing pressure on the Earth's climate system. Unbridled anthropogenic emissions of greenhouse gases, notably of carbon dioxide, have already caused an increase in global mean surface temperature of about 1 °C since the beginning of instrumental temperature records. Earth system analysis is regarded as a powerful method to gain new insights into geophysical and biogeochemical fundamentals of the climate system.

Mitigating future climate change to avoid the transgression of dangerous thresholds and tipping points of crucial elements in the Earth system is currently one of the biggest challenges of humanity. Therefore, Earth system analysis is an indispensable tool in assessing planetary boundaries and guiding decision processes by political stakeholders.

Invited Talk SYCE 1.2 Thu 14:00 Audimax 1

Towards a carbon-free energy system: Expectations from R&D in renewable energy technologies — •Bernd Rech[1,2] and Rutger Schlatmann[3,4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [2]Technische Universität Berlin, Marchstr. 23, 10587 Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, PVcomB Schwarzschildstraße 3 12489 Berlin, Germany — [4]HTW - Hochschule für Technik und Wirtschaft Berlin, Renewable Energies, Wilhelminenhofstraße 75A, 12459 Berlin, Germany

The future global society needs a sustainable, climate-friendly energy supply largely based on a massive expansion of renewable energy sources. Photovoltaics (PV) and wind energy will become key technological pillars according to most scenarios and already today provide very low levelized cost of electricity (LCOE) in many regions and for several applications. It is important to note that for the long term the development of a system capable of trading, distributing and storing renewable energy will become necessary. This needs to be facilitated by the conversion of primary renewable energy into transportable and storable energy carriers.

Recent progress, opportunities and challenges in R&D will be highlighted for wind energy, solar thermal power plants and artificial photosynthesis on different technology readiness levels. In more detail we will discuss the development of new PV devices surpassing today*s efficiency limits as a case study how new renewable energy technologies may speed up the transition towards a sustainable energy system.

Invited Talk SYCE 1.3 Thu 14:30 Audimax 1

Decarbonizing the Heating Sector - Challenges and Solutions — •Florian Weiser — MVV Energie AG, Mannheim, Germany

The German climate targets cannot be reached without decarbonizing the heating sector that currently accounts for approximately one third of Germany's yearly CO2 emissions. Green heating technologies are already technically available for decentralized applications as well as for district heating systems, e.g. electrical heat pumps and biomass-fired systems. However, despite technical progress, green heating technologies will continue to be significantly more expensive than fossil-fired heating systems. Closing the CO2 gap between a "businesses as usual" path with current policies and a path consistent with the climate targets in the building heating sector will cost approximately 9 billion euros in the year 2030. The MVV study "Take-Off Wärmewende" proposes a mixture of instruments in order to accelerate the decarbonization of the building heating sector consisting of a CO2 tax on fossil fuels, CO2 limits for the building stock, municipal heat plans as well as funding schemes for green heat and energy efficiency. Furthermore, decarbonization policies for the building heating sector in Switzerland, Denmark, UK and France are analyzed.

15 min. break

Invited Talk SYCE 1.4 Thu 15:15 Audimax 1

A carbon-free Energy System in 2050: Modelling the Energy Transition — •Christoph Kost, Philip Sterchele, and Hans-Martin Henning — Fraunhofer-Institut für Solare Energiesysteme ISE, Freiburg, Germany

By 2050, Germany has committed to aim a carbon-free energy system under the Paris Agreement. This transition of the energy system from the 2020-system still based on high shares of fossil fuels to a system with zero carbon emissions from fossil fuels will completely change the energy world in Germany, in the power sector, building and industry sector, as well as in the transport sector. Modeling and analyzing this transition with the powerful tool for the German energy sector REMod creates insights how this challenging transformation can be carried out in the short-, medium and long-term by 2050. The model results show huge degradants for exchanges of technologies and applications in all four sectors.

Invited Talk SYCE 1.5 Thu 15:45 Audimax 1

The transition of the electricity system to 100% renewable energy: agent-based modeling of investment decisions under climate policies — •Kristian Lindgren — Department of Space, Earth and Environment, Chalmers University of Technology, Gothenburg, Sweden

A future energy system that to a large extent depends on variable renewable energy sources, like wind and solar power, involves new challenges for securing a reliable supply of electricity. The economic basis for such an electricity system differs significantly from the one we have today, and one can expect that prices will be more volatile and risk for shortages in supply increases.

We explore the transition towards a 100% renewable electricity system, driven by climate policies. These policies affect the investment decisions taken by companies, and we consider these to constitute the driving mechanism for the transition. This results in an agent-based (or mechanistic) model, in which companies are agents with possibly different bases for decisions as well as limitations in knowledge about the future. This is in contrast with the standard optimisation approach that identifies the cost-optimal allocation of investments generally assuming perfectly informed agents.

Several characteristics of the transition, like electricity prices, volatility, and roles of different technologies are discussed, and the dependence on different agent features is illustrated.

Symposium Curvilinear condensed matter (SYCL)

jointly organized by
the Magnetism Division (MA),
the Chemical and Polymer Physics Division (CPP), and
the Surface Science Division (O)

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Physical properties of living but also synthetic systems in condensed and soft matter are determined by the interplay between the physical order parameters, geometry and topology. Specifically to condensed matter, spin textures, static and dynamic responses become sensitive to bends and twists in physical space. In this respect, curvature effects emerged as a novel tool in various areas of physics to tailor electromagnetic properties and responses relying on geometrical deformations. Until recently, the impact of a curvature on electronic and magnetic properties of solids was mainly studied theoretically. The remarkable development in nanotechnology, e.g. preparation of high-quality extended thin films and nanowires as well as the potential to arbitrarily reshape those architectures after their fabrication, has enabled first experimental insights into the fundamental properties of 3D shaped semiconducting, superconducting, and magnetic nanoarchitectures. The investigation of physical effects governing the responses of curved nanoobjects to electric and magnetic fields has become a general trend in multiple disciplines, including electronics, photonics, plasmonics and magnetics. Considering the rapid development of the field, it is the purpose of this symposium to push the emergent topic of curvature-induced effects in condensed matter systems to a matured independent research direction in the modern condensed matter physics.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 2)

Invited Talks

SYCL 1.1	Wed	10:00–10:30	Audimax 2	**Curvature Effects and Topological Defects in Chiral Condensed and Soft Matter** — •Avadh Saxena
SYCL 1.2	Wed	10:30–11:00	Audimax 2	**Topology and Transport in nanostructures with curved geometries** — •Carmine Ortix
SYCL 2.1	Wed	11:15–11:45	Audimax 2	**Superconductors and nanomagnets evolve into 3D** — •Oleksandr Dobrovolskiy
SYCL 2.2	Wed	11:45–12:15	Audimax 2	**Properties of domain walls and skyrmions in curved ferromagnets** — •Volodymyr Kravchuk
SYCL 2.3	Wed	12:15–12:45	Audimax 2	**X-ray three-dimensional magnetic imaging** — •Valerio Scagnoli

Sessions

SYCL 1.1–1.2	Wed	10:00–11:00	Audimax 2	**Curvilinear condensed matter 1**
SYCL 2.1–2.3	Wed	11:15–12:45	Audimax 2	**Curvilinear condensed matter 2**

Sessions

– Invited Talks –

SYCL 1: Curvilinear condensed matter 1

Time: Wednesday 10:00–11:00 Location: Audimax 2

Invited Talk SYCL 1.1 Wed 10:00 Audimax 2

Curvature Effects and Topological Defects in Chiral Condensed and Soft Matter — •Avadh Saxena — Theoretical Division, Los Alamos National Lab, USA

The interplay of geometry and topology underlies many novel and intriguing properties of a variety of hard and soft materials including chiral magnets, nematic liquid crystals, and biological vesicles. These materials harbor a gamut of topological defects ranging from domain walls, dislocations, disclinations, solitons, vortices, skyrmions and merons to monopoles, Dirac strings, hopfions and boojums among many others. I will illustrate this rich interplay with three distinct physical examples. (i) Curvature induced quantum potential on minimal surfaces such as helicoids and catenoids (ii) Controlled motion and confinement of liquid crystal skyrmions near curved boundaries using the Q-tensor (as opposed to director) based free energy where the twist acts as the analogue of Dzyloshinskii-Moriya interaction in chiral magnets. (iii) Deformation of biological membranes and vesicles using Canham-Helfrich free energy and Bogomolnyi decomposition technique to determine equilibrium shapes. Finally, I will briefly describe specific applications of these ideas in memory devices, drug delivery systems as well as active matter and nonlinear relativistic systems.

Invited Talk SYCL 1.2 Wed 10:30 Audimax 2

Topology and Transport in nanostructures with curved geometries — •Carmine Ortix — Institute for Theoretical Physics, Utrecht University, Princetonplein 5, 3584 CC, Utrecht Netherlands — Dipartimento di Fisica "E. R. Caianiello", Universita' di Salerno, I-84084 Fisciano (Salerno), Italy

Recent advances in nanostructuring techniques have enabled the synthesis of compact three-dimensional nanoarchitectures: constructs of one- or two-dimensional nanostructures assembled in curved geometries, such as nanotubes and nanohelices. In this talk, I will discuss examples of unique geometry-driven topological and transport properties. These include the appearance of a non-linear Hall effect with time-reversal symmetry due to the Berry curvature dipole in corrugated bilayer graphene [1,2], the geometric control of spin transport properties in curved metallic nanochannels [3], the prediction of a strongly directional magnetotransport in carbon nanoscrolls [4], and the generation of topological insulating phases in shape-deformed semiconducting nanowires [5].

[1] R. Battilomo, N. Scopigno, C. Ortix, Physical Review Letters 123, 196403 (2019). [2] S.-C. Ho, C.-H. Chang, Y.-C. Hsieh, S.-T. Lo, B. Huang, T.-H.-Yen Vu, C. Ortix, T.-M. Chen, Nature Electronics 4, 116 (2021). [3] K. S. Das, D. Makarov, P. Gentile, M. Cuoco, B. J. van Wees, C. Ortix, I. J. Vera-Marun, Nano Letters 19, 6839 (2019). [4] C.-H. Chang, C. Ortix, Nano Letters 17, 3076 (2017). [5] P. Gentile, M. Cuoco, C. Ortix, Physical Review Letters 115, 256801 (2015).

SYCL 2: Curvilinear condensed matter 2

Time: Wednesday 11:15–12:45 Location: Audimax 2

Invited Talk SYCL 2.1 Wed 11:15 Audimax 2

Superconductors and nanomagnets evolve into 3D — •Oleksandr Dobrovolskiy — Superconductivity and Spintronics Laboratory, Nanomagnetism and Magnonics, Faculty of Physics, University of Vienna, Währinger Str. 17, 1090 Vienna, Austria

Patterned superconductors and nanomagnets are traditionally 2D planar structures. However, recent work is expanding superconductivity and nanomagnetism into the third dimension [1]. This expansion is triggered by advanced synthesis methods and the discovery of novel geometry- and topology-induced effects. In addition to self-assembled systems, a high level of maturity is now reached in direct-write nanofabrication by focused electron and focused ion beam induced deposition (FEBID and FIBID, respectively) [2, 3].

In this overview talk, a selection of shape- and curvature-induced effects in 3D superconducting and ferromagnetic structures will be outlined. A particular focus will be on the effects relevant for novel spintronic functionalities relying upon (i) the dynamics of Abrikosov vortices in superconductors [4], (ii) the dynamics of spin waves in ferromagnets [5], and (iii) the interplay of superconductivity and magnetism in heterostructures [6].

[1] D. Makarov *et al.*, Adv. Mater. **33** (2021) 2101758.
[2] M. Huth *et al.*, Microelectron. Engin. **185-186** (2018) 9.
[3] A. Fernandez-Pacheco *et al.*, Mater. **13** (2020) 3774.
[4] O. Dobrovolskiy *et al.*, Appl. Phys. Lett. **118** (2021) 132405.
[5] O. Dobrovolskiy *et al.*, Nat. Commun. **11** (2020) 3291.
[6] O. Dobrovolskiy *et al.*, Nat. Phys. **15** (2019) 477.

Invited Talk SYCL 2.2 Wed 11:45 Audimax 2

Properties of domain walls and skyrmions in curved ferromagnets — •Volodymyr Kravchuk — Karlsruhe Institute of Technology, Germany. — Bogolyubov Institute for Theoretical Physics, Kyiv, Ukraine

In the presence of the curvature, the topological magnetic solitons (domain walls, skyrmions, vortices) gain a number of new properties. A spatially localized curvature defect can generate the pinning as well as the repulsion potential for domain walls and skyrmions (depending on the signs of the curvature and topological charge of the soliton and also on its helicity). For a large amplitude defect, the pinned skyrmion demonstrates a multiplet of equilibrium states forming the ladder for the energy levels. The transitions between the levels can be controlled by pulses of the external magnetic field. Curvature drastically changes the dynamical properties of the topological solitons: the current-driven domain wall can demonstrate the negative mobility in three-dimensional curvilinear wire with torsion; the curvature gradients result in the driving force acting on domain walls and magnetic skyrmions; curvature enriches the spectrum of the spin eigenexitations of the skyrmion. Curvature generally couples the geometrical chirality of the magnet and spin chirality of the magnetic texture. This results in the chirality symmetry breaking effects, e.g. for the domain wall on the Moebius stripe, in the core switching process for a magnetic vortex on a spherical shell.

Invited Talk SYCL 2.3 Wed 12:15 Audimax 2

X-ray three-dimensional magnetic imaging — •Valerio Scagnoli — Laboratory for Mesoscopic Systems, Department of Materials, ETH Zurich, Zurich, Switzerland — Paul Scherrer Institute, Villigen, Switzerland

Three dimensional magnetic systems hold the promise to provide new functionality associated with greater degrees of freedom. Over the last years we have worked towards developing methods to fabricate and characterize three dimensional magnetic structures. Specifically, we have combined X-ray magnetic imaging with new iterative reconstruction algorithms to achieve X-ray magnetic tomography and laminography [1-4]. In a first demonstration, we have determined the three-dimensional magnetic nanostructure within the bulk of a soft GdCo2 magnetic micropillar and we have identified the presence of Bloch points of different types [1] as well as three-dimensional structures forming closed vortex loops [3]. Subsequently, we have used the flexibility provided by the laminography geometry to perform time resolved measurements of the magnetization dynamics in a two-phase micrometer size GdCo disk. Therefore, X-ray magnetic three-dimensional imaging, with its recent extension to the soft X-ray regime [5], has now reached sufficient maturity that will enable to unravel complex three-dimensional magnetic structures for a range of magnetic systems.

[1] C. Donnelly et al., Nature 547, 328 (2017) [2] C. Donnelly et al., New J. Phys. 20, 083009 (2018) [3] C. Donnelly et al., Nat. Phys. 17, 316 (2021) [4] C. Donnelly et al., Nat. Nanotechnol. 15, 356 (2020) [5] K. Witte et al., Nano Letters 20, 1305 (2020)

Symposium: The Physics of CoViD Infections (SYCO)

jointly organised by
the Biological Physics Division (BP),
the Dynamics and Statistical Physics Division (DY), and
the Physics of Socio-economic Systems Division (SOE)

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Viral diseases involve a combination of physical, chemical, and biological mechanisms – from the development of a viral infection in an organism to the spreading of the disease in a population. The physical understanding of these mechanisms involves on the molecular and cellular level, the structure and dynamics of viral proteins, their interaction with the cell membrane, and the development of drugs to prevent cell entry. On the level of transmission of the disease from person to person, it concerns the dynamics of droplet formation and breakup, and the areo- and hydrodynamics of droplet distribution. Finally, on the population level, simulation studies of the spreading of the disease in large groups help to predict the spreading dynamics and to develop strategies that can be employed to prevent spreading. This also concerns the development of strategies to use of a limited amount of a vaccine most efficiently in the early stages of a viral disease.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 1)

Invited Talks

SYCO 1.1	Mon	13:30–14:00	Audimax 1	**A Tethered Ligand Assay to Probe SARS-CoV-2:ACE2 Interactions** — Magnus Bauer, Sophia Gruber, Adina Hausch, Lukas Milles, Thomas Nicolaus, Leonard Schendel, Pilar Lopez Navajas, Erik Procko, Daniel Lietha, Rafael Bernadi, Hermann Gaub, •Jan Lipfert
SYCO 1.2	Mon	14:00–14:30	Audimax 1	**From molecular simulations towards antiviral therapeutics against COVID-19** — •Rebecca Wade
SYCO 1.3	Mon	14:45–15:15	Audimax 1	**The physical phenotype of blood cells is altered in COVID-19** — Markéta Kubánková, Martin Kräter, Bettina Hohberger, •Jochen Guck
SYCO 1.4	Mon	15:15–15:45	Audimax 1	**Extended lifetime of respiratory droplets in a turbulent vapor puff and its implications on airborne disease transmission** — •Detlef Lohse, Kai Leong Chong, Chong Shen Ng, Naoki Hori, Morgan Li, Rui Yang, Roberto Verzicco
SYCO 1.5	Mon	15:45–16:15	Audimax 1	**Beyond the demographic vaccine distribution: Where, when and to whom should vaccines be provided first?** — •Benno Liebchen, Jens Grauer, Fabian Schwarzendahl, Hartmut Löwen

Sessions

SYCO 1.1–1.5	Mon	13:30–16:15	Audimax 1	**The Physics of CoViD Infections**

Sessions

– Invited Talks –

SYCO 1: The Physics of CoViD Infections

Time: Monday 13:30–16:15 Location: Audimax 1

Invited Talk SYCO 1.1 Mon 13:30 Audimax 1

A Tethered Ligand Assay to Probe SARS-CoV-2:ACE2 Interactions — Magnus Bauer[1], Sophia Gruber[1], Adina Hausch[1], Lukas Milles[2], Thomas Nicolaus[1], Leonard Schendel[1], Pilar Lopez Navajas[3], Erik Procko[4], Daniel Lietha[3], Rafael Bernadi[5], Hermann Gaub[1], and •Jan Lipfert[1] — [1]LMU Munich — [2]University of Washington — [3]Spanish National Research Council — [4]University of Illinois — [5]Auburn University

SARS-CoV-2 attaches to the ACE2 receptor on human hosts cells via its receptor-binding domain (RBD) on the Spike protein. This critical first step occurs in dynamic environments, where external forces act on the binding partners, creating an urgent need for assays that can quantitate SARS-CoV-2 interactions with ACE2 under mechanical load. We present a tethered ligand assay that comprises the RBD and the ACE2 ectodomain joined by a flexible peptide linker. Using magnetic tweezers and atomic force spectroscopy, we investigate the RBD:ACE2 interaction over the whole physiologically relevant force range. Combined with steered molecular dynamics simulations, we observe and assign fully consistent unbinding and unfolding events across the three techniques and establish ACE2 unfolding as a molecular fingerprint. We quantify the force dependence and kinetics of the RBD:ACE2 bond in equilibrium and find significant differences between SARS-CoV-1 and 2, which helps to rationalize the different infection patterns of the two viruses. Finally, we probe how different RBD mutations affect force stability and speculate how mechanical coupling promotes increased transmissibility in variants of concern.

Invited Talk SYCO 1.2 Mon 14:00 Audimax 1

From molecular simulations towards antiviral therapeutics against COVID-19 — •Rebecca Wade — Heidelberg Institute for Theoretical Studies — ZMBH, Heidelberg University, Germany

Despite advancing vaccination campaigns against COVID-19, the emergence of new variants of SARS-CoV-2 and the difficulties of achieving high vaccination levels demonstrate the importance of developing antiviral therapeutics. During the pandemic, the international computational molecular biophysics community has worked towards this goal by applying simulation techniques to study viral infection and to discover new antiviral agents. One of the challenges for such studies is the highly dynamic nature of virus protein drug targets, such as the main protease and the spike glycoprotein.

To identify inhibitors of the main protease, we applied our TRAPP toolbox (1) to analyze the druggability of ca. 30000 protein conformations and found that small structural variations in the binding site dramatically impact ligand binding (2). Virtual screening against selected conformations led to the prediction and experimental validation of novel inhibitors.

Heparin is used to prevent thrombosis in COVID-19 patients but also has antiviral activity. We are carrying out simulations to investigate how heparin polysaccharide binds to the spike and to design of new heparin derivatives for antiviral therapy. Our results reveal three mechanisms by which heparin can exert its antiviral effects (3).

(1) https://trapp.h-its.org/ (2) Gossen et al., ACS Pharmacol. Transl. Sci. 2021, 4, 1079 - 1095. (3) Paiardi et al., arXiv:2103.07722

15 min. break

Invited Talk SYCO 1.3 Mon 14:45 Audimax 1

The physical phenotype of blood cells is altered in COVID-19 — Markéta Kubánková[1], Martin Kräter[1], Bettina Hohberger[2], and •Jochen Guck[1,3] — [1]Max Planck Institute for the Science of Light & Max Planck Zentrum für Physik und Medizin, Erlangen, Germany — [2]Department of Ophthalmology, Friedrich-Alexander-Universität, Erlangen, Germany — [3]Department of Physics, Friedrich-Alexander-Universität, Erlangen, Germany

The clinical syndrome coronavirus disease 2019 (COVID-19) induced by SARS-CoV-2 continues to be a major health concern worldwide. While the pathology is not yet fully understood, a hyper-inflammatory response and thrombotic events leading to congestion of microvessels are key signatures of disease pathogenesis. Until now, the physical changes of blood cells have not been considered in the context of COVID-19 related vascular occlusion and organ damage. Here we report an evaluation of multiple physical parameters including the mechanical features of five frequent blood cell types, namely erythrocytes, lymphocytes, monocytes, neutrophils, and eosinophils. In total, more than 4 million blood cells of 17 COVID-19 hospitalized patients at different levels of severity, 24 volunteers free from infectious or inflammatory diseases, and 14 recovered COVID- 19 patients were analyzed. We found significant changes in lymphocyte stiffness, monocyte size, neutrophil size and deformability, and heterogeneity of erythrocyte deformation and size. While some of these changes reverted to normal values after hospitalization, others persisted for months after hospital discharge, evidencing the long-term imprint of COVID-19 on the body.

Invited Talk SYCO 1.4 Mon 15:15 Audimax 1

Extended lifetime of respiratory droplets in a turbulent vapor puff and its implications on airborne disease transmission — •Detlef Lohse, Kai Leong Chong, Chong Shen Ng, Naoki Hori, Morgan Li, Rui Yang, and Roberto Verzicco — Physics of Fluids Group, University of Twente, Enschede, The Netherlands

Long-range airborne transmissions of viruses encapsulated in droplets play a major role in the transmission of respiratory diseases. I will show direct numerical simulations of a typical respiratory aerosol within a Lagrangian-Eulerian approach, coupled to the ambient velocity, temperature, and humidity fields to allow for exchange of mass and heat and to realistically account for the droplet evaporation. We found that for an ambient relative humidity of 50% the lifetime of the smallest droplets of our study with initial diameter of 10 μm gets extended by a factor of more than 30 as compared to what is suggested by the classical picture of Wells, mainly due to the role of the respiratory humidity, while the larger droplets basically behave ballistically. With increasing ambient relative humidity the extension of the lifetimes of the small droplets further increases and goes up to 150 times for 90% relative humidity, implying more than two meters advection range of the respiratory droplets within one second. For low ambient temperatures the problem is even more serious, as the humidity saturation level of air goes down with decreasing temperature. We anticipate our approach to be a starting point for larger parameter studies and for optimizing ventilation and indoor humidity controlling concepts, which both will be key in mitigating the COVID-19 pandemic.

Invited Talk SYCO 1.5 Mon 15:45 Audimax 1

Beyond the demographic vaccine distribution: Where, when and to whom should vaccines be provided first? — •Benno Liebchen[1], Jens Grauer[2], Fabian Schwarzendahl[2], and Hartmut Löwen[2] — [1]Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt — [2]Heinrich-Heine-Universität Düsseldorf, Universitätsstrasse 1, 40225 Düsseldorf

Once vaccines become available in a pandemic disease they are typically distributed demographically. This is in line with vaccination guidelines which largely focus on the question "to whom first?". In this talk we explore if lives could potentially be saved by asking also "where and when to provide vaccines first". To answer this question we propose alternative (non-demographic) vaccine distribution strategies and test their impact on the disease evolution within a newly developed nonuniform statistical mean-field model [1]. We find that a sequential prioritization of regions where infection numbers currently spread fastest is generically more effective than distributing vaccines demographically. These results are meant as a starting point to inspire systematic explorations of non-demographic vaccine distribution strategies aiming to find the optimal compromise between the prioritization of risk groups and highly affected regions. Towards the end of the talk we discuss recent results on possible mutation-induced phenomena in infectious-diseases and their response to vaccination [2].

[1] J. Grauer, H. Löwen, B. Liebchen, Sci. Rep. 10, 1 (2020)
[2] F. Schwarzendahl, J. Grauer, B. Liebchen, H. Löwen, medRxiv (2021)

Symposium Multidimensional coherent spectroscopy of functional nanostructures (SYCS)

jointly organised by
the Semiconductor Physics Division (HL),
the Chemical and Polymer Physics Division (CPP), and
the Surface Science Division (O)

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Overview of Invited Talks and Sessions

(Lecture hall Audimax 1)

Invited Talks

SYCS 1.1	Tue	10:00–10:30	Audimax 1	**Multidimensional coherent spectroscopy of perovskite nanocrystals** — •Steven Cundiff, Albert Liu, Diogo Almeida, Gabriel Nagamine, Lazaro Padilha
SYCS 1.2	Tue	10:30–11:00	Audimax 1	**Coherent multidimensional techniques for the characterization of nanomaterials** — •Elisabetta Collini
SYCS 1.3	Tue	11:00–11:30	Audimax 1	**Exciton Dynamics revealed by Multidimensional Coherent Spectroscopies applied to Light-Harvesting Systems** — •Thomas L.C. Jansen
SYCS 1.4	Tue	11:45–12:15	Audimax 1	**Revealing couplings with action-based 2D microscopy** — •Tobias Brixner
SYCS 1.5	Tue	12:15–12:45	Audimax 1	**Low-frequency phonons affect charge carrier dynamics in hybrid perovskites** — •Mischa Bonn

Sessions

SYCS 1.1–1.5	Tue	10:00–12:45	Audimax 1	**Symposium: Multidimensional coherent spectroscopy of functional nanostructures**

Sessions

– Invited Talks –

SYCS 1: Symposium: Multidimensional coherent spectroscopy of functional nanostructures

Multidimensional coherent spectroscopy has recently enabled fundamentally new insight into non-equilibrium quantum dynamics underlying elementary photophysical and photochemical processes, energy relaxation, charge transfer, and strong coupling phenomena in biological and artificial molecular systems, and semiconductors nanostructures. This knowledge has significant implications for the design of functional materials and for their application in optoelectronics. The aim of this Symposium is to bring together international leading experts to address the most recent developments and future research directions in multidimensional coherent spectroscopy techniques for the study of elementary light-driven processes in functional materials and nanostructures.

Organizers: Antonietta De Sio, Christoph Lienau (Universität Oldenburg)

Time: Tuesday 10:00–12:45 Location: Audimax 1

Invited Talk SYCS 1.1 Tue 10:00 Audimax 1

Multidimensional coherent spectroscopy of perovskite nanocrystals — •Steven Cundiff[1], Albert Liu[1], Diogo Almeida[1,2], Gabriel Nagamine[2], and Lazaro Padilha[2] — [1]University of Michigan, Ann Arbor, MI, USA — [2]University of Campinas, Campinas, SP, Brazil

Perovskite nanocrystals, including nanocubes and nanoplatelets, have attracted signficant attention recently due to their novel optoelectronic properties, in particular their high fluorescence quantum efficiency. However there are still debates about their properties, including electronic structure and optical linewidths. Measurements of these properties are hindered by the inhomogeneous broadening due to size dispersion.

We use optical multidimensional coherent spectroscopy at low temperatures to remove the effects of inhomogeneous broadening and elucidate the intrinsic properties of the nanocrystals. This include insight into the ordering of the bandedge states, dephasing rates of triple coherences and dependence of the dephasing excitonic dephasing on the number of layers in nanoplatelets.

Invited Talk SYCS 1.2 Tue 10:30 Audimax 1

Coherent multidimensional techniques for the characterization of nanomaterials — •Elisabetta Collini — Department of Chemical Sciences, University of Padova, via Marzolo 1, 35131 Padova, Italy

2D electronic spectroscopy (2DES) techniques have gained particular interest given their capability of following ultrafast processes in real-time. These techniques have been primarily applied to biological complexes but are now gaining ground to characterize transport processes in artificial nanomaterials and nanodevices. In this lecture, I will highlight the enormous potential of 2DES techniques to impact the field of nanosystems, quantum technologies, and quantum devices. The attention will be focused in particular on recent results obtained on semiconductor nanocrystals (*quantum dots*) in solid-state devices and metal-organic hybrid systems.

Invited Talk SYCS 1.3 Tue 11:00 Audimax 1

Exciton Dynamics revealed by Multidimensional Coherent Spectroscopies applied to Light-Harvesting Systems — •Thomas L.C. Jansen — University of Groningen, Zernike Institute for Advanced Materials, Groningen, The Netherlands

Natural light-harvesting systems as found in plants, algae, and especially bacteria are efficient in absorbing photons and transporting their energy to reaction centers, where the energy is converted to chemical energy. Time-resolved multidimensional coherent spectroscopies as Two-Dimensional Electronic Spectroscopy and Fluorescence-Detected Two-Dimensional Electronic Spectroscopy allow the detailed study of the mechanism and dynamics of the underlying light harvesting process. However, these spectra are often challenging to interpret. I will discuss how simulations can be used to distinguish between different processes as energy transport, exciton delocalization, electronic coherence, nuclear coherence, and exciton annihilation. Increasingly detailed models of light-harvesting systems allow increasingly refined understanding of the molecular scale dynamics directing the light-harvesting process. The understanding of what the spectroscopic methods reveal also pave the way for their application in other areas of research on functional nanostructures including organic, inorganic, and hybrid opto-electronic systems. This may aid the design of future artificial light-harvesting systems for photo-voltaic applications or help improving crop yield.

15 min. break.

Invited Talk SYCS 1.4 Tue 11:45 Audimax 1

Revealing couplings with action-based 2D microscopy — •Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Coherent two-dimensional (2D) electronic spectroscopy provides frequency resolution both for the excitation and the probe step. We have developed “action-based” 2D micro-spectroscopy variants using either fluorescence detection (with additional 260 nm spatial resolution) or electron detection (3 nm spatial resolution). In several exemplary applications on nanostructured systems, it will be discussed how various types of quantum-mechanical couplings can be retrieved. First, we investigate a $MoSe_2$ monolayer and observe long-term quantum beating as a function of population time. We analyze the data with a Franck–Condon model and retrieve quantitatively the exciton–phonon coupling strength at room temperature, a quantity previously unknown for 2D materials. Further, we embed a WSe_2 van-der-Waals heterostructure into a microcavity and observe a rich multi-peak structure in 2D spectra which has not been captured in conventional photoluminescence. Simulations reveal hybridized exciton–photon–phonon states, and time-dependent beating signals indicate further fine structure. Lastly, we apply 2D spectroscopy within photoemission electron microscopy (PEEM) on a nanoslit resonator. We find that multiplasmon quantum excitations are required to understand photoemission, going beyond the commonly employed classical linear response model.

Invited Talk SYCS 1.5 Tue 12:15 Audimax 1

Low-frequency phonons affect charge carrier dynamics in hybrid perovskites — •Mischa Bonn — Max Planck Institute for Polymer Research

We study the effect of the gigahertz dielectric response of organic cations and the terahertz phonon response of the inorganic sublattice on the properties, in particular of charge carriers, of hybrid organic-inorganic perovskite materials. We show that electron-phonon coupling is efficient, as evidenced by the timescale of coupling of nascent charge carriers to low-frequency phonon modes occurring on the timescale of the oscillation time of the phonon. We reveal direct coupling between the phonon mode and the bandgap, explaining the anomalous increase of the bandgap of hybrid perovskites with increasing temperature. We also show that there is remarkably efficient coupling between the organic and inorganic sublattices in the perovskite, despite the lack of covalent bonds between the two sublattices.

Symposium Spain as Guest of Honor (SYES)

jointly organized by
the DPG Condensed Matter Division (SKM),
the EPS Condensed Matter Division (EPS-CMD), and
the División de Física de la Materia Condensada (DFMC-GEFES) de la Real Sociedad Española de Física (RSEF)

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The 'Guest of Honor' Symposia celebrate the European physics community in general and the cooperation of the respective learned societies in particular. Thereby, the German Physical Society aims to further collaborations between individual scientists, research groups and institutions.

This year's 'Guest of Honor' Symposium honors the numerous ties between Spanish and German physicists by highlighting five fields of common interests.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 2)

Invited Talks

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Sessions

SYES 1.1–1.6	Wed	13:30–16:15	Audimax 2	**Spain as Guest of Honor**

Sessions

– Invited Talks –

SYES 1: Spain as Guest of Honor

The 'Guest of Honor' Symposia celebrate the European physics community in general and the cooperation of the respective learned societies in particular. Thereby, the German Physical Society aims to further collaborations between individual scientists, research groups and institutions.

This year's 'Guest of Honor' Symposium honors the numerous ties between Spanish and German physicists by highlighting five fields of common interests.

Time: Wednesday 13:30–16:15 Location: Audimax 2

Invited Talk SYES 1.1 Wed 13:30 Audimax 2
DFMC-GEFES — •Julia Herrero-Albillos — Dpto. Ciencia y Tecn. de Materiales y Fluidos, Universidad de Zaragoza and Instituto de Nanociencia y Materiales de Aragón (CSIC-UNIZAR). Zaragoza, Spain
I will shortly present DFMC-GEFES* activities with special emphasis on its role in Spanish and European physics.

*DFMC-GEFES: División de Física de la Materia Condensada de la Real Sociedad Española de Física (http://gefes-rsef.org)

Invited Talk SYES 1.2 Wed 13:40 Audimax 2
Towards Phononic Circuits based on Optomechanics — •Clivia M. Sotomayor Torres — Catalan Institute of Nanoscience and Nanotechnology ICN2, Campus UAB, 08193 Bellaterra, Spain
The optomechanical (OM) interaction using suspended nanobeams where overlapping confined mechanical and optical modes coexist is chosen to realise phononic circuit elements. Room temperature mechanical quality factors reached Q > 103. We demonstrated a coherent phonon emitter at 0.3 GHz via self-pulsing and up to 5 GHz via dynamical back-action. The nanobeam is coupled evanescently via a tapered fibre either directly to the OM cavity or to an integrated photonic waveguide. The non-linear interactions can be controlled to reach a chaotic regime and, with an external laser, the coherent phonon emission can be modulated. The physics of synchronisation, of nanobeams coupled to optical waveguides and the coupling to surface acoustic waves to excite and detect phononic signals have been studied and reproducible functionalities demonstrated. We report on the successful integration of circuit elements in a proof-of-concept phononics chip.

Work in collaboration with D. Navarro-Urrios, M. Colombano, G. Arregui, J. Maire, N. Capuj, A. Griol, A. Martinez, J. Ahopelto, T. Makkonen, A. Pitanti, S. Zanotto, B. Djafari-Rouhani, Y. Pennec, D. Mencarelli and L. Pierantoni , partners of the EU H2020 FET Open project PHENOMEN (713450) www.phenomen-project.eu and G. Madiot

Invited Talk SYES 1.3 Wed 14:10 Audimax 2
Adding magnetic functionalities to epitaxial graphene — •Rodolfo Miranda — IMDEA Nanociencia, Madrid, Spain — Universidad Autónoma Madrid, Madrid, Spain
The intrinsic magnetic properties of pristine graphene are negligible, but we show here that, by either adsorption of suitable molecules or intercalation of heavy or magnetic metal atoms, one can i) create long range magnetic order in hybrid graphene systems, ii) introduce a giant spin-orbit coupling into the π bands of graphene or iii) produce chiral magnetic domain walls stabilized and protected by graphene even at 300 K.

i)A monolayer of TCNQ molecules on graphene grown on Ru(0001) acquire charge and a magnetic moment. The TCNQ monolayer develops spatially extended, spin-split, electronic bands and a magnetically ordered ground-state as visualized by spin-polarized STS. The long range magnetic order is due to direct exchange interaction mediated by overlapping frontier orbitals of the molecules.

ii)Pb-intercalated Graphene grown on Ir(111) develops a giant (70-100 meV) spin-orbit coupling in the π bands of graphene, as detected by spin-ARPES. The system is a suitable candidate for the observation of Spin Hall Effect in graphene

iii)Finally, epitaxial graphene/Co(111)/Pt(111) stacks grown on MgO(111) exhibit enhanced Perpendicular Magnetic Anisotropy for Co layers up to 4 nm thick and generate left-handed Néel-type chiral Domain Walls stabilized by interfacial DMI interaction. The magnetic texture, protected by graphene is stable at 300 K in air.

5-Minute Break

Invited Talk SYES 1.4 Wed 14:45 Audimax 2
Bringing nanophotonics to the atomic scale — •Javier Aizpurua — Center for Materials Physics in San Sebastian (CSIC-UPV/EHU), Spain
A plasmonic nanogap is a superb configuration to explore the interplay between light and matter. Light scattered off, or emitted from a nanogap carries the information of the surrounding electromagnetic environment with it. In metallic nanocavities with ultrasmall gaps, electron currents across the gap at optical frequencies efficiently produce a strong nonlinear optical response. All these effects can be further controlled when a bias is applied across the gap, enabling the possibility of active control of light emitted from the cavity. This situation becomes even more appealing when a molecule is located in the gap of the plasmonic cavity or in its proximity, with the molecule playing an active role either in the electromagnetic coupling with the cavity, or even participating in processes of charge injection and transfer, which can be revealed through molecular electroluminescence. Here, we will address situations of light emission in electron tunneling configurations where atomic-scale resolution is achieved due to the presence of picocavities within the gap. The process of interaction between a molecular emitter and a tunneling cavity will be addressed both in the weak and strong coupling regimes, as revealed in light absorption and in emission. Strong coupling between a molecule and a plasmonic cavity shows great technological potential as it produces hybrid molecule-cavity polaritonic states which can be used for quantum information or in induced chemical reactivity.

Invited Talk SYES 1.5 Wed 15:15 Audimax 2
Hydrodynamics of collective cell migration in epithelial tissues — •Jaume Casademunt — University of Barcelona - UBICS, Barcelona, Spain
Collective migration of cohesive groups of cells is a hallmark of the tissue remodeling events that underlie embryonic morphogenesis, wound repair and cancer invasion. In this collective migration, supra-cellular properties such as collective polarization or force generation emerge and eventually control large- scale tissue organization. This suggests that a coarse-grained approach based on a hydrodynamic description of tissues as continuous active materials may shed some light into our understanding of large-scale tissue dynamics. Specifically, an appealing open question is to what extent the complex biological regulation at play can be encoded in a series of material parameters within a purely mechanical description. Here we present an overview of hydrodynamic modeling of cell tissues as active polar fluids, and discuss some examples where this approach has been instrumental to elucidate physical mechanisms behind collective cell behavior in epithelia: the occurrence of elastic-like waves, the wetting-dewetting transition in spreading cell monolayers, and the understanding of morphological instabilities of tissues.

Invited Talk SYES 1.6 Wed 15:45 Audimax 2
Understanding the physical variables driving mechanosensing — •Pere Roca-Cusachs — Institute for Bioengineering of Catalonia and University of Barcelona, Barcelona, Spain
Cell response to force regulates essential processes in health and disease. However, the fundamental mechanical variables that cells sense and respond to remain largely unknown. During this talk, I will discuss how this process of mechanosensing can be understood in physical terms, and used to predict cell response to both external force application, and passive mechanical properties such as Extracellular Matrix (ECM) rigidity.

Symposium Hybrid Nanomaterials: From Novel Physics and Multi-Scale Self-Organization to Functional Diversity on the Device Scale (SYHN)

jointly organised by
the Chemical and Polymer Physics Division (CPP),
the Dynamics and Statistical Physics Division (DY),
the Crystalline Solids and their Microstructure Division (KFM), and
the Metal and Material Physics Division (MM)

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The interplay of interfacial determinacy and geometric constraint leads to new, often surprising physicochemical behavior in many nanostructured materials. Particularly in the combination of soft and hard matter, this also results in special functionalities and mechanical properties that have the potential to completely rethink virtually all technological areas, especially energy generation, storage and conversion but also the biomedical field.

However, the resulting hybrid systems are usually characterized by strong electro-mechanical, chemo-mechanical and thermo-photonic couplings that have so far eluded fundamental understanding. In recent years, nanoscience has also increasingly focused on the question to what extent the combination of soft and hard matter opens up the possibility of using multiscale self-assembly and phase transitions, similar to many biological systems, to transport nanoscale effects from the mesoscale to the macroscale in order to design hybrid structural materials with integrated multifunctionality for robust components.

This interdisciplinary symposium will focus on these issues at the interface between soft matter physics and chemistry and materials science. A special focus will be put on porous hybrid systems but also on multiscale assembly of nano-objects (nanoparticles) with respect to the interplay of mechanics and function. As application fields electro-mechanical sensors/actuators, fluidics and photonics will be in the center.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 1)

Invited Talks

SYHN 1.1	Thu	10:00–10:30	Audimax 1	**Scaling behavior of stiffness and strength of hierarchical network nanomaterials** — •Shan Shi
SYHN 1.2	Thu	10:30–11:00	Audimax 1	**Functional and programmable DNA nanotechnology** — •Laura Na Liu
SYHN 1.3	Thu	11:15–11:45	Audimax 1	**Multivalent nanoparticles for targeted binding** — •Stefano Angioletti-Uberti
SYHN 1.4	Thu	11:45–12:15	Audimax 1	**Programming Nanoscale Self-Assembly** — •Oleg Gang
SYHN 1.5	Thu	12:15–12:45	Audimax 1	**Achieving Global Tunability via Local Programming of a Structure's Composition** — •Jochen Mueller

Sessions

SYHN 1.1–1.5	Thu	10:00–12:45	Audimax 1	**Hybrid Nanomaterials: From Novel Physics and Multi-Scale Self-Organization to Functional Diversity on the Device Scale**

Sessions

– Invited Talks –

SYHN 1: Hybrid Nanomaterials: From Novel Physics and Multi-Scale Self-Organization to Functional Diversity on the Device Scale

Time: Thursday 10:00–12:45 Location: Audimax 1

Invited Talk SYHN 1.1 Thu 10:00 Audimax 1

Scaling behavior of stiffness and strength of hierarchical network nanomaterials — •Shan Shi — Institut für Werkstoffmechanik, Helmholtz-Zentrum Hereon, Geesthacht — Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg, Hamburg

Structural hierarchy is known to optimize mechanical behavior in deliberately designed structures and natural materials. The benefits of hierarchy implementing the high strength of nanoscale objects into hierarchical structures would lead to even more interesting mechanical characteristics. Yet, truly nanoscale structures with a prohibitive number of struts in any macroscopic bodies have not been demonstrated in load-bearing form that could be subjected to mechanical tests.

Here, we prepared macroscopic, crack-free nested network nanomaterials ”hierarchical nanoporous gold” by two-stage self-organization processes of dealloying, which processes allow for large samples contained over trillions of struts to be synthesized. Macro-compression tests indicate the hierarchical architecture affords enhanced strength and stiffness. The experiments are well supported by our proposed scaling laws for the stiffness and strength for nested network with different numbers of hierarchy levels and by atomistic simulations. Therefore, this work for the first time demonstrated that structural hierarchy brings enhanced mechanics for truly nanoscale network materials.

Invited Talk SYHN 1.2 Thu 10:30 Audimax 1

Functional and programmable DNA nanotechnology — •Laura Na Liu — 2. Physics Institute, University of Stuttgart, Stuttgart, Germany

A fundamental design rule that nature has developed for biological machines is the intimate correlation between motion and function. One class of biological machines is molecular motors in living cells, which directly convert chemical energy into mechanical work. They coexist in every eukaryotic cell, but differ in their types of motion, the filaments they bind to, the cargos they carry, as well as the work they perform. Such natural structures offer inspiration and blueprints for constructing DNA-assembled artificial systems, which mimic their functionality. In this talk, I will discuss a variety of DNA-assembled architectures with different motion and functions. I will also outline ongoing research directions and conclude that DNA nanotechnology has a bright future ahead.

15 min. break

Invited Talk SYHN 1.3 Thu 11:15 Audimax 1

Multivalent nanoparticles for targeted binding — •Stefano Angioletti-Uberti — Department of Materials, Imperial College London, United Kingdom

Ligand-coated nanoparticles are a leading candidate for various applications where targeted binding is necessary, e.g. drug-delivery or biosensing, to name just two.

In this system, the main idea is that binding to the target occurs via the formation of ligand-receptor bonds. In fact, typically many of such bonds will form and in various competing patterns that vary not only depending on the bond strength but also on features such as grafting densities, or the geometry of binding. This results in highly tuneable binding affinities and more generally peculiar (and not yet fully exploited) novel binding properties that arise from the statistical nature of the binding, properties that could be exploited to achieve new functionalities.

In this talk, I will present some of our recent work to understand these so-called multivalent nanoparticles, showing how theory and simulations have been used to both rationalise and predict the behaviour of experiments and point the consequences of our findings for the development of nanomedicine applications based on multivalent binding.

Invited Talk SYHN 1.4 Thu 11:45 Audimax 1

Programming Nanoscale Self-Assembly — •Oleg Gang — Columbia University, New York, NY, USA — Brookhaven National Lab, Upton, NY, USA

The ability to organize rationally functional nanoscale components into the targeted architectures promises to enable a broad range of nanotechnological applications, from designed biomaterials to photonic devices and information processing systems. However, we are currently lacking a broadly applicable methodology for the bottom-up nano-fabrication with ability to prescribe a structure and to integrate different types of components. The talk will discuss our progress on uncovering guiding principles and establishing a practical platform for assembly of designed large-scale and finite-size nano-architectures from diverse nanocomponents through the DNA-programmable assembly. The recent advances in creating periodic and hierarchical organizations from inorganic nanoparticles and proteins will be presented. The use of the developed assembly approaches for generating nanomaterials with nano-optical, electrical, and biochemical functions will be demonstrated.

Invited Talk SYHN 1.5 Thu 12:15 Audimax 1

Achieving Global Tunability via Local Programming of a Structure's Composition — •Jochen Mueller — Johns Hopkins University, Baltimore, MD, United States

Once fabricated, structures and devices typically maintain their properties throughout their lifetime. In recent years, various stimuli, including temperature, pressure, and magnetic fields, have been implemented to actively change the mechanical and other physical properties after fabrication. Yet, most such approaches are limited to individual properties, specific geometries, or require high structural complexity. Inspired by this work – and by these challenges – we propose a framework for programmable and thermally reconfigurable multimaterial systems. The initial structure is monolithically fabricated via 3D printing and programmed by integrating active materials that can change their mechanical properties from virtually identical to over two orders of magnitude in difference with respect to a passive base material. By varying the temperature, the programmed structure can actively adapt a wide range of mechanical properties and deformation behaviors, including the deformation mode, Poisson's ratio, and effective relative density. We anticipate the proposed framework to enable significant progress in numerous technological fields, such as aerospace, biomedical, and robotics.

Symposium Novel phases and dynamical properties of magnetic skyrmions (SYMS)

jointly organised by
the Low Temperature Physics Division (TT),
the Magnetism Division (MA),
the Surface Science Division (O), and
the Crystalline Solids and their Microstructure Division (KFM)

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The discovery of skyrmions in cubic chiral ferromagnets over a decade ago, featuring non-trivial topological winding and greatly enhanced sensitivity to spin transfer torques, stimulated intense research into the suitability of skyrmions for technical applications. The symposium focusses on the recent identification of symmetry-broken phases and new forms of driven dynamical states of skyrmions in ferromagnetic host materials vis a vis the discovery of skyrmionic order in geometrically frustrated and antiferromagnetic magnets and their dynamical properties. The symposium this way highlights the intimate relationship of non-trivial topology and exceptional spin dynamics in different skyrmion-hosting systems.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 2)

Invited Talks

SYMS 1.1	Tue	10:00–10:30	Audimax 2	**Imaging skyrmions in synthetic antiferromagnets by single spin relaxometry** — •Aurore Finco
SYMS 1.2	Tue	10:30–11:00	Audimax 2	**Microwave spectroscopy of the skyrmionic states in a chiral magnetic insulator** — •Aisha Aqeel, Jan Sahliger, Takuya Taniguchi, Stefan Maendl, Denis Mettus, Helmuth Berger, Andreas Bauer, Markus Garst, Christian Pfleiderer, Christian H. Back
SYMS 1.3	Tue	11:15–11:45	Audimax 2	**Archimedean Screw in Driven Chiral Magnets** — •Nina del Ser
SYMS 1.4	Tue	11:45–12:15	Audimax 2	**Frustration-driven magnetic fluctuations as the origin of the low-temperature skyrmion phase in $Co_7Zn_7Mn_6$** — •Jonathan White, Victor Ukleev, Kosuke Karube, Peter Derlet, Chennan Wang, Hubertus Luetkens, Daisuke Morikawa, Akiko Kikkawa, Lucile Mangin-Thro, Andrew Wildes, Yuichi Yamasaki, Yuichi Yokoyama, Le Yu, Cinthia Piamonteze, Nicolas Jaouen, Yusuke Tokunaga, Henrik Rønnow, Taka-hisa Arima, Yoshinori Tokura, Jonathan White
SYMS 1.5	Tue	12:15–12:45	Audimax 2	**Magnetic Skyrmions as Topological Multi-Media Influencers** — •Sebastián A. Díaz

Sessions

SYMS 1.1–1.5	Tue	10:00–12:45	Audimax 2	**Novel phases and dynamical properties of magnetic skyrmions**

Sessions

– Invited Talks –

SYMS 1: Novel phases and dynamical properties of magnetic skyrmions

Time: Tuesday 10:00–12:45 Location: Audimax 2

Invited Talk SYMS 1.1 Tue 10:00 Audimax 2

Imaging skyrmions in synthetic antiferromagnets by single spin relaxometry — •Aurore Finco — Laboratoire Charles Coulomb, Université de Montpellier and CNRS, Montpellier, France

Antiferromagnets attract a great interest for spintronics owing to the robustness of the hosted magnetic textures and their fast dynamics. NV-center magnetometry has emerged in the last years as a powerful technique to investigate them. Here we introduce a new imaging mode of the NV magnetometer which relies on the detection of noise originating from spin waves interacting with the textures of interest.

We demonstrate this method on synthetic antiferromagnets (SAF). We first image domain walls and prove that we perform noise-based imaging by measuring spin relaxation times. Calculations of the spin wave dispersions as well as maps of simulated noise intensity enable us to conclude that we probe spin waves channelled in the domain walls. Going further, we tune the composition of the SAF stacks in order to stabilize spin spirals or skyrmions. In both cases, our relaxometry-based technique is able to image the non-collinear structures, demonstrating its efficiency and opening new avenues of exploration in the characterization of complex structures in magnetically-compensated materials.

This work was done in collaboration with the UMR CNRS/Thalès and the C2N in Palaiseau, France. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 846597 and from the DARPA TEE Program.

Invited Talk SYMS 1.2 Tue 10:30 Audimax 2

Microwave spectroscopy of the skyrmionic states in a chiral magnetic insulator — •Aisha Aqeel[1], Jan Sahliger[1], Takuya Taniguchi[1], Stefan Maendl[1], Denis Mettus[1], Helmuth Berger[2], Andreas Bauer[1], Markus Garst[3], Christian Pfleiderer[1], and Christian H. Back[1,4] — [1]Technical University of Munich, Garching, Germany — [2]École polytechnique Federale de Lausanne, Lausanne, Switzerland — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

In the cubic chiral magnet Cu2OSeO3 a low-temperature skyrmion state (LTS) and a concomitant tilted conical state are observed for magnetic fields applied along specific crystallographic directions (<100>). In this work, we investigated the dynamic resonances of these novel magnetic states. We have used the broadband microwave spectroscopy to study these resonance modes. By comparing the results to linear spin-wave theory, we clearly identify the gyrational and breathing modes associated with the LTS, as well as the hybridization of the breathing mode with a dark octupole gyration mode mediated by the magnetocrystalline anisotropies. Interestingly, our findings suggest that under decreasing fields the hexagonal skyrmion lattice becomes unstable, resulting in the formation of elongated skyrmions.

15 min. break

Invited Talk SYMS 1.3 Tue 11:15 Audimax 2

Archimedean Screw in Driven Chiral Magnets — •Nina del Ser — Institute for Theoretial Physics, University of Cologne, Cologne, Germany

In chiral magnets a magnetic helix forms where the magnetization winds around a propagation vector $\mathbf{q}$. We show theoretically that a magnetic field $\mathbf{B}_\perp(t) \perp \mathbf{q}$, which is spatially homogeneous but oscillating in time, induces a net rotation of the texture around $\mathbf{q}$. This rotation is reminiscent of the motion of an Archimedean screw and is equivalent to a translation with velocity $\mathbf{v}_{\text{screw}}$ parallel to $\mathbf{q}$. Due to the coupling to a Goldstone mode, this non-linear effect arises for arbitrarily weak $\mathbf{B}_\perp(t)$ with $v_{\text{screw}} \propto B_\perp^2$ as long as pinning by disorder is absent. The effect is resonantly enhanced when internal modes of the helix are excited and the sign of $\mathbf{v}_{\text{screw}}$ can be controlled either by changing the frequency or the polarization of $\mathbf{B}_\perp(t)$. The Archimedean screw can be used to transport spin and charge and thus the screwing motion is predicted to induce a voltage parallel to $\mathbf{q}$. Using a combination of numerics and Floquet spin wave theory, we show that the helix becomes unstable upon increasing $\mathbf{B}_\perp$, forming a 'time quasicrystal' which oscillates in space and time for moderately strong drive.

Invited Talk SYMS 1.4 Tue 11:45 Audimax 2

Frustration-driven magnetic fluctuations as the origin of the low-temperature skyrmion phase in $Co_7Zn_7Mn_6$ — •Jonathan White[1], Victor Ukleev[1], Kosuke Karube[2], Peter Derlet[1], Chennan Wang[1], Hubertus Luetkens[1], Daisuke Morikawa[2], Akiko Kikkawa[2], Lucile Mangin-Thro[3], Andrew Wildes[3], Yuichi Yamasaki[4,5], Yuichi Yokoyama[4], Le Yu[1,6], Cinthia Piamonteze[1], Nicolas Jaouen[7], Yusuke Tokunaga[8], Henrik Rønnow[6], Taka-hisa Arima[2,8], Yoshinori Tokura[2,8], and Jonathan White[2] — [1]Paul Scherrer Institut, Switzerland — [2]RIKEN CEMS, Japan — [3]Institut Laue-Langevin, France — [4]NIMS, Japan — [5]PRESTO, Japan — [6]EPFL, Switzerland — [7]Synchrotron Soleil, France — [8]University of Tokyo, Japan

Magnetic skyrmion phases in noncentrosymmetric magnets are an established testbed for topological quantum matter research. In chiral cubic Co-Zn-Mn compounds, Bloch-type skyrmion phases are easily tuned according to composition, and display, amongst other phenomena, remarkable metastable skyrmion behaviour. Here we focus on $Co_7Zn_7Mn_6$, which we showed recently to host two thermodynamically distinct equilibrium skyrmion phases. In addition to a conventional A-phase stable near T_c, the second phase is instead stable at much lower temperature. From our most recent quantum beam experiments, we find the stability of the low temperature phase is uniquely derived from a novel cooperative interplay between chiral magnetism and magnetic frustration-induced spin fluctuations generated by a magnetic hyper-kagome motif embedded in the crystal structure.

Invited Talk SYMS 1.5 Tue 12:15 Audimax 2

Magnetic Skyrmions as Topological Multi-Media Influencers — •Sebastián A. Díaz — University of Duisburg-Essen, Duisburg, Germany

Magnetic skyrmions are stable, particle-like spin configurations whose real-space topology affords them with fascinating properties. Soon after their experimental observation and motivated by the prospect of using them as information carriers, research focused on mastering their manipulation via their coupling to applied fields, electric currents, and temperature gradients. However, the spectrum of novel phenomena goes beyond these initial milestone discoveries. Recently, magnetic skyrmions have been shown to be fertile substrates for multiple topological media. This talk will focus on two of our latest theoretical proposals: topological magnon insulating phases supported by skyrmion crystals[1] and topological superconductivity induced by antiferromagnetic skyrmion chains[2]. The hallmarks of the former are robust magnonic states localized at the sample boundaries. These states are suitable for applications in magnonics, the harnessing of magnons as information carriers. Exploiting the mobility of antiferromagnetic skyrmions, our proposed topological superconductivity platform could provide the so far elusive smoking gun evidence of the non-Abelian exchange statistics of Majorana bound states localized at the ends of the chain.

[1] S. A. Díaz et al., PRL 122, 187203 (2019); S. A. Díaz et al., PRR 2, 013231 (2020); T. Hirosawa et al., PRL 125, 207204 (2020)

[2] S. A. Díaz et al., arXiv:2102.03423

Symposium Advanced neuromorphic computing hardware: Towards efficient machine learning (SYNC)

jointly organised by
the Semiconductor Physics Division (HL),
the Thin Films Division (DS), the Dynamics and Statistical Physics Division (DY), and
Physics of Socio-economic Systems Division (SOE)

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Recently novel computational approaches such a neural networks are revolutionizing computation. At the same time, we experience that the performance growth of digital microchips is saturating and the energy consumption of classical digital electronic processors is becoming a serious issue. This impasse has re-invigorated learning from the brain with its amazing intelligence-per-watt ratio and the exploration of unconventional physical substrates and nonlinear phenomena.

Our symposium will present the recent progress and future perspectives of neuro-inspired computing based on solid-state systems and their relation to machine learning. This includes not only important aspects of novel computational architectures in unconventional substrates but also new theoretical concepts of computing in non-digital, "brain-like" physical substrates.

The chosen topic is highly interdisciplinary as we aim at bringing together researchers from material science, machine learning, computer engineering, nonlinear dynamics with exciting talks of renowned international experts in the field.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 1)

Invited Talks

SYNC 1.1	Wed	10:00–10:30	Audimax 1	**Equilibrium Propagation: a Road for Physics-Based Learning** — •Damien Querlioz
SYNC 1.2	Wed	10:30–11:00	Audimax 1	**Machine Learning and Neuromorphic Computing: Why Physics and Complex Systems are Indispensable** — •Ingo Fischer
SYNC 1.3	Wed	11:00–11:30	Audimax 1	**Photonic Tensor Core Processor and Photonic Memristor for Machine Intelligence** — •Volker Sorger
SYNC 1.4	Wed	11:45–12:15	Audimax 1	**Material learning with disordered dopant networks** — •Wilfred van der Wiel
SYNC 1.5	Wed	12:15–12:45	Audimax 1	**In-memory computing with non-volatile analog devices for machine learning applications** — •John Paul Strachan

Sessions

SYNC 1.1–1.5	Wed	10:00–12:45	Audimax 1	**Symposium: Advanced neuromorphic computing hardware: Towards efficient machine learning**

Sessions

– Invited Talks –

SYNC 1: Symposium: Advanced neuromorphic computing hardware: Towards efficient machine learning

Time: Wednesday 10:00–12:45 Location: Audimax 1

Invited Talk SYNC 1.1 Wed 10:00 Audimax 1
Equilibrium Propagation: a Road for Physics-Based Learning — •Damien Querlioz — Université Paris-Saclay, CNRS, C2N, Palaiseau, France.
Neuromorphic computing takes inspiration from the brain to create highly energy-efficient hardware for information processing, capable of sophisticated tasks. The resulting systems are most often preprogrammed: training neuromorphic systems on-chip to perform new tasks remains a formidable challenge. The flagship algorithm for training neural networks, backpropagation, is indeed not hardware-friendly. It requires a mathematical procedure to compute gradients, external memories to store them, and an external dedicated circuit to change the neural network parameters according to these gradients. The brain, by contrast, does not learn this way. It learns intrinsically, and its synapses evolve directly through the spikes applied by the neurons they connect, using their biophysics. This technique is very advantageous in terms of energy efficiency and device density. In this talk, I will introduce our approach towards reproducing this brain strategy of intrinsic learning exploiting device physics. I will show through simulations how we take advantage of the physical roots of an algorithm called Equilibrium Propagation (1) to design dynamical circuits that learn intrinsically with high accuracy (2-4).

1. B. Scellier, Y. Bengio, Front. Comput. Neurosci. 11 (2017). 2. M. Ernoult, J. Grollier, D. Querlioz, Y. Bengio, B. Scellier, Proc. NeurIPS, pp. 7081 (2019). 3. A. Laborieux et al., Front. Neurosci. 15 (2021). 4. E. Martin et al., iScience. 24 (2021).

Invited Talk SYNC 1.2 Wed 10:30 Audimax 1
Machine Learning and Neuromorphic Computing: Why Physics and Complex Systems are Indispensable — •Ingo Fischer — Instituto de Física Interdisciplinar y Sistemas Complejos IFISC (UIB-CSIC), Campus UIB, 07122 Palma de Mallorca, Spain
Advances in Machine Learning have recently boosted neuromorphic computing and its implementation in analog hardware. We discuss why physics and complex systems science provide valuable perspectives and tools for understanding existing methods and developing novel transdisciplinary approaches and their hardware implementation.

Invited Talk SYNC 1.3 Wed 11:00 Audimax 1
Photonic Tensor Core Processor and Photonic Memristor for Machine Intelligence — •Volker Sorger — George Washington University, Washington DC, USA
Photonic technologies are at the forefront of the ongoing 4th industrial revolution of digitalization supporting applications such as 5G networks, virtual reality, autonomous vehicles, and electronic warfare. With Moores law and Dennard scaling now being limited by fundamental physics, the trend in processor heterogeneity suggests the possibility for special-purpose photonic processors such as neural networks or RF-signal & image filtering. Here unique opportunities exist, for example, given by algorithmic parallelism of analog and distributed non-van Neuman architectures enabling non-iterative O(1) processors with ps-short delay towards real-time decision making. Here, I will share our latest work on photonic information processors to include a photonic tensor core including multistate photonic nonvolatile random-access memory [Appl. Phys. Rev.], and a massively parallel Fourier-optics convolutional processor [Optica]. In summary, photonics connects the worlds of electronics and optics, thus enabling new concepts of efficient intelligence information processing via algorithm-hardware homomorphism empowered by the distinctive properties of light.

15 min. break.

Invited Talk SYNC 1.4 Wed 11:45 Audimax 1
Material learning with disordered dopant networks — •Wilfred van der Wiel — BRAINS Center for Brain-Inspired Nano Systems, MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands
The implementation of machine learning in digital computers is intrinsically wasteful and one has started looking at natural information processing systems, in particular the brain, that operate much more efficiently. Whereas the brain utilizes wet, soft tissue for information processing, one could in principle exploit any material and its physical properties to solve a problem. Here we give examples of how nanomaterial networks can be trained using the principle of Material Learning to take full advantage of the computational power of matter.

We have shown that a designless network of gold nanoparticles can be configured into Boolean logic gates using artificial evolution. We further demonstrated that this principle is generic and can be transferred to other material systems. By exploiting the nonlinearity of a nanoscale network of boron dopants in silicon, we can significantly facilitate classification. Using a convolutional neural network approach, it becomes possible to use our device for handwritten digit recognition. An alternative Material Learning is approach is followed by first mapping our Si:B network on a deep neural network model, which allows for applying standard Machine Learning techniques in finding functionality. Finally, we show that the widely applied machine learning technique of gradient descent can be directly applied in materio, opening up the pathway for autonomously learning hardware systems.

Invited Talk SYNC 1.5 Wed 12:15 Audimax 1
In-memory computing with non-volatile analog devices for machine learning applications — •John Paul Strachan — Peter Grünberg Institute (PGI-14), Forschungszentrum Jülich GmbH, Jülich, Germany — RWTH Aachen University, Aachen, Germany
I describe our work to build non-von Neumann computing systems for machine learning and other computing applications. We are able to improve speed and power by leveraging emerging non-volatile and analog devices (e.g., memristors) and combining with mature CMOS technology, enabling the construction of novel circuits and architectures. We describe the acceleration of linear algebra operations and also complex pattern storage and retrieval, which are core operations in modern deep learning and broader machine learning workloads. We also build improved Content Addressable Memory (CAM) circuits that can be used in a variety of computing applications from network security, genomics, and many types of data classification. We forecast significant improvement over CPUs, GPUs, and custom ASICs using these new architectures. I will also describe work in addressing the types of errors often observed in analog systems, both in mitigating their effects as well as harnessing them productively.

Symposium Potentials for NVs sensing magnetic phases, textures and excitations (SYNV)

jointly organised by
the Low Temperature Physics Division (TT),
the Magnetism Division (MA),
the Metal and Material Physics (MM), and
the Semiconductor Division (HL)

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The understanding of ordered magnetic phases is essential from fundamental and application perspectives. While ferromagnets are currently used in non-volatile, high-density data storage devices, topologically trivial and non-trivial magnetic phases are discussed for future low-energy information processing schemes. An overarching scientific quest towards achieving high performance devices, is to obtain a detailed understanding of the stabilization of magnetic phases, the interactions at play, the resulting magnetic textures, and their excitations. Color centers such as nitrogen vacancies (NV) in diamond represent a modern platform to access key magnetization parameters on the nanoscale and therefore represent an important method to provide a deeper insight into the mechanisms at play. This symposium brings together experts from different but overlapping fields of static and dynamic NV sensing, using tip-based single NV scanning methods as well as ensemble-based widefield imaging concepts. The speakers will provide an overview of the recent and exciting developments of this spectroscopy technique with a particular emphasis on material science questions.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 2)

Invited Talks

SYNV 1.1	Mon	13:30–14:00	Audimax 2	**Harnessing Nitrogen Vacancy Centers in Diamond for Next-Generation Quantum Science and Technology** — •Chunhui Du
SYNV 1.2	Mon	14:00–14:30	Audimax 2	**Nanoscale imaging of spin textures with single spins in diamond** — •Patrick Maletinsky
SYNV 1.3	Mon	14:30–15:00	Audimax 2	**Spin-based microscopy of 2D magnetic systems** — •Jörg Wrachtrup
SYNV 1.4	Mon	15:15–15:45	Audimax 2	**Exploring antiferromagnetic order at the nanoscale with a single spin microscope** — •Vincent Jacques
SYNV 1.5	Mon	15:45–16:15	Audimax 2	**Nanoscale magnetic resonance spectroscopy with NV-diamond quantum sensors** — •Dominik Bucher

Sessions

SYNV 1.1–1.5	Mon	13:30–16:15	Audimax 2	**Potentials for NVs sensing magnetic phases, textures and excitations**

Sessions

– Invited Talks –

SYNV 1: Potentials for NVs sensing magnetic phases, textures and excitations

Time: Monday 13:30–16:15 Location: Audimax 2

Invited Talk SYNV 1.1 Mon 13:30 Audimax 2
Harnessing Nitrogen Vacancy Centers in Diamond for Next-Generation Quantum Science and Technology — •Chunhui Du — University of California, San Diego, California, United State

Advanced quantum systems are integral to both scientific research and modern technology enabling a wide range of emerging applications. Nitrogen vacancy (NV) centers, optically active atomic defects in diamond, are directly relevant in this context due to their single-spin sensitivity and remarkable functionality over a broad temperature range. In this talk, I will present our recent efforts on developing NV-based quantum sensing and imaging techniques and their potential to address the challenges in both condensed matter physics and quantum science and technologies. Specifically, we have achieved: 1) electrical control of coherent spin rotations of NV spin qubits in NV-magnon based hybrid systems, 2) nanoscale imaging of magnetic flux and magnetization of a topological superconductor by NV wide-field microscopy, and 3) local non-invasive measurements of thermal environment of Mott insulators by NV centers. Our results illustrate the unique capability enabled by NV centers in exploring the exotic spin, heat, and charge transport in emergent quantum materials. The demonstrated coupling between NV centers and magnons in hybrid quantum devices further points to the possibility to establish macroscale entanglement between distant spin qubits and paves the way for developing transformative NV-based quantum computer.

Invited Talk SYNV 1.2 Mon 14:00 Audimax 2
Nanoscale imaging of spin textures with single spins in diamond — •Patrick Maletinsky — Department of Physics, Basel University, Switzerland

Quantum two-level systems offer attractive opportunities for sensing and imaging at the nanoscale. Since its inception, this idea [1] has advanced from proof of concept [2] to a mature quantum technology [3], which finds applications in condensed matter physics, materials science and engineering. In this talk, I will discuss our approach to realizing such quantum sensors [4] and highlight some particularly rewarding applications in the imaging of nanoscale spin textures.

Specifically, I will discuss how we employ single electronic spins in diamond for nanoscale probing of antiferromagnetic systems [5,6] and high-resolution imaging of atomically thin van der Waals magnets [7]. For both, the combination of sensitivity, spatial resolution and quantitative imaging enables unprecedented insights into nanoscale domains and domain-walls down to the atomic monolayer limit.

I will conclude with an outlook of future developments of single spin magnetometers for extreme conditions, such as high magnetic fields, mK temperatures or high-frequency sensors to probe the dynamics of nanomagnetic systems.

[1] B. Chernobrod et al., J. Appl. Phys. 97, 014903 [2] G. Balasubmaranian et al., Nature 455, 644 [3] P. Appel et al., Rev. Sci. Instr. 87, 063703 [4] N. Hedrich et al. Phys. Rev. Appl. 14, 064007 [5] P. Appel et al., Nano Lett. 19, 1682 [6] N. Hedrich et al., Nature Phys. 17, 574 [7] L. Thiel et al., Science 364, 973

Invited Talk SYNV 1.3 Mon 14:30 Audimax 2
Spin-based microscopy of 2D magnetic systems — •Jörg Wrachtrup — 3rd Physics Institute, University of Stuttgart, Stuttgart, Germany

The investigation of magnetic order in 2D materials requires dedicated probes. While conventional probes of magnetism with nanoscale resolution, like Lorenz microscopy or MFM fail for few layer- or monolayer samples, STM requires dedicated sample preparation. NV-based magnetic probes on the other hand are very well suited to provide quantitative data with a few ten nm spatial resolution and sufficient sensitivity, even for monolayer samples. In the talk I will describe experiments on CrBr3 which show the domain structure of the material [1]. Upon imaging material with different number of layers we gained insight into interlayer coupling and it impact on magnetic order. We also measure magnetic order over a wide range of temperatures and derive information on the physics of the phase transition of CrBr3. In addition, I will show measurements on CrI3 samples of different thickness and relative orientation where we find signatures of Moiré patterns in twisted multilayers [2].

[1] Qi-Chao Sun et al. Magnetic domains and domain wall pinning in atomically this CrBr3 revealed by nanoscale imaging, Nature Comm. 12, 1989 (2021) [2] Qi-Chao Sun et al. Direct visualization of magnetic domains and moiré magnetism in twisted two-dimensional magnets, submitted (2021)

15 min. break

Invited Talk SYNV 1.4 Mon 15:15 Audimax 2
Exploring antiferromagnetic order at the nanoscale with a single spin microscope — •Vincent Jacques — Laboratoire Charles Coulomb, Université de Montpellier and CNRS, 34095 Montpellier, France

Experimental methods allowing for the detection of single spins in the solid-state, which were initially developed for quantum information science, open new avenues for the development of highly sensitive quantum sensors. In that context, the electronic spin of a single nitrogen-vacancy (NV) defect in diamond can be used as an atomic-sized magnetometer, providing an unprecedented combination of spatial resolution and magnetic sensitivity under ambient conditions [1]. In this talk, I will illustrate how scanning-NV magnetometry can be used as a powerful tool for exploring condensed-matter physics, focusing on chiral spin textures in antiferromagnetic materials [2,3].

References: [1] L. Rondin et al., Rep. Prog. Phys. 77, 056503 (2014) [2] I. Gross et al., Nature 549, 252 (2017) [3] A. Finco et al., Nat. Comm. 12, 767 (2021)

Invited Talk SYNV 1.5 Mon 15:45 Audimax 2
Nanoscale magnetic resonance spectroscopy with NV-diamond quantum sensors — •Dominik Bucher — Technical University of Munich, Physical Chemistry, Garching, Germany

Recently, optically probed nitrogen-vacancy (NV) point defects in diamond have emerged as a new class of quantum sensors allowing the detection of magnetic fields on unprecedented length scales. This technique allows the measurement of magnetic resonance signals on the nanoscale down to a single electronic or nuclear spin. In the first part of this talk, I will introduce the concept of quantum sensing with NV-centers, in particular, the detection of oscillating magnetic fields, important for magnetic resonance spectroscopy applications. In the second part, I will report on recent progress on probing thin films and 2D materials with this technique. In the concluding part, possible applications in sensing magnetic phases, textures and excitations will be discussed.

Symposium The Rise of Photonic Quantum Technologies – Practical and Fundamental Aspects (SYPQ)

jointly organised by
the Semiconductor Physics Division (HL),
the Magnetism Division (MA),
the Metal and Material Physics Division (MM),
the Low Temperature Physics Division (TT), and
the Working Group young Leader in Physics (AGyouLeaP)

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Overview of Invited Talks and Sessions

(Lecture hall Audimax 2)

Invited Talks

SYPQ 1.1	Fri	10:00–10:30	Audimax 2	**Quantum dots operating at telecom wavelengths for photonic quantum technology** — •Simone Luca Portalupi
SYPQ 1.2	Fri	10:30–11:00	Audimax 2	**Photonic graph states for quantum communication and quantum computing** — •Stefanie Barz
SYPQ 1.3	Fri	11:00–11:30	Audimax 2	**Rare-earth ion doped solids at sub-Kelvins: practical and fundamental aspects** — •Pavel Bushev
SYPQ 1.4	Fri	11:45–12:15	Audimax 2	**Quantum Light and Strongly Correlated Electronic States in a Moiré Heterostructure** — •Brian Gerardot
SYPQ 1.5	Fri	12:15–12:45	Audimax 2	**Quantum communication in fibers and free-space** — •Rupert Ursin

Sessions

SYPQ 1.1–1.5	Fri	10:00–12:45	Audimax 2	**Symposium: The Rise of Photonic Quantum Technologies – Practical and Fundamental Aspects**

Sessions

– Invited Talks –

SYPQ 1: Symposium: The Rise of Photonic Quantum Technologies – Practical and Fundamental Aspects

Within the so-called second quantum revolution many research fields undergo a transition from basic research in solid-state physics and quantum optics towards applications of photonic quantum technologies, which will prospectively have a large impact to our future daily life. In this light, our Symposium brings together leading experts and early career scientists from different fields, reporting their recent progress on quantum technologies. The topics will illuminate practical but also fundamental aspects at the intersections between the fields of semiconductor and solid-state physics, spin systems, quantum optics, quantum communication, and quantum computing.

Organizers: Tobias Heindel (TU Berlin), Kai Müller (TU München), Nadezhda Kukharchyk (Walther Meißner Institute, Garching)

Time: Friday 10:00–12:45 Location: Audimax 2

Invited Talk SYPQ 1.1 Fri 10:00 Audimax 2
Quantum dots operating at telecom wavelengths for photonic quantum technology — •Simone Luca Portalupi — IHFG-University of Stuttgart
In recent years, strong efforts have been made in order to realize out-of-the-lab demonstrations using quantum science. In particular, the broad range of photonic quantum technologies became highly attractive for the real world implementation of quantum information, quantum communication and quantum network tasks. Long distance realizations would benefit from the possibility of using photons as carriers of information. For these purposes, the use of quantum light in the so-called telecom O- (centred around 1310 nm) and C-band (centred around 1550 nm) would have the advantages of experiencing minimal photon wavepacket dispersion and absorption. Semiconductor quantum dots are considered one of the most appealing sources of quantum light, in particular the ones based on the GaAs material system. In this talk, we will discuss the techniques that can be employed to realize In(Ga)As/GaAs quantum dots emitting in the telecom O- and C-bands [1]. Furthermore, we will discuss advanced fabrication techniques [2] and optical resonators that can be employed to sensibly enhance the source brightness and performances, even operating at liquid nitrogen temperature [3].

[1] S. L. Portalupi, et al., Semicond. Sci. Technol. 34, 053001 (2019)
[2] M. Sartison, et al., Appl. Phys. Lett. 113, 032103 (2018)
[3] S. Kolatschek, et al., arXiv:2107.03316 (2021)

Invited Talk SYPQ 1.2 Fri 10:30 Audimax 2
Photonic graph states for quantum communication and quantum computing — •Stefanie Barz — Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — Centre for Integrated Quantum Science and Technologies, University of Stuttgart, Germany
Multipartite entanglement and, in particular, graph states are useful resources both for quantum computing and quantum communication, especially in networked settings.

In this talk, I will show a few examples where multipartite entanglement offers an advantage over classical or bipartite approaches.

In particular, I will present how photonic graph states can serve as a resource for computation and, vice versa, how computation can be used as a tool to test certain states.

Furthermore, I will show how graph states offer an advantage for communication protocols, in particular in networked settings and where one aims at keeping the identity of the communicating parties private.

I will present implementations of these concepts and discuss challenges in scaling up photonic quantum technologies.

Invited Talk SYPQ 1.3 Fri 11:00 Audimax 2
Rare-earth ion doped solids at sub-Kelvins: practical and fundamental aspects — •Pavel Bushev — JARA-Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, 52425 Jülich
Rare-earth ion-doped solids are promising candidates with a great variety of potential applications in quantum information processing and quantum communication. Due to the existence of addressable and long-lived transitions at microwave and optical frequencies these materials might be deployed as quantum memories in circuit QED, quantum memories for itinerary optical photons, and as quantum transducers between microwaves and light. Some of the above-listed applications require the use of ultra-low temperatures, i.e. $T < 0.1$ Kelvin. At this temperature, one may expect the resolving of single microwave photons at GHz frequency as well as the increase of spin and nuclear coherence times. In my talk, I will review the experimental state-of-the-art and discuss practical and fundamental aspects of the deep freezing of spin-doped solids.

15 min. break.

Invited Talk SYPQ 1.4 Fri 11:45 Audimax 2
Quantum Light and Strongly Correlated Electronic States in a Moiré Heterostructure — •Brian Gerardot — Institute for Photonics and Quantum Sciences, Heriot-Watt University, Edinburgh, UK
The unique physical properties of two-dimensional materials, combined with the ability to stack unlimited combinations of atomic layers with arbitrary crystal angle, has unlocked a new paradigm in designer quantum materials. For example, when two different monolayers are brought into contact to form a heterobilayer, the electronic interaction between the two layers results in a spatially periodic potential-energy landscape: the moire superlattice. The moire superlattice can create flat bands and quench the kinetic energy of electrons, giving rise to strongly correlated electron systems. Further, single particle wave packets can be trapped in the moire potential pockets with three-fold symmetry to form quantum dots which can emit single photons. Here I will present magneto-optical spectroscopy of $MoSe_2/WSe_2$ heterobilayer devices with a small relative twist. I will discuss moire-trapped inter-layer excitons, which can emit quantum light, and intra-layer excitons, which are sensitive to a large number of strongly correlated electron and hole states as a function of fractional filling.

Invited Talk SYPQ 1.5 Fri 12:15 Audimax 2
Quantum communication in fibers and free-space — •Rupert Ursin — Institute for Quantum Optics and Quantum Information - Vienna of the Austrian Academy of Sciences, Austria — Quantum Technology Laboratories GmbH, Vienna, Austria
Quantum communication is by far the most technically advanced and mature field within the emerging field of quantum technologies. It gained a lot of attention over the recent years because of the remarcable achievements in China on satellite links and in fibre based communication networks. I will present the quantum links we've successfully implemented from the Chinese satellite MICIUS to an optical ground station in Graz, Austria. Then I will present our effort to build scalable quantum networks on deployed fibres in the city of Bristol, UK and a quantum link between Malta and Italy on a submarine optical fibre cable. Last but not least I will present the recent efforts to built very bright entangled photon sources and preliminary results from an international collaboration to connects the Central European capital cities around Vienna with quantum optical fibre links.

Symposium Facets of many-body quantum chaos (SYQC)

jointly organised by
the Low Temperature (TT),
the Dynamics and Statistical Physics Division (DY), and
the Magnetism Division (MA)

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Many-body systems share the essential and surprising property that often simple effective descriptions emerge as a result of complex chaotic dynamics. Recent years have seen significant progress in the understanding of such complex dynamics in the quantum many-body context, both theoretically and experimentally, with impact onto areas as diverse as quantum gravity (via ADS/CFT dualities) or quantum information theory. It is the central goal of this Symposium to embody a broad spectrum of these recent developments with a particular focus on its cross-disciplinary aspects ranging from quantum statistical mechanics, atomic and condensed matter physics to high-energy physics.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 2)

Invited Talks

SYQC 1.1	Tue	13:30–14:00	Audimax 2	**Holographic interpretation of SYK quantum chaos** — •Alexander Altland
SYQC 1.2	Tue	14:00–14:30	Audimax 2	**Non-Fermi liquids and the lattice** — •Sean Hartnoll
SYQC 1.3	Tue	14:30–15:00	Audimax 2	**Dual-unitary circuits: non-equilibrium dynamics and spectral statistics** — •Bruno Bertini
SYQC 1.4	Tue	15:15–15:45	Audimax 2	**Post-Ehrenfest many-body quantum interferences in ultracold atoms** — •Steven Tomsovic
SYQC 1.5	Tue	15:45–16:15	Audimax 2	**Dynamics in unitary and non-unitary quantum circuits** — •Vedika Khemani

Sessions

SYQC 1.1–1.5	Tue	13:30–16:15	Audimax 2	**Facets of many-body quantum chaos**

Sessions

– Invited Talks –

SYQC 1: Facets of many-body quantum chaos

Time: Tuesday 13:30–16:15 Location: Audimax 2

Invited Talk SYQC 1.1 Tue 13:30 Audimax 2

Holographic interpretation of SYK quantum chaos — •Alexander Altland — Institute for theoretical physics, University of Cologne, Germany

Since its introduction in 2015, the SYK model has been intensively researched, and at this point is the perhaps best understood model system of many body quantum chaos. However, when Kitaev first proposed the model, his motivation was to define the boundary theory of a two-to-one dimensional holographic correspondence. In this talk, we will address the question what the lessons learned about the SYK system in the past five years can teach us about the nature of candidate bulk theories. Looking at the problem through the lens of quantum chaos, we will argue that perturbative studies inspired by periodic orbit analysis go a long way, but not all, in identifying the gravitational bulk. The solution of the problem might lie in a symmetry breaking principle realized in all universality classes of quantum chaos, but not so far in the proposed bulk duals. We will suggest that this symmetry breaking must be present in bulk duals of chaotic boundary theories, and that the search for it might turn into a creative resource.

Invited Talk SYQC 1.2 Tue 14:00 Audimax 2

Non-Fermi liquids and the lattice — •Sean Hartnoll — Stanford University

Non-Fermi liquids are electronic systems with strong electronic interactions. For example, the electrons may be quantum critical. Therefore, the electrons are expected to thermalize quickly. However, heat must also be able to leave the electronic degrees of freedom – for example, this will happen by Joule heating upon applying a current. In a metal Joule heating goes via the lattice degrees of freedom. I will explain a new formalism for computing the timescales over which the electronic and lattice degrees of freedom thermalize each other in a non-Fermi liquid.

Invited Talk SYQC 1.3 Tue 14:30 Audimax 2

Dual-unitary circuits: non-equilibrium dynamics and spectral statistics — •Bruno Bertini — University of Oxford

I will discuss the quantum non-equilibrium dynamics and the spectral statistics of a recently introduced class of “statistically solvable” many-body quantum systems: the dual-unitary circuits. These systems furnish a minimal modelling of generic, locally interacting, many-body quantum systems. In particular, I will show that generic dual-unitary circuits display behaviours typically associated with many-body quantum chaos.

15 min. break

Invited Talk SYQC 1.4 Tue 15:15 Audimax 2

Post-Ehrenfest many-body quantum interferences in ultracold atoms — •Steven Tomsovic — Department of Physics and Astronomy, Washington State University, Pullman, WA USA

Far out-of-equilibrium many-body quantum dynamics in isolated systems necessarily generate interferences beyond an Ehrenfest time scale, where quantum and classical expectation values diverge. Ultracold atomic gases provide a promising setting to explore these phenomena. Theoretically speaking, the heavily-relied-upon truncated Wigner approximation leaves out these interferences. We develop a semiclassical theory of coherent state propagation for many-body bosonic systems, which properly incorporates such missing quantum effects. For mesoscopically populated Bose-Hubbard systems, it is shown that this theory captures post-Ehrenfest quantum interference phenomena very accurately, and contains relevant phase information to perform many-body spectroscopy with high precision.

Invited Talk SYQC 1.5 Tue 15:45 Audimax 2

Dynamics in unitary and non-unitary quantum circuits — •Vedika Khemani — Stanford University

Symposium Topological constraints in biological and synthetic soft matter (SYSM)

jointly organised by
the Chemical and Polymer Physics Division (CPP),
the Biological Physics Division (BP), and
the Dynamics and Statistical Physics Division (DY)

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This focus session illustrates the importance of topology-related phenomena and processes in various areas of soft matter physics. The examples cover topological constraints in synthetic and biological polymer melts and gels, the role of knots in proteins, and topological defects in liquid-crystalline materials.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 1)

Invited Talks

SYSM 1.1	Mon	10:00–10:30	Audimax 1	**Interphase Chromatin Undergoes a Local Sol-Gel Transition Upon Cell Differentiation** — •Alexandra Zidovska
SYSM 1.2	Mon	10:30–11:00	Audimax 1	**Topological Tuning of DNA Mobility in Entangled Solutions of Supercoiled Plasmids** — •Jan Smrek, Jonathan Garamella, Rae Robertson-Anderson, Davide Michieletto
SYSM 1.3	Mon	11:15–11:45	Audimax 1	**Dynamics of macromolecular networks under topological and environmental constraints: some outstanding challenges** — •Dimitris Vlassopoulos
SYSM 1.4	Mon	11:45–12:15	Audimax 1	**Supercoiling in a Protein Increases its Stability** — •Joanna Sulkowska, Szymon Niewieczerzał
SYSM 1.5	Mon	12:15–12:45	Audimax 1	**Topology for soft matter photonics** — •Igor Musevic

Sessions

SYSM 1.1–1.5	Mon	10:00–12:45	Audimax 1	**Topological constraints in biological and synthetic soft matter**

Sessions

– Invited Talks –

SYSM 1: Topological constraints in biological and synthetic soft matter

Time: Monday 10:00–12:45 Location: Audimax 1

Invited Talk SYSM 1.1 Mon 10:00 Audimax 1
Interphase Chromatin Undergoes a Local Sol-Gel Transition Upon Cell Differentiation — •Alexandra Zidovska — Center for Soft Matter Research, New York University, New York, NY, USA
Cell differentiation, the process by which stem cells become specialized cells, is associated with chromatin reorganization inside the cell nucleus. Here, we measure the chromatin distribution and dynamics in embryonic stem cells *in vivo* before and after differentiation. We find that undifferentiated chromatin is less compact, more homogeneous and more dynamic than differentiated chromatin. Further, we present a noninvasive rheological analysis using intrinsic chromatin dynamics, which reveals that undifferentiated chromatin behaves like a Maxwell fluid, while differentiated chromatin shows a coexistence of fluid-like (sol) and solid-like (gel) phases. Our data suggest that chromatin undergoes a local sol-gel transition upon cell differentiation, corresponding to the formation of the more dense and transcriptionally inactive heterochromatin [Eshghi I, Eaton JA and Zidovska A, *Phys. Rev. Lett.*, 126(22): 228101 (2021)].

Invited Talk SYSM 1.2 Mon 10:30 Audimax 1
Topological Tuning of DNA Mobility in Entangled Solutions of Supercoiled Plasmids — •Jan Smrek[1], Jonathan Garamella[2], Rae Robertson-Anderson[2], and Davide Michieletto[3,4] — [1]Faculty of Physics, University of Vienna, Austria — [2]Department of Physics and Biophysics, University of San Diego, USA — [3]School of Physics and Astronomy, University of Edinburgh, UK — [4]MRC Human Genetics Unit, Institute of Genetics and Molecular Medicine, University of Edinburgh, UK
Ring polymers in dense solutions are among the most intriguing problems in polymer physics. Thanks to its natural occurrence in circular form, DNA has been extensively employed as a proxy to study the fundamental physics of ring polymers in different topological states. Yet, torsionally constrained – such as supercoiled – topologies have been largely neglected so far. Here we address this gap by coupling large-scale Molecular Dynamics simulations with Differential Dynamic Microscopy of entangled supercoiled DNA plasmids. We discover that, unexpectedly, larger supercoiling increases the size of entangled plasmids and concomitantly induces an enhancement in DNA mobility. These findings are reconciled as due to supercoiling-driven asymmetric and double-folded plasmid conformations which reduce inter-plasmids entanglements and threadings. Our results suggest a way to topologically tune DNA mobility via supercoiling. In addition, I will highlight the importance of threading topological constraints in other complex polymeric fluids in- and out of equilibrium.

15 min. break

Invited Talk SYSM 1.3 Mon 11:15 Audimax 1
Dynamics of macromolecular networks under topological and environmental constraints: some outstanding challenges — •Dimitris Vlassopoulos — FORTH and University of Crete, 100 N. Plastira St., Heraklion 70013, Greece
One of the biggest successes of soft matter physics has been the understanding of the rheological consequences of polymeric entanglements. It has set the stage for further advances which continue to date. Examples range from the viscoelastic spectrum of wormlike micelles to shear thinning of entangled polymers. Yet, a number of outstanding challenges remain, and here we present recent work addressing two of them: (i) Entangled linear polymers under strong shear exhibit a rich transient response whose interpretation remains controversial. We focus on the weak undershoot following the (well understood) overshoot of shear stress growth coefficient, which is often hard to detect experimentally. Modeling provides a rationalization by invoking the idea of tumbling which itself stems from simulation results. We designed a set of experiments with homopolymer blends to further elucidate its origin and identify the experimental and molecular parameters governing its appearance. (ii) Supramolecular assemblies based on hydrogen bonding motifs in apolar solvents exhibit rheological signatures which sensitively depend on traces (0.01%wt) of dissolved water. Hence, the relative humidity affects the viscoelastic response of the formed physical networks. We present results from linear and nonlinear rheometry which allow to quantify this overlooked effect and provide the ability to tune the rheology of supramolecular networks at molecular level.

Invited Talk SYSM 1.4 Mon 11:45 Audimax 1
Supercoiling in a Protein Increases its Stability — •Joanna Sulkowska and Szymon Niewieczerzał — Centre of New Technologies, University of Warsaw, Banacha 2c, 02-097 Warsaw, Poland
Currently it is known that at least 6% of proteins possess nontrivial topology (i.e. are entangled) and form structures called knots, slipknots, lassos, links and theta curves. A lasso is a structure that contains a covalent loop (closed by a cysteine, amide, or other bridge), crossed by at least one free end of a protein.

The supercoiling motif is the most complex type of nontrivial topology found in proteins with lasso motif. Based on a protein from extremophilic species with such a motif, with a coarse-grained protein model I will show that this protein can knot itself; however, the supercoiling changes a smooth landscape observed in reduced conditions into a two-state folding process in the oxidative conditions, with a deep intermediate state. The protein takes advantage of the hairpin-like motif to overcome the topological barrier and thus to supercoil. I will also show that the depth of the supercoiling motif, i.e. the length of the threaded terminus, has a crucial impact on the folding rates of the studied protein. Finally, I will show that fluctuations of the minimal surface area (i.e. the area of a surface spanned on a covalent loop) can be used to measure local stability, and that supercoiling motif introduces stability into the protein. These results suggest that the supercoiling motif enables the studied protein to live in physically extreme conditions, which are detrimental to most life on Earth.

Invited Talk SYSM 1.5 Mon 12:15 Audimax 1
Topology for soft matter photonics — •Igor Musevic — J. Stefan Institute, Ljubljana, Slovenia
Topological defects in liquid crystals can be created by either rapid pressure or temperature quench across the isotropic-liquid crystal phase transition and are stabilized either by colloidal inclusions or confinement. Defects appear as point charges or small defect loops that carry integer topological charge. Because the total topological charge must be conserved, point charges and loops in nematic liquid crystals always appear in pairs with opposite topological charges or in chargeless loops. Topological defects in liquid crystals can be used to assemble and even knot and link colloidal structures and superstructures of particles dispersed in a liquid crystal with the colloidal binding energy of the order of several 1000 kT. It has been also shown that micro-droplets of liquid crystals are in fact optical micro-cavities that can be put into laser operation solely by light. Because of the fluid nature of liquid crystals, droplets can be self-transformed into liquid fibers that are excellent optical wave-guides. This makes it possible to realize complex photonic devices, where topological defects act as a binding matter and the liquid crystal has the role of photonic soft matter.

Symposium Physics of van der Waals 2D heterostructures (SYWH)

jointly organised by
the Semiconductor Physics Divison (HL),
the Thin Films Division (DS),
the Surface Science Division (O), and
the Low Temperature Physics Division (TT)

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Van-der-Waals heterostructures based on two-dimensional (2D) layered materials provide a unique platform to engineer and control electronic, magnetic, and optical properties, as also recently recognized by the DFG establishing a new SPP 2244 on "2D-Materialien – die Physik von van der Waals (Hetero-)Strukturen (2DMP)". Many exciting phenomena have been reported in stacked materials interacting by weak interactions. Most spectacular are strong correlations, magnetism, and superconductivity in twisted bilayer graphene, whose theoretical understanding is currently debated. The aim of this plenary symposium is to present an overview of those recent developments by leading experts in this forefront area of condensed matter physics. We plan to structure the symposium to make it appealing to low temperature, semiconductor, as well as magnetism communities, and to provide a communication platform to establish links between the various topics, which is possible by the very nature of van der Waals structures. We also wish to introduce the topic of the aforementioned SPP to a broader DPG audience.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 2)

Invited Talks

SYWH 1.1	Thu	13:30–14:00	Audimax 2	**Spin interactions in van der Waals topological materials and magnets** — •Saroj Dash
SYWH 1.2	Thu	14:00–14:30	Audimax 2	**Exciton optics, dynamics and transport in atomically thin materials** — •Ermin Malic, Samuel Brem, Raul Perea-Causin, Daniel Erkensten, Roberto Rosati
SYWH 1.3	Thu	14:30–15:00	Audimax 2	**Correlated Electrons in van der Waals Superlattices: Control and Understanding** — •Tim Wehling
SYWH 1.4	Thu	15:15–15:45	Audimax 2	**Exciton manipulation and transport in 2D semiconductor heterostructures** — •Andras Kis
SYWH 1.5	Thu	15:45–16:15	Audimax 2	**Chern Insulators, van Hove singularities and Topological Flat-bands in Magic-angle Twisted Bilayer Graphene*** — •Eva Andrei, Shuang Wu, Zhenyuan Zhang

Sessions

SYWH 1.1–1.5	Thu	13:30–16:15	Audimax 2	**Symposium: Physics of van der Waals 2D heterostructures**

Sessions

– Invited Talks –

SYWH 1: Symposium: Physics of van der Waals 2D heterostructures

Time: Thursday 13:30–16:15 Location: Audimax 2

Invited Talk SYWH 1.1 Thu 13:30 Audimax 2

Spin interactions in van der Waals topological materials and magnets — •Saroj Dash — Chalmers University of Technology, Gothenburg, Sweden

Two-dimensional (2D) quantum materials and their van der Waals heterostructures represent a novel platform to realize different spin-based phenomena. Here, we used large-area CVD graphene as a spin interconnect and demonstrated a spin majority logic gate operation (1). We further engineered 2D material heterostructures by combining the best of different materials in one ultimate unit for the creation of strong proximity induced spin-orbit coupling and magnetism in graphene (2,4,3). Recently, we detected current-induced spin-polarization in topological insulators and Weyl semimetal candidates and their graphene-based heterostructures up to room temperature (4,5). Finally, we demonstrated room temperature spin-valve devices using van der Waals itinerant ferromagnet in heterostructures with graphene (6). These findings open a novel platform for electrical creation and gate-control of spin polarization and provide new opportunities for all-2D heterostructure spintronic devices and integrated circuits.

1. Carbon 161, 892 (2020), Nature Commun. 6, 6766 (2015). 2. Nature Commun. 8, 16093 (2017). 3. 2D Materials 7 (1), 015026 (2019). 4. Nature Commun. 11, 3657 (2020). 5. Advanced Materials, 2000818 (2020). 6. preprint arXiv:2107.00310 (2021).

Invited Talk SYWH 1.2 Thu 14:00 Audimax 2

Exciton optics, dynamics and transport in atomically thin materials — •Ermin Malic[1,2], Samuel Brem[1], Raul Perea-Causin[2], Daniel Erkensten[2], and Roberto Rosati[1] — [1]Philipps-University of Marburg, Germany — [2]Chalmers University of Technology, Sweden

Monolayer transition metal dichalcogenides (TMDs) exhibit a remarkable excitonic landscape including bright and a variety of dark exciton states. Solving 2D material Bloch equations for excitons, phonons and photons, we obtain a microscopic access to the interplay of optics, ultrafast dynamics and diffusion of excitons in TMDs. In joint theory-experiments studies we shed light on the importance of momentum-dark excitons in low-temperature photoluminescence spectra [1], non-equilibrium exciton dynamics visualized in tr-ARPES experiments [2], temperature-resolved exciton-exciton annihilation processes [3], phonon-driven dissociation of excitons [4], and accelerated hot-exciton diffusion [5]. The gained microscopic insights into the spatiotemporal exciton dynamics are crucial for understanding and controlling many-particle phenomena governing exciton optics, dynamics and transport in technologically promising 2D materials.

[1] S. Brem et al., Nano Lett. 20, 2849 (2020)
[2] R. Wallauer et al., Nano Lett. 21, 5867 (2021)
[3] D. Erkensten et al., arXiv 2106.05035 (2021)
[4] R. Perea-Causin et al., Nanoscale 13, 1884 (2021)
[5] R. Rosati et al., arXiv 2105.10232 (2021)

Invited Talk SYWH 1.3 Thu 14:30 Audimax 2

Correlated Electrons in van der Waals Superlattices: Control and Understanding — •Tim Wehling — University of Bremen, 28359 Bremen, Germany

The interplay of electronic correlations, lattice degrees of freedom and topology holds the promise for the realization of exotic states of quantum matter. Here, we discuss routes to understand and control this interplay in van der Waals superlattice systems. The nature of superconducting order presents a recurring overarching open question in this context. We will first address doping fingerprints of superconductivity arising from spin and lattice fluctuations in moiré superlattice systems [1]. We will show how doping-dependent measurements of the superconducting transition temperature provide direct access to probing the superconducting pairing mechanism in twisted van der Waals materials. We will then analyze possibilities of Coulomb and superlattice engineering in these systems. We will discuss confinement and deconfinement [2] pathways to create correlated Dirac fermions in stacks of transition metal dichalcogenides and identify knobs to control topology, electron correlations and emergent order in these systems.

[1] N. Witt, J. M. Pizarro, T. Nomoto, R. Arita, T. O. Wehling, arXiv:2108.01121 (2021).

[2] J. M. Pizarro, S. Adler, K. Zantout, T. Mertz, P. Barone, R. Valentí, G. Sangiovanni, T. O. Wehling, npj Quantum Materials 5, 79 (2020).

15 min. break.

Invited Talk SYWH 1.4 Thu 15:15 Audimax 2

Exciton manipulation and transport in 2D semiconductor heterostructures — •Andras Kis — École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

New opportunities are enabled by the band structure of transition metal dichalcogenides (TMDCs) in which we could harness the valley degree of freedom for valleytronics and next-generation photonics. Long-lived interlayer excitons in van der Waals heterostructures based on TMDCs have recently emerged as a promising platform for this, allowing control over exciton diffusion length, energy and polarization. I will show here how by using MoS2/WSe2 van der Waals heterostructures, we can realize excitonic transistors with switching action, confinement and control over diffusion length at room temperature in a reconfigurable potential landscape. On the other hand, the weak interlayer interaction and small lattice mismatch in MoSe2/WSe2 heterostructures results in brightening of forbidden optical transitions, allowing us to resolve two separate interlayer transitions with opposite helicities and meV-scale linewidths.Our more advanced excitonic devices now also offer the way to manipulate the motion of valley (spin) polarized excitons.

Invited Talk SYWH 1.5 Thu 15:45 Audimax 2

Chern Insulators, van Hove singularities and Topological Flat-bands in Magic-angle Twisted Bilayer Graphene* — •Eva Andrei, Shuang Wu, and Zhenyuan Zhang — Dept. of Physics, Rutgers University, Piscatay NJ 08904, USA

Magic-angle twisted bilayer graphene exhibits intriguing quantum phase transitions triggered by enhanced electron-electron interactions when its flat-bands are partially filled. These phases and their experimental manifestations provide clues to the underlying non-trivial band topology. In particular, transport measurements revealed a succession of doping-induced phase transitions at integer moiré fillings. We have shown that these transitions are accompanied by van Hove singularities (VHS) which facilitate the emergence of correlation-induced gaps and topologically non-trivial sub-bands. In the presence of a magnetic field, well quantized Hall plateaus at filling of 1, 2, 3 carriers per moiré-cell reveal the sub-band topology and signal the emergence of Chern insulators. Surprisingly, for magnetic fields exceeding 5T we observe a VHS at a filling of 3.5, suggesting the emergence of a fractional Chern insulator.

Shuang Wu, Zhenyuan Zhang, K. Watanabe, T. Taniguchi, Eva Y. Andrei, Nature Materials, 20 (2021) p488

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Overview of Invited Talks and Sessions

(Lecture halls H1 and H6; Posters P)

Invited Talks

BP 1.1	Mon	10:00–10:30	H1	**Physics-Informed Deep Learning for Characterizing Perturbed Cell Growth** — •Robert Endres, Henry Cavanagh, Rob Lind, Andreas Mosbach, Gabriel Scalliet
BP 2.1	Mon	11:30–12:00	H1	**PINCH-1 promotes migration in extracellular matrices and influences the mechanophenotype** — •Claudia Tanja Mierke
BP 3.1	Thu	10:00–10:30	H1	**SARS-CoV-2 induced membrane remodeling in infected cells revealed by in celullo cryo-ET** — Steffen Klein, Liv Zimmermann, Sophie Winter, Mirko Cortese, Moritz Wachsmuth-Melm, Christopher Neufeldt, Berati Cerikan, Megan Stanifer, Steeve Boulant, Ralf Bartenschlager, •Petr Chlanda
BP 6.1	Thu	13:30–14:00	H6	**How do lipids and proteins diffuse in cell membranes, and what do the diffusion experiments actually measure?** — •Ilpo Vattulainen
BP 7.1	Thu	15:00–15:30	H6	**Shaping embryos through controlled tissue phase transitions** — •Otger Campàs

Invited talks of the joint symposium Topological constraints in biological and synthetic soft matter (SYSM)

See SYSM for the full program of the symposium.

SYSM 1.1	Mon	10:00–10:30	Audimax 1	**Interphase Chromatin Undergoes a Local Sol-Gel Transition Upon Cell Differentiation** — •Alexandra Zidovska
SYSM 1.2	Mon	10:30–11:00	Audimax 1	**Topological Tuning of DNA Mobility in Entangled Solutions of Supercoiled Plasmids** — •Jan Smrek, Jonathan Garamella, Rae Robertson-Anderson, Davide Michieletto
SYSM 1.3	Mon	11:15–11:45	Audimax 1	**Dynamics of macromolecular networks under topological and environmental constraints: some outstanding challenges** — •Dimitris Vlassopoulos
SYSM 1.4	Mon	11:45–12:15	Audimax 1	**Supercoiling in a Protein Increases its Stability** — •Joanna Sulkowska, Szymon Niewieczerzał
SYSM 1.5	Mon	12:15–12:45	Audimax 1	**Topology for soft matter photonics** — •Igor Musevic

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium The Physics of CoViD Infections (SYCO)

See SYCO for the full program of the symposium.

SYCO 1.1	Mon	13:30–14:00	Audimax 1	**A Tethered Ligand Assay to Probe SARS-CoV-2:ACE2 Interactions** — Magnus Bauer, Sophia Gruber, Adina Hausch, Lukas Milles, Thomas Nicolaus, Leonard Schendel, Pilar Lopez Navajas, Erik Procko, Daniel Lietha, Rafael Bernadi, Hermann Gaub, •Jan Lipfert
SYCO 1.2	Mon	14:00–14:30	Audimax 1	**From molecular simulations towards antiviral therapeutics against COVID-19** — •Rebecca Wade
SYCO 1.3	Mon	14:45–15:15	Audimax 1	**The physical phenotype of blood cells is altered in COVID-19** — Markéta Kubánková, Martin Kräter, Bettina Hohberger, •Jochen Guck
SYCO 1.4	Mon	15:15–15:45	Audimax 1	**Extended lifetime of respiratory droplets in a turbulent vapor puff and its implications on airborne disease transmission** — •Detlef Lohse, Kai Leong Chong, Chong Shen Ng, Naoki Hori, Morgan Li, Rui Yang, Roberto Verzicco
SYCO 1.5	Mon	15:45–16:15	Audimax 1	**Beyond the demographic vaccine distribution: Where, when and to whom should vaccines be provided first?** — •Benno Liebchen, Jens Grauer, Fabian Schwarzendahl, Hartmut Löwen

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Active nematics: From 2D to 3D (SYAN)

See SYAN for the full program of the symposium.

SYAN 1.1	Fri	10:00–10:30	Audimax 1	**Corrugated patterns made from an active nematic sheet** — •Anis Senoussi, Shunichi Kashida, Raphaël Voituriez, Jean-Christophe Galas, Ananyo Maitra, Estevez-Torres André
SYAN 1.2	Fri	10:30–11:00	Audimax 1	**Wrinkling instability in 3D active nematics** — •Isabella Guido
SYAN 1.3	Fri	11:15–11:45	Audimax 1	**Three-dimensional active nematic defects and their energetics** — •Miha Ravnik
SYAN 1.4	Fri	11:45–12:15	Audimax 1	**Liquid-crystal organization of liver tissue** — •Benjamin M Friedrich, Hernan Morales-Navarrete, Andre Scholich, Hidenori Nonaka, Fabian Segovia Miranda, Steffen Lange, Jens Karschau, Yannis Kalaidzidis, Frank Jülicher, Marino Zerial
SYAN 1.5	Fri	12:15–12:45	Audimax 1	**Machine learning active nematic hydrodynamics** — •Vincenzo Vitelli

Sessions

BP 1.1–1.4	Mon	10:00–11:15	H1	**Statistical physics of biological systems (joint session BP/DY)**
BP 2.1–2.4	Mon	11:30–12:45	H1	**Cytoskeleton**
BP 3.1–3.3	Thu	10:00–11:00	H1	**Protein Structure and Dynamics**
BP 4.1–4.11	Thu	11:15–12:15	P	**Posters Biological Physics**
BP 5.1–5.5	Thu	11:45–13:00	H2	**Active Matter (joint session DY/BP/CPP)**
BP 6.1–6.4	Thu	13:30–14:45	H6	**Membranes and Vesicles**
BP 7.1–7.4	Thu	15:00–16:15	H6	**Cell Mechanics, Cell Adhesion and Migration, Multicellular Systems**
BP 8	Thu	18:00–19:00	MVBP	**Annual General Meeting**
BP 9.1–9.5	Fri	11:15–12:30	H2	**Machine Learning in Dynamical Systems and Statistical Physics (joint session DY/BP)**

Annual General Meeting of the Biological Physics Division

Thu 18:00–19:00 MVBP

- Bericht
- Wahl
- Verschiedenes

Sessions

– Invited Talks, Contributed Talks, and Posters –

BP 1: Statistical physics of biological systems (joint session BP/DY)

Time: Monday 10:00–11:15 Location: H1

Invited Talk BP 1.1 Mon 10:00 H1

Physics-Informed Deep Learning for Characterizing Perturbed Cell Growth — •Robert Endres[1], Henry Cavanagh[1], Rob Lind[2], Andreas Mosbach[3], and Gabriel Scalliet[3] — [1]Imperial College London, UK — [2]Syngenta International Research Centre, UK — [3]Syngenta Crop Protection AG, Switzerland

The morphodynamical analysis of cells can be a powerful and cost-effective way of understanding the phenotypic effects of perturbations, but current techniques often only work for stationary cell behaviour. Here, we introduce a novel framework that extends the morphodynamic analysis to nonstationary dynamics during early-stage growth of the soybean rust P. pachyrhizi. At its core, our approach learns the 2-dimensional feature space of cell shape using variational autoencoders from deep learning, and subsequently models how populations of cells develop over this space using two simple differential equations, each capturing complementary aspects of the dynamics with parameters depending on the perturbations. First, a Fokker-Planck model to describe the diffusive development on a Waddington-type energy landscape, providing a global perspective on the dynamics, and second, a cell-mechanical model describing local growth as a persistent random walk. Informative perturbation-dependent parameters are found by fitting simulations to the shape-space embeddings, representing a powerful tool for linking machine-learning and biophysical modelling.

BP 1.2 Mon 10:30 H1

Collisions increase self-diffusion in odd-diffusive systems — •Erik Kalz[1,2], Iman Abdoli[1], Hidde Derk Vuijk[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theory der Polymere, 01069 Dresden — [2]Technische Universität Dresden, Institut für Theoretische Physik 01069 Dresden

It is generally believed that collisions of particles reduce the self-diffusion coefficient. We show that in odd-diffusive systems, which are characterized by diffusion tensors with anti-symmetric elements, collisions surprisingly can enhance the self-diffusion. In these systems, due to an inherent curving effect, the motion of particles is facilitated, instead of hindered by collisions. We refer to this as an overdamped swing-by effect. Consistent with this we find that the collective diffusion remains unaffected. We demonstrate this counterintuitive behavior in a system of Brownian particles under Lorentz force. Using a geometric model, we theoretically predict a magnetic-field governed crossover from a reduced to an enhanced self-diffusion. The physical interpretation is quantitatively supported by the force-autocorrelation function, which turns negative with increasing magnetic field. Using Brownian dynamic simulations, we show that the predictions are also valid for active chiral particles as another odd-diffusive system.

BP 1.3 Mon 10:45 H1

How is anomalous diffusion compatible with thermodynamics in biophysical systems? — •David Hartich and Aljaz Godec — Mathematical bioPhysics Group, MPI-BPC, Göttingen, Germany

In a finite system driven out of equilibrium by a constant external force the thermodynamic uncertainty relation (TUR) bounds the variance of the conjugate current variable by the thermodynamic cost of maintaining the non-equilibrium stationary state. Here we highlight a new facet of the TUR by showing that it also bounds the time-scale on which a finite system can exhibit anomalous kinetics. In particular, we demonstrate that the TUR bounds subdiffusion in a single file confined to a ring as well as a dragged Gaussian polymer chain even when detailed balance is satisfied. Conversely, the TUR bounds the onset of superdiffusion in the active comb model. Remarkably, the fluctuations in a comb model evolving from a steady state behave anomalously as soon as detailed balance is broken. Our work establishes a link between stochastic thermodynamics and the field of anomalous dynamics that will fertilize further investigations of thermodynamic consistency of anomalous diffusion models.

[1] DH, A. Godec, Phys Rev. Lett. (in press), arXiv:2102.06678.

BP 1.4 Mon 11:00 H1

Maximum likelihood estimates of diffusion coefficients from single-particle tracking experiments — •Jakob Tómas Bullerjahn[1] and Gerhard Hummer[1,2] — [1]Department of Theoretical Biophysics, MPI of Biophysics, Frankfurt am Main, Germany — [2]Institute of Biophysics, Goethe University, Frankfurt am Main, Germany

Single-molecule localization microscopy allows practitioners to locate and track labeled molecules in biological systems. When extracting diffusion coefficients from the resulting trajectories, it is common practice to perform a linear fit on mean-squared-displacement curves. However, this strategy is suboptimal and prone to errors. Recently, it was shown that the increments between the observed positions provide a good estimate for the diffusion coefficient, and their statistics are well-suited for likelihood-based analysis methods. Here, we revisit the problem of extracting diffusion coefficients from single-particle tracking experiments subject to static noise and dynamic motion blur using the principle of maximum likelihood. Taking advantage of an efficient real-space formulation, we extend the model to mixtures of subpopulations differing in their diffusion coefficients, which we estimate with the help of the expectation-maximization algorithm. This formulation naturally leads to a probabilistic assignment of trajectories to subpopulations. We employ the theory to analyze experimental tracking data that cannot be explained with a single diffusion coefficient, and test how well the data conform to the model assumptions. https://doi.org/10.1063/5.0038174

BP 2: Cytoskeleton

Time: Monday 11:30–12:45 Location: H1

Invited Talk BP 2.1 Mon 11:30 H1

PINCH-1 promotes migration in extracellular matrices and influences the mechano-phenotype — •Claudia Tanja Mierke — University of Leipzig, Biological Physics, Leipzig, Germany

Cell migration performs a critical function in numerous physiological processes, including tissue homeostasis or wound healing, and pathological processes that include malignant cancer progression. The efficiency of migration appears to be based on the mechano-phenotype of the cytoskeleton. Cytoskeletal properties depend on intercellular and environmental factors. Thus, connections between the cell and its microenvironment are established by cell-matrix adhesion receptors. Upon activation, focal adhesion proteins such as PINCH-1 are recruited to sites where focal adhesions form. PINCH-1 specifically couples through interactions with ILK, which binds to cell-matrix receptors and the actomyosin cytoskeleton. However, the role of PINCH-1 in cell mechanics regulating cellular motility in 3D-collagen matrices is elusive. PINCH-1 is thought to facilitate 3D-motility by regulating cellular mechanical properties, such as stiffness. Therefore, PINCH-1 wild-type and knock-out cells were examined for their ability to migrate in dense extracellular 3D-matrices and cellular deformability. PINCH-1 wild-type cells migrated more numerous and deeper in 3D-matrices. PINCH-1 wild-type cells are less deformable (stiffer) compared to PINCH-1 knock-out cells. Migration and deformability were reduced by drug-dependent inhibition of Arp2/3 complex or actin polymerization. Finally, PINCH-1 appears to be essential for providing cellular mechanical stiffness, which regulates 3D motility.

BP 2.2 Mon 12:00 H1

A novel second PI(4,5)P_2 binding site determines PI(4,5)P_2 sensitivity of the tubby domain — Veronika Thallmair[1], Lea Schultz[1], Wencai Zhao[1], Siewert J. Marrink[2], Dominik Oliver[1], and •Sebastian Thallmair[2,3] — [1]Philipps-University Marburg, Germany — [2]University of Groningen, The Netherlands — [3]Frankfurt Institute for Advanced Studies, Frankfurt, Germany

Phosphoinositides (PIs) are important signaling lipids multitasking in diverse cellular signaling pathways. They operate by recruiting proteins to the membrane surface by means of PI recognition domains. One of the recognition domains for PI(4,5)P_2 lipids, which is the major PI species in the plasma membrane, is the tubby domain. It is conserved in the tubby-like protein (TULP) family and plays an important role in targeting proteins into cilia.

We used coarse-grained (CG) molecular dynamics (MD) simulations with the re-parametrized Martini 3 force field to explore the PI(4,5)P_2 affinity of the C-terminal tubby domain (tubbyCT). Our CG MD simulations revealed a novel second binding site consisting of a conserved cationic cluster at the protein-membrane interface. The simulations together with mutation experiments in living cells showed that the second binding site substantially contributes to the fine-tuned $PI(4,5)P_2$ affinity of tubbyCT. We will discuss the computational and experimental characterization of the novel binding site, its importance for the membrane targeting properties of tubbyCT, and for its ability to recognize distinct $PI(4,5)P_2$ pools in the plasma membrane.

BP 2.3 Mon 12:15 H1

Motor proteins generate the curved shape of the mitotic spindle — •Arian Ivec[1], Maja Novak[1], Nenad Pavin[1], and Iva Tolić[2] — [1]Department of Physics, Faculty of Science, University of Zagreb, Bijenička cesta 32, 10000 Zagreb, Croatia — [2]Division of Molecular Biology, Ruder Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

The mitotic spindle is a complex micro-machine made up of microtubules and associated proteins that are highly ordered in space and time to ensure its proper biological functioning. A functional spindle has a characteristic shape, which includes curved bundles of microtubules that are twisted around the pole-to-pole axis. An in-depth understanding of both how the linear and rotational forces define the overall shape of the mitotic spindle and how the twisted shapes arise as a result of interactions between microtubules and motor proteins is still unclear. To answer this, we introduce a model in which motor proteins generate forces at the poles and along the microtubule bundles, thereby regulating the shapes of microtubule bundles. The model provides predictions for forces in the spindle, including that the shape of the entire spindle is predominately determined by rotational forces, and that a difference in bending forces explains the disparity in the shapes of inner and outer bundles.

BP 2.4 Mon 12:30 H1

Bottom-up assembly of functional DNA-based cytoskeletons for synthetic cells — •Kevin Jahnke[1,2], Pengfei Zhan[3,4], Na Liu[3,4], and Kerstin Göpfrich[1,2] — [1]Max Planck Institute for Medical Research, Heidelberg, Germany — [2]Heidelberg University, Heidelberg, Germany — [3]Stuttgart University, Stuttgart, Germany — [4]Max Planck Institute for Solid State Research, Stuttgart, Germany

Bottom-up synthetic biology aims at reconstructing a cell from biomolecular constituents. However, the combination of multiple elements and functions remained elusive, which stimulates endeavors to explore entirely synthetic bioinspired solutions towards engineering life. To this end, DNA nanotechnology represents one of the most promising routes, given the inherent sequence specificity, addressability, and programmability of DNA. Here, we demonstrate functional DNA-based cytoskeletons operating in microfluidic cell-sized compartments and lipid vesicles. The synthetic cytoskeletons consist of DNA tiles self-assembled into filament networks. These filaments can be rationally designed and controlled to imitate features of natural cytoskeletons, including dynamic instability, ATP-triggered polymerization, and vesicle transport in cell-sized confinement. Also, they possess engineerable characteristics, including assembly and disassembly powered by DNA hybridization or aptamer-target interactions and autonomous transport of gold nanoparticles. This work underpins DNA nanotechnology as a key player in building synthetic cells.

BP 3: Protein Structure and Dynamics

Time: Thursday 10:00–11:00 Location: H1

Invited Talk BP 3.1 Thu 10:00 H1

SARS-CoV-2 induced membrane remodeling in infected cells revealed by in celullo cryo-ET — Steffen Klein, Liv Zimmermann, Sophie Winter, Mirko Cortese, Moritz Wachsmuth-Melm, Christopher Neufeldt, Berati Cerikan, Megan Stanifer, Steeve Boulant, Ralf Bartenschlager, and •Petr Chlanda — Heidelberg University Hospital, Heidelberg, Germany

Coronavirus replication in the host cell causes extensive remodeling of cellular membranes. To better understand the governing mechanisms of SARS-CoV-2 membrane remodeling during RNA replication and virus assembly we visualized hubs of virus replication and assembly using cryo-electron tomography of infected cells. Our data reveal the architecture of double-membrane vesicles which are associated with viral genome replication. Viral RNA filaments inside these compartments show a diameter consistent with double-stranded RNA and displayed frequent branching, likely representing secondary structures. Virion assembly sites were found at cisternae enriched in spike trimers and viral ribonucleoprotein complexes (vRNPs) at the cytoplasmic side. We further structurally analyzed the viral genome in newly assembled virions and revealed that the viral RNA is encased by multiple individual cylindrical vRNPs. We propose that this arrangement allows the incorporation of the unusually large coronavirus genome into the virion while maintaining high steric flexibility between the vRNPs during virion assembly.

BP 3.2 Thu 10:30 H1

Size-dependent deviations from the colloidal prediction: about the diffusion of proteins in a cellular environment — •Christian Beck[1,2], Felix Roosen-Runge[3], Tilo Seydel[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [2]Institut Laue-Langevin, 38042 Grenoble Cedex 9, France — [3]Department of Biomedical Science, Malmö University, Sweden

Diffusive properties are of fundamental importance for biological processes. For their quantitative understanding, the short-time diffusive properties are of huge interest. Previous studies investigated the volume fraction dependence of short-time diffusive properties for different pure proteins solutions [1] and recently in controlled poly-disperse cell-like environments [2]. In cooperation with the ILL life science group, we now investigated the diffusive properties of different sized proteins in the presence of deuterated lysate. In contrast to the previous study [2], the apparent global diffusion of the different proteins investigated does significantly deviate from the total volume fraction dependence of the pure protein solutions. While small proteins have a higher diffusion coefficient in the presence of lysate compared with the pure protein solution, big proteins, however, are slowed down. These results give a new insight into the diffusive properties of proteins in cells and might contribute significantly to a quantitative understanding of biological processes.

[1] M. Grimaldo, et al., Quart. Rev. Biophys. 52 (2019) e7, 1;
[2] M. Grimaldo, et al., J. Phys. Chem. Lett. 10 (2019) 1709

BP 3.3 Thu 10:45 H1

Scattering techniques: powerful tools to elucidate the molecular mechanisms of Wilson's disease — •Olga Matsarskaia — Institut Laue-Langevin, Grenoble, France

Copper (Cu) is an essential element for mammals and its metabolism is thus tightly regulated [1]. In the case of Wilson's disease, however, Cu metabolism is impaired, leading to abnormal Cu levels in the body [2]. Severe, often lethal, consequences ensue, such as liver and neurological damage [3,4] as well as the destruction of hemoglobin (Hb) and red blood cells (RBCs) [5]. The latter two symptoms are believed to be due to Cu-induced aggregation of Hb [6,7]. The current understanding of Wilson's disease is predominantly phenomenological. Thus, this project applies an interdisciplinary array of techniques including neutron and X-ray scattering to deepen the understanding of this highly complex condition. Scattering data recently obtained using human RBCs and purified human Hb will be presented, demonstrating real-time effects of Cu addition to these systems. The results obtained will be discussed in the broader context of medical research with the goal of inspiring an interdisciplinary dialogue between fundamental science and clinical applications.

[1] Löffler & Petrides, Springer Heidelberg (2007); [2] Riordan & Roger, J.Hepatol. (2001) 34, 433-48; [3] Ala et al., The Lancet (2007), 369, 397-408; [4] Gitlin, Gastroenterol. (2003), 125, 1868-77; [5] Ferenci, Metab. Brain Dis. (2004), 19, 229-39; [6] Rifkind, Blood (1965), 26, 433-48; [7] Jandl, Engle, Allen, J. Clin. Invest. (1960), 39, 1818-36

BP 4: Posters Biological Physics

Time: Thursday 11:15–12:15 Location: P

BP 4.1 Thu 11:15 P

Gelation dynamics upon pressure-induced liquid-liquid phase separation in a water-lysozyme solution — Marc Moron[1], •Ahmed Al-Masoodi[2], Clementine Lovato[2], Mario Reiser[3], Lisa Randolph[2], Göran Surmeier[1], Jennifer Bolle[1], Fabian Westermeier[4], Michael Sprung[4], Metin Tolan[1], Roland Winter[5], Michael Paulus[1], and Christian Gutt[2] — [1]Fakultät Physik / DELTA, TU Dortmund, 44221 Dortmund, Germany — [2]Department Physik, Universität Siegen, 57072 Siegen, Germany — [3]Department of Physics, Stockholm University, 10691 Stockholm, Sweden — [4]Deutsches Elektronen Synchrotron DESY, 22607 Hamburg, Germany — [5]Fakultät Chemie und Chemische Biologie, Physikalische Chemie, TU Dortmund, 44221 Dortmund, Germany

Phase transitions in concentrated protein solutions have been in the focus of research for years. For example, many diseases can be attributed to protein aggregation or liquid-liquid phase separation in human cells. Lysozyme represents a well-studied model protein. We investigated the effect of hydrostatic pressure on concentrated lysozyme solutions in different environments and were able to show that besides temperature, protein concentration, cosolvents and ionic strength also the hydrostatic pressure modulates the protein-protein interaction. Up to now, only the static properties of the lysozyme solutions were characterized. In this work, we present first pressure dependent X-ray photon correlation spectroscopy (XPCS) measurements on concentrated lysozyme solutions to study the dynamics of pressure-induced liquid-liquid phase transitions.

BP 4.2 Thu 11:15 P

Nonlinear viscoelastic behavior and hysteresis in hydrated collagen fibrils — •Martin Dehnert, Paul Zech, and Robert Magerle — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany

We study the nanomechanical properties of hydrated collagen fibrils with AFM-based nanoindentation measurements. Force–distance (FD) data measured with tip velocities $< 1\ \mu$m/s and different indentation protocols (force relaxation, creep, and cyclic loading) display nonlinear viscoelastic and elastoplastic behavior: (a) stress relaxation with a time constant $\tau_R \sim 0.1$ s, (b) creep with a time constant $\tau_C \sim 5$ s, and (c) approximately rate-independent hysteretic behavior with return point memory at intermediate time scales. The main cause of the hysteresis is the elastoplastic deformation of collagen fibrils in the leathery regime. We explore the variations of these nanomechanical properties in sets of unfixed hydrated collagen fibrils isolated from native chicken achilles tendon and compare it with collagen fibrils embedded in the natural tendon. AFM imaging in air with controlled humidity preserves the tissue's native water content and allows for high-resolution imaging the assembly of collagen fibrils beneath an approximately 5 to 10-nm-thick layer of the fluid components of the interfibrillar matrix. This sheds new light on the role of interfibrillar bonds, the mechanical properties of the interfibrillar matrix, and the biomechanics of native tendon.

BP 4.3 Thu 11:15 P

Optical Stretcher for Adherent Cells — •Alexander Janik[1], Tobias Neckernuss[1], Nathalie Neffgen[2], Jonas Pfeil[1], Mika Lindén[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University — [2]Institute of Inorganic Chemistry II, Ulm University

We have demonstrated a method to stretch adherent cells with a parallel laser beam to probe their mechanical properties. This contribution focuses on improvements of the setup as well as on interactions between cells and the illumination light. Progress has recently been made in the detection of the z position of the upper cell membrane, which is now achieved by tracking fluorescent beads on the cell. This yields a high z resolution and eliminates artefacts resulting from laser induced aberrations, which affect mainly detection rays entering the objective at small angles.

BP 4.4 Thu 11:15 P

Identifying malignant tissue using fs-Laser Induced Breakdown Spectroscopy (LIBS) and Neural Networks — •Elena Ramela Ciobotea, Christoph Burghard Morscher, Cristian Sarpe, Bastian Zielinski, Hendrike Braun, Arne Senftleben, and Thomas Baumert — Kassel Universität, Kassel, Germany

The problem of differentiating cancerous tissue from a healthy one is currently solved in the diagnostic process through microscopic imaging of stained biopsy sections by pathologists. During surgical removal of cancerous tissue oncological safety margins must be established to ensure the complete removal of the tumor without affecting much of the neighboring healthy tissue. For this purpose, on-site pathological analysis is done on freshly frozen, stained cuts which is time consuming. We investigate a new approach of minimizing the time of discrimination between malign and benign tissue by an in situ, non-contact spectroscopic analysis. In a proof of principle experiment, a plasma is generated by focusing an 800 nm femtosecond laser on the pathologic postoperative sample. The spectrum of plasma radiation contains information on the element composition of the ablated tissue. Since the recorded spectra are complex and full of information, neural networks are employed to find differences between malign and benign tissue with a high speed and accuracy. In this contribution we present the experimental parameters that allow for the best possible differentiation of some biological tissues through fs-LIBS by minimizing deviations between the measurements.

BP 4.5 Thu 11:15 P

Epigenetic relevance of quantum phenomena in DNA — •Mirko Rossini and Joachim Ankerhold — Institute for Complex Quantum systems and IQST, Ulm University, Germany

The behaviour of excited particles along the DNA strand inside a cell has been a topic of foremost interest in the field of biophysics in the last 20 years. On one hand, understanding how the dynamics of such particles can affect the geometry and structural properties of the DNA, locally or globally, can lead to new insights in the field of epigenetics [1]. On the other hand, the DNA strand itself has been analysed to explore its potential as a molecular conducting nano-wire.

With this poster we provide a description of different tight-binding models with dissipative background, exploring their population dynamics and coherence properties. The choice of the parameters for the models is taken to mimic some specific DNA sequences which are relevant in the epigenetic field of research. We provide then some experimental results which justify our interest in this topic and in this methods. Apart from single charge dynamics, we also consider excitonic dynamics in various DNA sequences, in particular with respect to charge separation and localization.

[1] E. R. Bittner, J. Chem. Phys. **125**, 094909 (2006).

BP 4.6 Thu 11:15 P

Swimming vesicles propelled by flagellated bacteria in membrane tubes — •Lucas Le Nagard[1], Aidan Brown[1], Alexander Morozov[1], Angela Dawson[1], Vincent Martinez[1], Margarita Staykova[2], and Wilson Poon[1] — [1]The University of Edinburgh, United Kingdom — [2]Durham University, United Kingdom

Recent simulation studies have predicted that giant unilamellar vesicles submitted to a collection of local internal forces should display enhanced fluctuations and a fascinating diversity of shape changes, from the formation of membrane tubes to deformations leading to vesicle division. Experimental investigation of those phenomena, based on the encapsulation of self-propelled particles or swimming bacteria into giant lipid vesicles, has only recently started. Such minimal systems can be used to study the interactions between an active suspension and a confining (deformable) boundary. They should also help deepen the understanding of biological processes where membrane deformation under local forcing is important. In this work, we encapsulate motile *Escherichia coli* bacteria in low-tension giant lipid vesicles. We observe that the bacteria apply local forces on the membrane, deforming it to generate membrane tubes reminiscent of those seen in eukaryotic cells infected by *Listeria monocytogenes*. Strikingly, these bacteria-enclosing tubes can propel the vesicles. We show that the propulsive force arises from a tight coupling between the bacteria's well-bundled flagella and the membrane tubes, which become rotating helices turning the initially passive vesicles into active micro-swimmers.

BP 4.7 Thu 11:15 P

Effect of Liquid-Liquid Phase Separation of Pol II on gene regulation — •Arya Changiarath Sivadasan and Lukas Stelzl — Johannes Gutenberg University, Mainz

Liquid Liquid phase separation(LLPS) plays an important role in the regulation of cellular processes. In particular, LLPS underpins the formation of localized nuclear hubs of RNAP II during the transcription of genes. Recent experimental studies revealed that the disordered Carboxy terminal domain (CTD) of the largest subunit of RNAP II, has a very strong tendency to phase separate. In our research, we are trying to understand the molecular basis of phase separation of RNAP II using multiscale molecular dynamic simulations. Our initial preliminary studies show the effects of temperature on CTD phase behavior and the influence of polymer length on critical temperature of phase separation. The results show that critical temperature increases with polymer length as expected. As a next step, we are interested in studying the phase separation of phosphorylated RNAP II and the effect of noise in the biochemical signaling on phase behavior. Moreover, we are also keen to understand the phase separation of a complex mixture of biomolecules such as CTD and RNA binding protein FUS. This would give insights into how the LLPS of CTD and other biomolecules regulates the transcription process in cells and will enable us to elucidate how the regulation of genes by LLPS is affected by noise.

BP 4.8 Thu 11:15 P

Bio-inspired Magnetic Nanoprobes For Subcellular Manipulation Studies in Single Cells — •Andreas Neusch[1], Iuliia Novoselova[1], Julia-Sarita Brand[1], Marius Otten[1], Matthias Karg[1], Michael Farle[2], Ulf Wiedwald[2], and Cornelia Monzel[1] — [1]Heinrich-Heine-University, Düsseldorf — [2]University of Duisburg-Essen, Duisburg

Cellular signals rely on characteristic temporal and spatial distributions of signaling molecules, but hitherto it is unclear which patterns trigger which cellular response. In recent years, Magnetogenetics emerged as an approach where magnetic nanoparticles (MNPs) and magnetic fields are used to spatially manipulate molecules to trigger cellular processes in order to mimic and study natural signaling patterns [Monzel et al. (2017), DOI: 10.1039/C7SC01462G]. Here, we compared two MNPs regarding their use as nanoagents of cellular functions. First, a bio-inspired semisynthetic nanoparticle - Magnetoferritin (MFt) - was chosen, which consists of the iron storage protein ferritin and a synthetic magnetic iron oxide core. MFt is genetically equipped with mEGFP for microscopic observation and bio-orthogonal targeting [Lisse et al. (2017), DOI: 10.1002/adma.201700189]. Furthermore, synthetic iron-oxide MNPs (synomag, micromod, Rostock) were studied. After examining basic properties, we assessed methods of transfer into cells and probed MNP manipulation in the cytoplasm. Using external magnetic fields, MNPs were spatially redistributed and kinetically analyzed. Our magnetic manipulation approach bears the perspective to achieve an understanding of how cell signals evolve.

BP 4.9 Thu 11:15 P

On the adhesion-velocity relation and multistability of the motile state of MDA MB 231 cells on fibronectin lanes — Christoph Schreiber[1], Behnam Amiri[2], •Johannes Heyn[1], Joachim Rädler[1], and Martin Falcke[2,3] — [1]Ludwig-Maximilians-Universität München (LMU), Fakultät für Physik, Geschwister-Scholl-Platz 1, 80539 München, Germany — [2]Max Delbrück Center for Molecular Medicine in the Helmholtz Association, Robert Rössle Str. 10, 13125 Berlin, Germany — [3]Dept. of Physics, Humboldt University, Newtonstr. 15, 12489 Berlin, Germany

Migration of eukaryotic cells is a fundamental process for embryonic development, wound healing, immune responses, and tumour metastasis. A universal observation is the well-known biphasic adhesion-velocity relation. There is, however, little quantitative understanding of how adhesion and intracellular forces control cell velocity. We study the motion of MDA-MB-231 cells on microlanes with fields of alternating Fibronectin densities to address this topic and derive a mathematical model from the leading-edge force balance and the force-dependent polymerization rate. It reproduces quantitatively our measured adhesion-velocity relation. All motion-related forces are controlled by adhesion and velocity, which allows motion even with higher Fibronectin density at the rear than at the front. At transitions between different Fibronectin densities, steady motion is perturbed which changes the front and rear velocity. We then discuss the role of the biphasic relation between retrograde flow velocity and friction force for transitions of motile states.

BP 4.10 Thu 11:15 P

Exploring quantum features of the brain with MRI — •Christian Kerskens[1] and David Lopez Perez[1,2] — [1]Trinity College Institute of Neuroscience, Trinity College Dublin, Ireland — [2]Institute of Psychology, Polish Academy of Sciences, Warsaw, Poland

Recent proposals to explore quantum gravity have shown that if any physical system can mediate locally the generation of entanglement between two quantum systems, then it itself must be non-classical. Here, we adopted this idea to explore non-classicality in the human brain. Thereby, we considered an unknown brain function as the mediator which may or may not entangle the proton nuclear spins of free-diffusible bulk water. The challenge was to find a nuclear spin preparation that, together with a physiological condition, could facilitate the creation of quantum entanglement. For the spin preparation, we took the complementarity between magnetization and the likelihood of entanglement into account. As a result, we used a highly de-phased and saturated signal for our entanglement witness protocol, which was based on a hybrid multiple quantum coherence sequence. For the physiological condition, we assumed that some brain rhythms may influence the order at tissue level. Remarkably, we witnessed entanglement in the brains of our volunteers, if and only if, they were awake. Its temporal appearance showed a rhythm resembling heartbeat-evoked potentials. This link to conscious awareness underpins that the non-classical mediator may be used and manipulated in conscious-related computation, ergo we found indication that brain computation is non-classical.

BP 4.11 Thu 11:15 P

Revisiting the quantum brain — •Christian Kerskens — Trinity College Institute of Neuroscience, Trinity College Dublin, Ireland

More than 30 years ago, Penrose's published his pioneering ideas about the quantum brain, which was back then based on the knowledge at the time. This work, which marked an interim high in the field, received severe criticism. Meanwhile, many scientific areas relevant for the understanding of brain processes have evolved enormously. However, reservations remain. Here, we put some of those new jigsaw pieces together. We review findings from physics, quantum information, nematic, active matter, neuroscience, psychology, and philosophy which, we believe, could guide us towards a quantum brain theory. Thereby, we intend not to present a completed theory. We are aware that some direct translation from quantum physics to biology will, at the time, not hold a critical debate. However, we argue that the problem may be down to an insufficient understanding of physics, which needs to be solved. Biology may guide us (remember electrodynamics) once more to find in-depth insight into fundamental physics. Therefore, we divide the findings into those which resemble quantum computing but which can't be explained theoretically and into those which violate classicality in cognition and consciousness. We conclude that the brain may mimic a real brain quantum computer, which could potentially be based on topological quantum computing.

BP 5: Active Matter (joint session DY/BP/CPP)

Time: Thursday 11:45–13:00 Location: H2

See DY 12 for details of this session.

BP 6: Membranes and Vesicles

Time: Thursday 13:30–14:45 Location: H6

Invited Talk BP 6.1 Thu 13:30 H6

How do lipids and proteins diffuse in cell membranes, and what do the diffusion experiments actually measure? — •Ilpo Vattulainen — Department of Physics, University of Helsinki

There are various techniques able to gauge diffusion in biomembranes. For instance, quasi-elastic neutron scattering measures diffusion in a non-perturbative manner over nanosecond time scales, yet sampling in space is in these experiments done over large distances. Meanwhile, single-particle tracking allows one to measure the dynamics of individual molecules in almost nanometer resolution, but these measurements are based on the use of markers that may interfere with the diffusion process. Here we discuss nanoscale simulation studies designed to explore the underlying molecular-scale diffusion mechanisms of lipids and membrane proteins. We also discuss the bases of single-particle tracking experiments by considering the effects of streptavidin-functionalized Au nanoparticle probes on lateral diffusion. The results show that lipids diffuse in a concerted fashion as clusters of lipids whose motion is highly correlated, and membrane proteins move as dynamical complexes with tens of lipids bound to the protein. Lipids linked to a streptavidin-nanoparticle complex also turn out to move in a concerted manner but as a complex with the linker protein and numerous non-labeled lipids, slowing down the motion of the probe by an order of magnitude. The results highlight that prior to using any technique, it is crucial to understand the physical basis of the diffusion process that one aims to measure. Otherwise, interpretation of experimental data can be a surprisingly difficult task.

BP 6.2 Thu 14:00 H6

Fusion of virus and host membranes - the role of virus geometry and matrix proteins — •Gonen Golani[1], Sophie Winter[2], Steffen Klein[2], Petr Chlanda[2], and Ulrich S. Schwarz[1] — [1]Institute for Theoretical Physics and BioQuant, Heidelberg University, D-69120 Heidelberg, Germany — [2]Schaller Research Groups, Department of Infectious Diseases-Virology, Heidelberg University Hospital, D-69120 Heidelberg, Germany

Many medically important viruses are enveloped by a lipid membrane, therefore, a crucial step in the infection process is the fusion of the viral and cellular membranes. The fusion pathway involves a series of non-bilayer intermediates configurations: First, the monolayers of the two opposing membranes merge to form a hemifusion connection, referred to as the stalk. Next, expansion of the stalk brings the distal lipid monolayers together into a hemifusion diaphragm. Lastly, opening and expansion of a fusion pore within the diaphragm completes the fusion process. The formation of the stalk and expansion of the fusion pore constitute the two major energy barriers in the process. While formation of the stalk is directly driven by the viral fusion proteins and was extensity studied in the last decades, pore expansion is less well understood. Here we compute the stresses in the diaphragm and the resulting energy barrier to fusion pore expansion. We analyze, for the first time, effect of the virus geometry and membrane-matrix interaction on viral fusion rate. We also suggest a model for the role of interferon-induced transmembrane proteins (IFITMs) in inhibition of fusion by increasing the energy barrier of fusion pore expansion.

BP 6.3 Thu 14:15 H6

Calponin-homology domain mediated bending of membrane associated actin filaments — Saravanan Palani[1,2], Sayantika Ghosh[1], Esther Ivorra-Molla[1], Scott Clarke[1], Andrejus Suchenko[1], Mohan Balasubramanian[1], and •Darius Köster[1] — [1]Centre for Mechanochemcial Cell Biology and Warwick Medical School, Division of Biomedical Sciences, CV4 7AL Coventy, UK — [2]Department of Biochemistry, Division of Biological Sciences, Indian Institute of Science, Bangalore-560012, India

Actin filaments are central to cell function and the actin cytoskeleton exhibits a variety of geometries. Here, we show that 'curly', the actin-binding calponin-homology domain and a C-terminal unstructured domain from the IQGAP family of proteins, stabilizes individual actin filaments in a highly curved geometry when anchored to lipid membranes. Whereas F-actin is semi-flexible with a persistence length of $10\mu m$, binding of mobile curly within lipid membranes generates actin filament arcs and full rings of high curvature with radii below $1\mu m$. Higher rates of fully formed actin rings are observed in the presence of the actin-binding coiled-coil protein tropomyosin and when actin is directly polymerized on lipid membranes decorated with curly. Strikingly, curly induced actin filament rings contract upon the addition of muscle myosin II filaments and expression of curly in mammalian cells leads to highly curved actin structures in the cytoskeleton. Taken together, our work identifies a new mechanism to generate highly curved actin filaments, which opens a range of possibilities to control actin filament geometries in vitro and in vivo.

BP 6.4 Thu 14:30 H6

Fission mechanisms of cylindrical membrane tubes — •Russell Spencer and Marcus Müller — Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany

This work investigates the mechanisms and pathways for the fission of phospholipid membranes, in particular double-membrane fission as it occurs in mitochondrial division. We employ self-consistent field theory and utilize the string method to find the Minimum Free Energy Path (MFEP) connecting the metastable starting and ending states of different membrane topology in order to determine the most likely pathway for the transition. Our results suggest that the free energy barrier to membrane fission, as well as the dominant pathway, can be controlled by the tension experienced by the membrane. At high tension, the inner tube partially collapses into a worm-like micelle, which then ruptures, resulting in two capped tubes. The outer membrane then follows similarly. This pathway is non-leaky, i.e. the solvent inside the inner membrane, between the membranes and outside the outer membrane never mix. At lower tension, the barrier to forming a worm-like micelle becomes prohibitive, and instead, the inner and outer membranes fuse. This pathway is leaky as pores form close to the fusion sites.

BP 7: Cell Mechanics, Cell Adhesion and Migration, Multicellular Systems

Time: Thursday 15:00–16:15 Location: H6

Invited Talk BP 7.1 Thu 15:00 H6

Shaping embryos through controlled tissue phase transitions — •Otger Campàs — Physics of Life Excellence Cluster, TU Dresden, Germany — University of California, Santa Barbara, USA

During embryonic development, cells self-organize to build functional structures, like tissues and organs, and progressively shape the organism. While many key molecular players that orchestrate embryonic development are known, the physical mechanisms underlying embryonic morphogenesis remain largely unknown, mainly because of a lack in methodologies enabling direct in vivo and in situ measurements of forces and mechanical properties within developing 3D tissues and organs. For similar reasons, understanding the fundamental physical nature of active multicellular systems has been very challenging. We have recently developed novel microdroplet-based techniques that allow direct quantitative measurements of mechanical forces and material properties within 3D multicellular systems, including developing embryonic tissues. Using these techniques and focusing on the elongation of the body axis, a hallmark morphogenetic process in vertebrate development, we reveal a new physical mechanism of tissue morphogenesis whereby spatiotemporally controlled fluid-to-solid (rigidity) transitions in the tissue physical state, rather than patterned mechanical stresses, guide tissue flows to shape functional embryonic structures. Moreover, combining computational and experimental data, we show that active tension fluctuations control tissue fluidization in vivo.

BP 7.2 Thu 15:30 H6

Traction force microscopy with invertible neural networks — •Johannes Blumberg[1], Timothy Herbst[1,2], Ullrich Koethe[2], and Ulrich Schwarz[1] — [1]Institute for Theoretical Physics and Bioquant, Heidelberg University — [2]Visual Learning Lab, IWR, Heidelberg University

In traction force microscopy (TFM), the mechanical forces of cells adhering to an elastic substrate are estimated from the substrate displacements as measured by the movement of embedded fiducial marker beads. While the direct problem of calculating displacement from forces is well-defined by elasticity theory, the inverse problem of reconstructing forces from displacements is ill-posed. Usually an estimate is obtained by minimizing the mean squared distance between experimentally observed and predicted displacements. The standard method in this regard is Fourier Transform Traction Cytometry (FTTC), whose superior efficiency is based on the convolution theorem in Fourier space. Here we explore if the performance can be improved by using machine learning methods, in particular invertible neural networks, which recently have emerged as powerful method to solve ill-posed inverse problems.

BP 7.3 Thu 15:45 H6

An active gel model for optogenetic control of cell migration — •Oliver M. Drozdowski[1,2], Falko Ziebert[1,2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120 Heidelberg, Germany — [2]BioQuant, Heidelberg University, Im Neuenheimer Feld 267, 69120 Heidelberg, Germany

Optogenetics has emerged as a new powerful experimental method to control cellular processes in space and time, including actin filament polymerization and contractility of myosin II molecular motors. Here we report on a mathematical analysis of spatiotemporal activation patterns in a simple one-dimensional variant of active gel theory with the aim to predict how optogenetics can be used to control cell migration [1]. We first show that the model can describe the symmetrical flow of the actomyosin system observed in optogenetic experiments but not the long-lasting polarization required for cell migration. Motile solutions, however, become possible if cytoskeletal polymerization is included through the boundary conditions. Optogenetic activation of contraction can then initiate locomotion in a symmetrically spreading cell and strengthen motility in an asymmetrically polymerizing one. If designed appropriately, it can also arrest motility even for protrusive boundaries.

[1] https://arxiv.org/abs/2104.14636, to appear in Phys. Rev. E

BP 7.4 Thu 16:00 H6

Defect-mediated morphogenesis — •Ludwig A. Hoffmann, Livio N. Carenza, Julia Eckert, and Luca Giomi — Universiteit Leiden, The Netherlands

Growing experimental evidence indicates that topological defects could serve as organizing centers in the morphogenesis of tissues. We provide a quantitative explanation for this phenomenon, rooted in the buckling theory of deformable active polar liquid crystals. Using a combination of linear stability analysis and computational fluid dynamics, we demonstrate that confined cell layers are unstable to the formation of protrusions in the presence of disclinations. The instability originates from an interplay between the focusing of the elastic forces, mediated by defects, and the renormalization of the system's surface tension by the active flow. The post-transitional regime is also characterized by several complex morphodynamical processes, such as oscillatory deformations, droplet nucleation and active turbulence. Our findings offer an explanation of recent observations on tissue morphogenesis and shed light on the dynamics of active surfaces in general.

BP 8: Annual General Meeting

Time: Thursday 18:00–19:00 Location: MVBP

Annual General Meeting

BP 9: Machine Learning in Dynamical Systems and Statistical Physics (joint session DY/BP)

Time: Friday 11:15–12:30 Location: H2

See DY 16 for details of this session.

Chemical and Polymer Physics Division
Fachverband Chemische Physik und Polymerphysik (CPP)

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Overview of Invited Talks and Sessions

(Lecture halls H1 and H3; Poster P)

Invited Talks

CPP 2.1	Mon	13:30–14:00	H1	**On the permeability of dense polymer membranes** — •Joachim Dzubiella
CPP 3.1	Mon	13:30–14:00	H3	**Emulsion Templating: Unexpected Morphology of Monodisperse Macroporous Polystyrene** — •Cosima Stubenrauch, Lukas Koch, Sophia Botsch, Wiebke Drenckhan
CPP 3.4	Mon	14:30–15:00	H3	**Structural Transitions of Molecules on Surfaces** — •Angelika Kühnle
CPP 4.1	Tue	10:00–10:30	H3	**Adaptable amphiphilic co-networks: structure and properties in relation with multi-quantum NMR** — •Michael Lang, Reinhard Scholz, Lucas Löser, Carolin Bunk, Frank Böhme, Kay Saalwächter
CPP 4.2	Tue	10:30–11:00	H3	**Adaptive networks through supramolecular interactions** — •Ilja Voets
CPP 4.5	Tue	11:45–12:15	H3	**Tunable self-assembled hydrogels from block copolymers with thermoresponsive and pH-responsive blocks** — •Christine M. Papadakis, Florian A. Jung, Constantinos Tsitsilianis
CPP 7.1	Wed	10:00–10:30	H3	**Chemically Fueled Out-Of-Equilibrium Self-Assemblies and Autonomous Material Systems** — •Andreas Walther
CPP 7.4	Wed	11:15–11:45	H3	**The quest for robust superhydrophobic surfaces** — •Robin Ras
CPP 10.1	Thu	13:30–14:00	H3	**Nanophotonic structures by inkjet printing** — Yidenekachew J. Donie, Qiaoshuang Zhang, Guillaume Gomard, •Uli Lemmer
CPP 13.1	Fri	10:00–10:30	H3	**Electron-lattice relaxation effects in halide perovskites** — •David A. Egger
CPP 13.6	Fri	11:45–12:15	H3	**Light-actuated colloidal nano- and microparticles** — •Cornelia Denz, Matthias Rueschenbaum, Valeria Bobkova, Julian Jeggle, Raphael Wittkowski
CPP 15.1	Fri	13:30–14:00	H3	**Data-driven protein design and simulation** — •Andrew Ferguson

Invited talks of the joint symposium Topological constraints in biological and synthetic soft matter (SYSM)

See SYSM for the full program of the symposium.

SYSM 1.1	Mon	10:00–10:30	Audimax 1	**Interphase Chromatin Undergoes a Local Sol-Gel Transition Upon Cell Differentiation** — •Alexandra Zidovska
SYSM 1.2	Mon	10:30–11:00	Audimax 1	**Topological Tuning of DNA Mobility in Entangled Solutions of Supercoiled Plasmids** — •Jan Smrek, Jonathan Garamella, Rae Robertson-Anderson, Davide Michieletto
SYSM 1.3	Mon	11:15–11:45	Audimax 1	**Dynamics of macromolecular networks under topological and environmental constraints: some outstanding challenges** — •Dimitris Vlassopoulos
SYSM 1.4	Mon	11:45–12:15	Audimax 1	**Supercoiling in a Protein Increases its Stability** — •Joanna Sulkowska, Szymon Niewieczerzał
SYSM 1.5	Mon	12:15–12:45	Audimax 1	**Topology for soft matter photonics** — •Igor Musevic

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium Multidimensional coherent spectroscopy of functional nanostructures (SYCS)

See SYCS for the full program of the symposium.

SYCS 1.1	Tue	10:00–10:30	Audimax 1	**Multidimensional coherent spectroscopy of perovskite nanocrystals** — •Steven Cundiff, Albert Liu, Diogo Almeida, Gabriel Nagamine, Lazaro Padilha
SYCS 1.2	Tue	10:30–11:00	Audimax 1	**Coherent multidimensional techniques for the characterization of nanomaterials** — •Elisabetta Collini
SYCS 1.3	Tue	11:00–11:30	Audimax 1	**Exciton Dynamics revealed by Multidimensional Coherent Spectroscopies applied to Light-Harvesting Systems** — •Thomas L.C. Jansen
SYCS 1.4	Tue	11:45–12:15	Audimax 1	**Revealing couplings with action-based 2D microscopy** — •Tobias Brixner
SYCS 1.5	Tue	12:15–12:45	Audimax 1	**Low-frequency phonons affect charge carrier dynamics in hybrid perovskites** — •Mischa Bonn

Invited talks of the joint symposium Amorphous materials: structure, dynamics, properties (SYAM)

See SYAM for the full program of the symposium.

SYAM 1.1	Tue	13:30–14:00	Audimax 1	**Glassy dynamics of vitrimers** — •Liesbeth Janssen
SYAM 1.2	Tue	14:00–14:30	Audimax 1	**Liquid-Liquid Phase Transition in Thin Vapor-Deposited Glass Films** — •Zahra Fakhraai
SYAM 1.3	Tue	14:30–15:00	Audimax 1	**Connection between structural properties and atomic motion in ultraviscous metallic liquids close to the dynamical arrest** — •Beatrice Ruta, Nico Neuber, Isabella Gallino, Ralf Busch
SYAM 1.4	Tue	15:15–15:45	Audimax 1	**Signatures of the spatial extent of plastic events in the yielding transition in amorphous solids** — •Celine Ruscher, Daniel Korchinski, Joerg Rottler
SYAM 1.5	Tue	15:45–16:15	Audimax 1	**Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment** — •Olfa D'Angelo, W. Till Kranz

Invited talks of the joint symposium Curvilinear condensed matter (SYCL)

See SYCL for the full program of the symposium.

SYCL 1.1	Wed	10:00–10:30	Audimax 2	**Curvature Effects and Topological Defects in Chiral Condensed and Soft Matter** — •Avadh Saxena
SYCL 1.2	Wed	10:30–11:00	Audimax 2	**Topology and Transport in nanostructures with curved geometries** — •Carmine Ortix
SYCL 2.1	Wed	11:15–11:45	Audimax 2	**Superconductors and nanomagnets evolve into 3D** — •Oleksandr Dobrovolskiy
SYCL 2.2	Wed	11:45–12:15	Audimax 2	**Properties of domain walls and skyrmions in curved ferromagnets** — •Volodymyr Kravchuk
SYCL 2.3	Wed	12:15–12:45	Audimax 2	**X-ray three-dimensional magnetic imaging** — •Valerio Scagnoli

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Diversity on the Device Scale (SYHN)

See SYHN for the full program of the symposium.

SYHN 1.1	Thu	10:00–10:30	Audimax 1	**Scaling behavior of stiffness and strength of hierarchical network nanomaterials** — •Shan Shi
SYHN 1.2	Thu	10:30–11:00	Audimax 1	**Functional and programmable DNA nanotechnology** — •Laura Na Liu
SYHN 1.3	Thu	11:15–11:45	Audimax 1	**Multivalent nanoparticles for targeted binding** — •Stefano Angioletti-Uberti
SYHN 1.4	Thu	11:45–12:15	Audimax 1	**Programming Nanoscale Self-Assembly** — •Oleg Gang
SYHN 1.5	Thu	12:15–12:45	Audimax 1	**Achieving Global Tunability via Local Programming of a Structure's Composition** — •Jochen Mueller

Invited talks of the joint symposium Active nematics: From 2D to 3D (SYAN)

See SYAN for the full program of the symposium.

SYAN 1.1	Fri	10:00–10:30	Audimax 1	**Corrugated patterns made from an active nematic sheet** — •Anis Senoussi, Shunichi Kashida, Raphaël Voituriez, Jean-Christophe Galas, Ananyo Maitra, Estevez-Torres André
SYAN 1.2	Fri	10:30–11:00	Audimax 1	**Wrinkling instability in 3D active nematics** — •Isabella Guido
SYAN 1.3	Fri	11:15–11:45	Audimax 1	**Three-dimensional active nematic defects and their energetics** — •Miha Ravnik
SYAN 1.4	Fri	11:45–12:15	Audimax 1	**Liquid-crystal organization of liver tissue** — •Benjamin M Friedrich, Hernan Morales-Navarrete, Andre Scholich, Hidenori Nonaka, Fabian Segovia Miranda, Steffen Lange, Jens Karschau, Yannis Kalaidzidis, Frank Jülicher, Marino Zerial
SYAN 1.5	Fri	12:15–12:45	Audimax 1	**Machine learning active nematic hydrodynamics** — •Vincenzo Vitelli

Sessions

CPP 1.1–1.7	Mon	11:15–13:00	H3	**2D materials and their heterostructures (joint session DS/HL/CPP)**
CPP 2.1–2.3	Mon	13:30–14:30	H1	**Hydrogels and Microgels**
CPP 3.1–3.8	Mon	13:30–16:15	H3	**Polymer Physics**
CPP 4.1–4.7	Tue	10:00–12:45	H3	**Focus: The Physics of Adaptive Polymer Networks**
CPP 5.1–5.19	Tue	17:30–19:30	P	**Poster Session I**
CPP 6.1–6.26	Tue	17:30–19:30	P	**Poster Session II**
CPP 7.1–7.8	Wed	10:00–12:45	H3	**Soft Matter (joint session CPP/DY)**
CPP 8.1–8.32	Wed	17:30–19:30	P	**Poster Session III**
CPP 9.1–9.5	Thu	11:45–13:00	H2	**Active Matter (joint session DY/BP/CPP)**
CPP 10.1–10.9	Thu	13:30–16:15	H3	**Organic Electronics and Photovoltaics, Electrical and Optical Properties (joint session CPP/KFM)**
CPP 11.1–11.4	Thu	15:15–16:15	H5	**Thin Oxides and Organic Thin Films (joint session DS/CPP)**
CPP 12	Thu	17:30–18:30	MVCPP	**Annual General Meeting of the CPP Division (CPP Mitgliederversammlung)**
CPP 13.1–13.8	Fri	10:00–12:45	H3	**Molecular Electronics, Hybrid and Perovskite Photovoltaics**
CPP 14.1–14.4	Fri	10:00–11:00	H2	**Condensed-Matter Simulations augmented by Advanced Statistical Methodologies (joint session DY/CPP)**
CPP 15.1–15.5	Fri	13:30–15:00	H3	**Theory and Simulation (joint session CPP/DY)**

Annual General Meeting of the Chemical and Polymer Physics Division

Thursday 17:30–18:30 MVCPP

- Report of the current speaker team
- Election of the second deputy speaker
- Miscellaneous

Monday 27.09.21

Time	AM1	AM2	H1	H3
09:00–09:30	Viola Priesemann; Jukka Pekola			
09:45				
10:00–12:30	Topological constraints in biological and synthetic soft matter **(SYSM)**	SKM Dissertation Prize 2021 **(SYSD)**		
12:45–13:15				
13:30–16:00	The Physics of CoViD Infections **(SYCO)**	Potentials for NVs sensing magnetic phases, textures and excitations **(SYNV)**	**Hydrogels & Microgels**	**Polymer Physics**
16:15				
16:30–17:00	Raissa D'Souza; John A. Rogers			
17:15				
17:30–19:00				

Tuesday 28.09.21

Time	AM1	AM2	H3
09:00–09:30	Silke Bühler-Paschen; Manfred Bayer		
09:45			
10:00–12:30	Multidimensional coherent spectroscopy of functional nanostructures **(SYCS)**	Novel phases and dynamical properties of magnetic skyrmions **(SYMS)**	**Focus: The Physics of Adaptive Polymer Networks**
12:45–13:15	AKC		
13:30–16:00	Amorphous materials: structure, dynamics, properties **(SYAM)**	Facets of many-body quantum chaos **(SYQC)**	
16:15			
16:30–17:00	Cynthia A. Volkert; John Sipe		
17:15			
17:30–19:00	**POSTERSESSION I + II** 17.30-19:30		

Wednesday 29.09.21

Time	AM1	AM2	H3
09:00–09:30	Hélène Bouchiat; Rupert Huber		
09:45			
10:00–12:30	Advanced neuromorphic computing hardware: Towards efficient machine learning **(SYNC)**	Curvilinear condensed matter **(SYCL)**	**Soft Matter**
12:45–17:15			
17:30–19:00	**POSTERSESSION III** 17.30-19:30		

Thursday 30.09.21

Time	AM1	AM2	H3
09:00–09:30	Jian-Wei Pan; Robert Pitz-Paal		
09:45			
10:00–12:30	Hybrid Nanomaterials: From Novel Physics & Multi-Scale Self-Organization to Functional Diversity on the Device Scale **(SYHN)**	Attosecond and coherent spins: New frontiers **(SYAS)**	
12:45–13:15			
13:30–16:00	Climate and energy: Challenges and options from a physics perspectiv **(SYCE)**	Physics of van der Waals 2D heterostructures **(SYWH)**	**Organic Electronics & Photovoltaics, Electrical & Optical Properties**
16:15			
16:30–17:00	Alain Karma; Can Ming Hu		
17:15			
17:30–18:00	**Annual General Meeting of the CPP Division (Zoom Meeting)**		

Friday 01.10.21

Time	AM1	AM2	H3
09:00–09:30	Mikhail Eremets; Klaus-Robert Müller		
09:45			
10:00–12:30	Active nematics: From 2D to 3D **(SYAN)**	The Rise of Photonic Quantum Technologies – Practical and Fundamental Aspects **(SYPQ)**	**Molecular Electronics, Hybrid & Perovskite Photovoltaics**
12:45–13:15			
13:30–14:45			**Theory & Simulation**
15:00	Closing Remarks		
15:15–16:00	Jelena Vuckovic; Ulrich Wiesner		

Sessions

– Invited Talks, Contributed Talks, and Posters –

CPP 1: 2D materials and their heterostructures (joint session DS/HL/CPP)

Time: Monday 11:15–13:00 Location: H3

See DS 2 for details of this session.

CPP 2: Hydrogels and Microgels

Time: Monday 13:30–14:30 Location: H1

Invited Talk CPP 2.1 Mon 13:30 H1

On the permeability of dense polymer membranes — •Joachim Dzubiella — Institute of Physics, Freiburg University

The permeability of polymers for the selective transport of molecular penetrants (drugs, toxins, reactants, etc.) is a central property in the design of soft functional materials. However, the permeation of dense and hydrated polymer membranes is a complex molecular- level phenomenon, and our understanding of the underlying physicochemical principles is still very limited. Here, I present our recent modeling efforts using coarse-grained as well as atomistic computer simulations in combination with the linear-response solution-diffusion model to understand and quantify the permeability of dense polymer (networks). Our work reveals some universal physical principles, such as strong solute partitioning-diffusion cancellation effects for a wide parameter regime, as well as significant 'chemical' effects (such as solute polarity and shape) which all contribute to the control of permeability. The gained insights enable us to formulate semi-empirical rules and scaling laws to potentially describe and extrapolate the permeability also for other polymer/solute systems.

CPP 2.2 Mon 14:00 H1

Phase behavior of ultra-soft spheres shows stable bcc lattices — •Andrea Scotti — Institute of Physical Chemistry RWTH Aachen University

The phase behavior of super-soft spheres is explored using solutions of ultra-low crosslinked poly(N-isopropylacrylamide) based microgels as a model system. For these microgels, the effects of the electric charges on their surfaces can be neglected and, therefore, only the role of softness on the phase behavior is investigated. The samples show a liquid-to-crystal transition at higher volume fraction with respect to both hard spheres and stiffer microgels. Furthermore, stable body centered cubic (bcc) crystals are observed in addition to the expected face centered cubic (fcc) crystals. Small-angle X-ray and neutron scattering with contrast variation allow the characterization of both the microgel-to-microgel distance, and the architecture of single microgels in crowded solutions. The measurements reveal that the stable bcc crystals depend on the interplay between the collapse and the interpenetration of the external shell of the ultra-low crosslinked microgels.

CPP 2.3 Mon 14:15 H1

Co-polymerization of PNIPAM microgels with Dopamine Methacrylamide to increase adhesive properties — •Sandra Forg[1], Alexandra Karbacher[1], Regine von Klitzing[1], Zhishuang Ye[2], and Xuhong Guo[2] — [1]Soft Matter at Interfaces (SMI), Technical University of Darmstadt, Germany — [2]School of Chemical Engineering, East China University of Science and Technology, China

Microgels are cross-linked polymer particles, which are highly swollen in solvents such as water. One of those microgels is the stimuli-responsive PNIPAM, which undergoes deswelling when heated above its LCST at 32°C. The co-polymerization of PNIPAM is a well-defined technique to design unique microgel systems.

Dopamine methacrylamide (DMA) is a catechol-based monomer, which is main responsible for the adhesive properties of marine organisms. Combining the stimuli-responsiveness of PNIPAM with the adhesive properties of DMA bears a huge potential for biomedicine.

In literature the formation mechanisms of such microgel networks are shown. Furthermore, it is well-known that such catechol-based monomers like DMA have a high radical scavenging ability and thus cross-link the microgel. But, so far, a detailed understanding of the co-polymerization is missing. Therefore, the reaction kinetics of DMA during the microgel synthesis are presented in this work. The built-in DMA was verified by UV-VIS standard addition and NMR spectroscopy. First adhesion tests under water will be presented.

CPP 3: Polymer Physics

Time: Monday 13:30–16:15 Location: H3

Invited Talk CPP 3.1 Mon 13:30 H3

Emulsion Templating: Unexpected Morphology of Monodisperse Macroporous Polystyrene — •Cosima Stubenrauch[1], Lukas Koch[1], Sophia Botsch[1], and Wiebke Drenckhan[2] — [1]Institut für Physikalische Chemie, Universität Stuttgart, Deutschland — [2]Institute Charles Sadron, CNRS Strasbourg, Frankreich

We start with a monodisperse, hexagonally close-packed water-in-monomer high internal phase emulsion (HIPE). The polymerization of the continuous monomer phase with a water-soluble initiator leads to a monodisperse, macroporous polymer with an unexpected morphology: the pore cross-sections of this material are closed hexagons and the pore walls consist of three distinctive layers. Though this morphology has already been observed for two different systems, the mechanism leading to it has not been identified yet. Based on new experimental results we propose a surfactant-driven mechanism: excess surfactant is dissolved in the continuous phase, where it emulsifies water from the emulsion droplets. When the polymerization is initiated from the interface, the continuous phase becomes a poor solvent for both the surfactant and the emulsified water. As a consequence, they "flee" from the site of the polymerization (1) towards the water/monomer interface or (2) into the yet unpolymerized inside of the continuous phase. The first process may cause the emulsion droplets to change their shape from spherical to polyhedral and the second process may be responsible for the formation of the three observed layers in the pore wall. We will (a) discuss both processes in detail and (b) present the experimental results that clearly support them.

CPP 3.2 Mon 14:00 H3

Dissociation degree and pKa value of polyacid systems in solution and coatings determined by FTIR titration — Luise Wirth[1,2], Birgit Urban[1], Carolin Naas[1,2], and •Martin Müller[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Department Functional Colloidal Materials, Hohe Str. 6, D-01069 Dresden, Germany — [2]Technische Universität Dresden, Department Chemistry and Food Chemistry, D-01062 Dresden, Germany

Dissociation degree a and pKa of poly(acrylic acid) (PAA) and propionic acid (PA) 0.1 M solutions were determined by FTIR titration and potentiometric (POT) titration concept. Increasing subsequently the pH value from 2 to 12 by adding 1 M NaOH portions, FTIR spectra of PA and PAA show decrease of n(C=O) and increase of n(COO-) band due to carboxyl (COOH) and carboxylate (COO-) groups, respectively. From the respective normalized band integrals A, the dissociation degree aIR=ACOO-/(ACOOH+ACOO-) can be calculated. pH was plotted versus aIR and fitted by pH=pKa+B log(aIR/(1-aIR)) related to Henderson-Hasselbalch equation with fit parameters pKa and empirical cooperativity factor B. The slight pKa deviation found for FTIR and POT titration, the respective deviation between monomeric PA and polymeric PAA and the PAA molecular weight trend (PAA-2K, PAA-50K, PAA-450K) are discussed based on the known two-phase model of polyelectrolyte solutions including Gibbs-Donnan potential concept. Furthermore, aIR of PAA within consecutively adsorbed polycation/PAA multilayer coatings was determined by FTIR titration showing significant effect of the outermost polyelectrolyte layer.

CPP 3.3 Mon 14:15 H3

New nanoscale gradient copolymer films fabricated via initiated chemical vapor deposition (iCVD) — •Stefan Schröder, Alexander M. Hinz, Oleksandr Polonskyi, Thomas Strunskus, and Franz Faupel — Kiel University, Institute for Materials Science, 24143 Kiel, Germany

Many structures found in the natural world are based on organic gradients. To reproduce these structures, polymers are an excellent choice, as they also enable the formation of gradient copolymers. This study reports on the fabrication of such gradient copolymers in the form of thin films via initiated chemical vapor deposition (iCVD). Solvent-free deposition and the mild deposition conditions are only two of the advantages of iCVD in order to produce high-quality polymer thin films on large-area substrates, complex geometries as well as temperature-sensitive samples. In addition, the process enables the combination of comonomers which typically lack a common solvent. For the transfer of the gradient film approach to the lower nanoscale, a detailed understanding and control of the vapor phase kinetics are required. This is solved in this study by a novel in-situ quadrupole mass spectrometry (QMS) extension combined with supporting ab-initio/density functional theory (DFT) calculations. It offers a better insight into the underlying reaction kinetics and enables enhances process control during the deposition. This facilitates the fabrication of gradient copolymer films with film thicknesses below 30 nm. They show completly new physical and chemical properties, which cannot be obtained with materials currently in use.

Invited Talk CPP 3.4 Mon 14:30 H3

Structural Transitions of Molecules on Surfaces — •Angelika Kühnle — Physical Chemistry I, Department of Chemistry, University Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

Molecular self-assembly constitutes a versatile strategy to create functional molecular structures at surfaces. Conventionally, self-assembly is associated with structures in thermodynamic equilibrium. In this talk, several examples will be given for molecular structures that are explained by thermodynamic equilibrium. However, observed structures might be kinetically trapped, and structural transitions can be induced by annealing. On the (111) surface of copper, dimolybdenum tetraacetate (MoMo) molecules are shown to undergo a reversible phase transition of molecular islands (2D solid phase) into mobile molecules (2D gas phase). Interestingly, while this phase transition is usually associate with heating, the mobilization of the MoMo molecules presented here is observed upon cooling. In this talk, the molecular-scale origin of this inverse phase transition is discussed.

15 min. break

CPP 3.5 Mon 15:15 H3

Tack Properties of Pressure-Sensitive Adhesive-Coated Fiber Assemblies — •Volker Körstgens, Jorge Corella Puertas, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

For the mechanical characterization of the adhesive bond of pressure-sensitive adhesives one has to take into account the geometry of the adherents and the kind of stress applied. We present a technique, which allows for the measurement of tack for assemblies of fibers coated with pressure-sensitive adhesives using customized cylindrical composite stamps [1]. Key element of the method is the proposed technique to achieve monolayers of parallel-aligned fibers as a fiber assembly. With the adapted probe tack test we investigated the tack properties of a polymer blend of poly(vinylpyrrolidone-co-vinylacetate) and polyethylene glycol (PEG) coated on human hair. This composition serves as a simple model system for hair styling products. The influence of different PEG contents and of the humidity on the tack is demonstrated. Nylon fibers with different diameters are studied as references. [1] V. Körstgens et al., ACS Appl. Polym. Mater. 2, 3189-3195 (2020).

CPP 3.6 Mon 15:30 H3

Thermoporometry Characterization of Mesoporous Materials: A Kernel-Based Approach — •Henry R. N. B. Enninful, Dirk Enke, and Rustem Valiullin — Leipzig University, Leipzig, Germany

Detailed characterization of the structure of mesoporous solids presents key insights into the tailored design for various industrial applications such as catalysis, molecular separations and adsorption, among others.

Thermoporometry, as a characterization technique, suffers from some inaccuracies which make it lag behind gas sorption for textural characterization.

Herein, we present a kernel-based approach for the thermoporometry characterization approach which accounts for a varying non-frozen layer thickness due to pore curvature and temperature and thermal fluctuations in especially, very small pores. Additionally, with the help of the serially-connected pore model (SCPM), we reveal disorder in cylindrical pores whose complex morphology results in cooperativity effects in thermodynamic phase behavior.

References [1] Enninful et 2019, Frontiers in Chemistry, doi: 10.3389/fchem.2019.00230. [2] Enninful et 2020, Microporous and Mesoporous Materials 309, 110534.

CPP 3.7 Mon 15:45 H3

Columnar Stacks of Azobenzene Stars Under Irradiation - Photoisomerization Kinetics and Light-Induced Defects — •Markus Koch, Marina Saphiannikova, and Olga Guskova — Institute Theory of Polymers, IPF Dresden, Germany

Azobenzenes (azo) are a class of molecules that photoisomerize between their trans and cis state, causing dramatic conformational changes. These chromophores are widely used to add light-responsive properties to various microscopic or macroscopic systems. The object of this study is a star-shaped molecule (TrisAzo) containing three azo groups connected via a BTA group. TrisAzo not only has a rich photoisomerization behavior [1]. In polar media, these molecules self-assemble into supramolecular structures, that undergo a reversible morphological transition upon UV-Vis light irradiation [2]. Our study focuses on modeling these systems via fully atomistic MD simulations. In particular, we investigate the effects of UV-Vis light on columnar TrisAzo stacks [3]. Using a detailed simulation approach, we can closely reproduce the photoisomerization kinetics in these systems. Moreover, the results demonstrate how light induces defects in the columns and how this is related to the intermolecular interactions of stacked TrisAzo molecules. We thank the German Research Foundation (DFG) for financial support, project GU 1510/5-1.

[1] M. Koch et al. J. Phys. Chem. B 121 (37), 8854-8867 (2017)
[2] S. Lee et al. Langmuir 29 (19), 5869-5877 (2013)
[3] M. Koch et al. Langmuir 35 (45), 14659-14669 (2019)

CPP 3.8 Mon 16:00 H3

Free energy considerations in confined heterocatalysis in a supported ionic liquid phase — •Takeshi Kobayashi[1], Hamzeh Kraus[2], Felix Ziegler[3], Michael Buchmeiser[3], Niels Hansen[2], and Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart — [2]Institute of Thermodynamics and Thermal Process Engineering, University of Stuttgart — [3]Institute of Polymer Chemistry, University of Stuttgart

The high potential of performing heterocatalysis in a confined mesoporous media within a supported ionic liquid phase (SILP) is studied using Molecular Dynamics (MD) simulations. Specifically, we investigate the possibility of immobilizing catalytic molecules in confined media in a biphasic solution consisting of an ionic liquid (IL) and heptane as the second phase within a pore with a lateral size of about 5 nm. Divalent cationic Ru-alkylidene N-heterocyclic carbene catalysts are placed in the solution. We were able to monitor the immobilization of the catalysts within the IL for achieving higher turnover rates in the catalytic reactions. We further analyze the accumulation and diffusion of the molecules within the pore, the influence of steric and IL-specific effects, the structuring of a solvent environment, and their synergistic interactions with the catalytic molecules. The free energy calculations reveal that the catalytic reaction must occur at the interface between the heptane and the IL. Our investigations are supported by experimental evidence and provide a deeper understanding of the inherent details that control a rational design of a linker-free catalyst immobilization in nanometer-sized templates for catalytic applications.

CPP 4: Focus: The Physics of Adaptive Polymer Networks

organized by Regine von Klitzing (TU Darmstadt) und Christian Holm (Universität Stuttgart).

Adaptive polymer networks and gels represent soft materials with dimensional stability and viscoelasticity, which can assume different states due to changes in environmental conditions. This makes them promising candidate materials for a variety of applications, such as membranes for separation techniques or perm-selective membranes, and sensors and actuators. A particularly versatile class of adaptive gels are amphiphilic networks, which combine components that swell selectively in different media. The investigation of these amphiphilic co-networks represents a topic of high current relevance in polymer sciences, which has been coordinated in Germany by the research group FOR2811 since 2019 (www.for2811.uni-mainz.de).

Time: Tuesday 10:00–12:45 Location: H3

Invited Talk CPP 4.1 Tue 10:00 H3
Adaptable amphiphilic co-networks: structure and properties in relation with multi-quantum NMR — •Michael Lang[1], Reinhard Scholz[1], Lucas Löser[2], Carolin Bunk[1], Frank Böhme[1], and Kay Saalwächter[2] — [1]Leibniz-Institut für Polymerforschung, Hohe Straße 6, 01069 Dresden, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physics - NMR Group, Betty-Heimann-Str. 7, 06120 Halle, Germany
Amphiphilic co-networks made by the hetero-complementary coupling of four arm star polymers are an interesting model system to understand the physics of adaptive co-networks and currently the focus of the DFG research unit FOR2811 in which we participate. We analyze these model networks in different states (preparation in co-solvent, swollen state, and "switched" states where one type of polymer is swollen and the other collapsed) with large scale Monte-Carlo simulations and experiments. We discuss the degree of swelling, the scattering function, chain extensions, etc. of these model systems briefly. A particular focus is put on data and models regarding proton multiple-quantum NMR. After a brief tutorial on what can be analyzed with this method, we sketch analytical models for NMR order parameters in a particular state and compare with the availabe simulation or experimental data in these states. This analysis provides useful information on the time average local properties of individual network strands including the strain distribution of network strands. Such information is hardly accessible with alternative methods and allows even for the analysis of cyclic network defects under appropriate conditions.

Invited Talk CPP 4.2 Tue 10:30 H3
Adaptive networks through supramolecular interactions — •Ilja Voets — Department of Chemical Engineering and Chemistry & Institute for Complex Molecular Systems, Eindhoven University of Technology
Supramolecular interactions offer a powerful tool to modulate self-assembly pathways to generate dynamic materials with adaptive properties. In this lecture I will showcase two versatile, supramolecular approaches to generate adaptive, polymer-based materials, based on electrostatically driven co-assembly of ionic-neutral block copolymers and on amphiphilic copolymers equipped with suitable motifs, such as C3-symmetrical discotics based on benzene-1,3,5-tricarboxamides (BTAs), encoded to form one-dimensional helical 'stacks'. I will discuss the structure and properties of the micellar and fibrillar objects that these materials form in dilute aqueous solution, and of the transient networks which emerge at elevated concentrations. Recent efforts and insights in e.g. polyelectrolyte complexation out-of-equilibrium, strain stiffening, high resolution optical imaging and templated polymerization will be addressed. In future, these concepts may be exploited to further custom-tailor gels towards a desired structure and associated mechanical response.

15 min.break

CPP 4.3 Tue 11:15 H3
Chain connectivity of tetra-PEG - tetra-PCL amphiphilic end-linked polymer model networks — •Lucas Löser[1], Carolin Bunk[2], Frank Böhme[2], and Kay Saalwächter[1] — [1]Inst. f. Physik - NMR, Martin-Luther-Universität Halle-Wittenberg — [2]Leibniz-Institut f. Polymerforschung Dresden e.V., Hohe Str. 6, Dresden
A new approach for the synthesis of model-like amphiphilic co-networks is introduced, and their structure analysed by static 1H time-domain nuclear magnetic resonance (NMR) methods. A novel approach of hetero-complementary end-linking [1] of two well-defined tetra-armed polyethylene glycol (PEG) stars based on Sakai et al. [2] is used and modified in a way, that amphiphilic gels are obtained. We link PEG stars with a hydrophobic poly-ϵ-caprolactone star (tetra-PCL) terminated with an oxazinone group, resulting in the formation of an amphiphilic network. By using static 1H-1H multiquantum-NMR, as initially performed by Lange et al. [3], we show that our method is capable of distinguishing different chain species in the swollen PEG-PCL networks, allowing quantification of network connectivity defects arising from the end-linking reaction of A4- and B4-type stars, as well as accurate quantification of inelastic material. The parameter space of the synthesis is explored and changes in microscopic network structure are studied depending on polymer concentration and different temperature programs during synthesis. [1] Jakisch et al. ; Macromol. Chem. Phys 2017, 219 [2] Sakai, T. et al.; Macromolecules 2008, 41 [3] Lange, F. et al.; Macromolecules 2011, 44

CPP 4.4 Tue 11:30 H3
Microscopic and macroscopic mechanical properties of amphiphilic model co-networks — •Nora Fribiczer[1], Kevin Hagmann[2], Carolin Bunk[3], Sebastian Seiffert[1], Regine von Klitzing[2], and Frank Böhme[3] — [1]Department of Chemistry, Johannes Gutenberg University Mainz, D-55128 Mainz — [2]Institute for condensed matter physics, Technische Universität Darmstadt, D-64289 Darmstadt — [3]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden
Amphiphilic polymer gels are composed of both hydrophilic and hydrophobic polymers, which makes their mechanical properties dependent on environmental conditions such as the solvent polarity. In this work, we present both a microscopic and macroscopic perspective of these properties using indentation atomic force microscopy and oscillatory shear rheology. With this, we aim to get a rational understanding of the interplay between the environmental conditions and the resulting mechanical properties in the bulk material and at the interface.

Next to the investigation of the mechanical properties under good and bad solvent conditions, we put special emphasis on the characterization of the gelation process during network formation. By variation of concentration and temperature the reactivity and network topology can be controlled due to the use of an innovative bi-functional coupling agent which connects the hydrophilic tetra-PEG and the hydrophobic tetra-PCL. Monitoring the network formation using shear rheology allows for determination of the respective gel points, which coincide with results obtained from nuclear magnetic resonance spectroscopy.

Invited Talk CPP 4.5 Tue 11:45 H3
Tunable self-assembled hydrogels from block copolymers with thermoresponsive and pH-responsive blocks — •Christine M. Papadakis[1], Florian A. Jung[1], and Constantinos Tsitsilianis[2] — [1]Physics Department, Technical University of Munich, Garching, Germany — [2]Department of Chemical Engineering, University of Patras, Greece
Pentablock terpolymers with thermoresponsive end blocks and a pH-responsive middle block form hydrogels in aqueous environment. By altering the stability of the crosslinks and the degree of bridging, the responsivities afford numerous possibilities to tune the mechanical properties. Small-angle neutron scattering revealed the underlying mesoscopic structures in dependence on temperature and the pH value [1]. The thin film geometry allows studying the microphase-separated structures in the dry state and during swelling in the vapor of water or organic solvents in situ using grazing-incidence small-angle X-ray scattering. The results reveal the role of the dielectric properties of the solvent for microphase separation and hydrogel formation [2].
[1] C. Tsitsilianis et al., *Macromolecules* **2018**, *51*, 2169. F. A. Jung et al., *Macromolecules* **2019**, *52*, 9746. M. M. S. Lencina, et al., *ACS Appl. Polym. Mater.* **2021**, *3*, 819.
[2] F. A. Jung et al., *Macromolecules* **2020**, *53*, 6255.

CPP 4.6 Tue 12:15 H3
Structural characterization of covalently connected amphiphilic star polymer conetworks — •Reinhard Scholz[1], Lucas Löser[2], Kay Saalwächter[2], Carolin Bunk[1], Frank Böhme[1], and Michael Lang[1] — [1]Leibniz Institut für Polymerforschung, 01005 Dresden, Germany — [2]Institut für Physik - NMR, Martin-Luther Univeristät Halle-Wittenberg, 061120 Halle, Germany
Polymer networks consisting of complementary four functional stars of poly ethylene glycol (PEG) and poly caprolactone (PCL) were synthesized via covalent coupling of complementary end groups. The equilibrium swelling in various solvents revealed either compatibility of both polymer components with good solvents for both components like in toluene, or a reduced swelling in solvents like THF or water, representing selective solvents for the PEG component only. Complementary X-ray scattering studies allowed to assign the structure factor to a swollen conetwork (in toluene), or to a swollen PEG component connect-

ing embedded clusters of PCL (in THF or water). These experimental results were accompanied by simulations of network formation as a function of polymer concentration during preparation, and subsequent swelling in a cosolvent or a selective solvent. The calculated structure factor arising from the simulated model networks reveals a typical length scale for the size and distance of the PCL clusters, in reasonable agreement with the dependence of the observed scattering intensity on wave vector.

CPP 4.7 Tue 12:30 H3

From four-arm block copolymers to electrostatically cross-linked gels — •Peter Johannes Mons[1], Nora Fribiczer[2], David Beyer[3], Felix Helmut Schacher[1], Sebastian Seiffert[2], and Christian Holm[3] — [1]Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich-Schiller-University Jena, D-07743 Jena — [2]Department of Chemistry, Johannes Gutenberg-University Mainz, D-55128 Mainz — [3]Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart

Reversibly electrostatically cross-linked polymer networks composed of oppositely charged four-armed star block copolymers feature favorable properties such as environmentally sensitive viscoelasticity and selective permeability. In this work, we present different double hydrophilic star-shaped block copolymers with oppositely charged polyelectrolytes that can form electrostatically cross-linked gels. A new class of reversible double hydrophilic or amphiphilic networks can be synthesized based on these gels.

The four-armed copolymers consist of a PEG-core block extended with sulfonated polystyrene or N,N-dimethylaminopropyl acrylamide (DMAPAa). The sulfonated polystyrene block carries a permanent anionic charge whereas the DMAPAa block carries a permanent cationic or pH-tunable charge. The gel formation upon mixing these block copolymers was verified by shear rheology, which showed a high dependence of the gel strength on the presence of counterions. Coarse-grained molecular dynamics simulations support the picture of well-gelated networks and give insight into the molecular conformations.

CPP 5: Poster Session I

Electrical, Dieelectrical and Optical Properties of Thin Films (1-7); Hybrid and Perovskite Photovoltaics (8-13); Organic Electronics and Photovoltaics (14-16); Molecular Electronics and Excited State Properties (17-19).

Time: Tuesday 17:30–19:30 Location: P

CPP 5.1 Tue 17:30 P

Thermal degradation of EMIM DCA post-treated PEDOT:PSS thermoelectric thin films, investigated via in-situ GISAXS — •Anna Lena Oechsle[1], Julian E. Heger[1], Nian Li[1], Shanshan Yin[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]ELETTRA Sincrotrone Trieste S. C. p. A., 34149 Basovizza TS, Italy — [3]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, 85748 Garching, Germany

The constantly increasing energy demand raises the need for renewable energies and the reduction of energy dissipation. Thermoelectric materials are promising in terms of waste heat recovery and the use of solar thermal energy, as they enable the direct conversion of a temperature gradient into electrical power. Nowadays great research focus is especially on thermoelectric polymers, as they are low or nontoxic, lightweight, flexible and allow a low-cost, large-scale solution-based production of thin films. In this work we show the positive influence of EMIM DCA post-treatment on the Seebeck coefficient and electrical conductivity of PEDOT:PSS thin films. However, for possible future applications it is also important to understand the behavior of these films during long-term operation at elevated temperature. Therefore, we reveal occurring morphology changes with in-situ GISAXS measurements of these films and try to link them to the observed decrease in the electrical conductivity.

CPP 5.2 Tue 17:30 P

Uncovering the enhancement mechanisms of thermoelectric performance of PEDOT: PSS films after physical-chemical dedoping — •Suo Tu, Ting Tian, Anna-Lena Oechsle, and Peter Müller-Buschbaum — Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

Organic semiconductors have attracted intense attention because of their potential use in mechanically flexible, lightweight, and inexpensive electronic devices. Especially* PEDOT: PSS is the most studied conducting polymer system due to their intrinsically high electrical conductivity, low thermal conductivity, and high mechanical flexibility in thermoelectric (TE) devices. It is generally acknowledged that it is difficult to achieve a high ZT value of TE materials, due to the fact that the interdependence of parameters as a function of charge carrier concentration. In this work, we adopt a combination of DMSO addition and subsequent DMSO/salt mixture post-treatment to improve the TE performance of PEDOT: PSS thin films. Results show that the as-obtained PEDOT: PSS film presents a maximum PF of 105.2 *W(m-1K-2), which is ~1750-fold leap larger than that of pristine film. The origin and mechanism of the underlying improvement are systematically investigated by various characterizations to gain a more profound understanding of the fundamental nature of the modified PEDOT: PSS films.

CPP 5.3 Tue 17:30 P

Measurement setup to characterize thermoelectric polymer thin films — •Simon Wegener[1], Anna Lena Oechsle[1], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The growing need to save fossil resources requires, besides their substitution, also their effective usage. This usage is mostly limited by the high amounts of wasted heat in the conversion from chemical energy to mechanical or electrical energy. Thermoelectric (TE) materials are a promising way to make use of this wasted energy. Particularly, they can be used in a wide range of applications to generate electricity. Nevertheless, these materials show lots of room for improvement in terms of their output power. Therefore, with our work, we aim to construct a setup, which focuses especially on the measurement of polymer-based TE materials for low-temperature applications. This setup consists of two mounting plates that can be heated or cooled individually to determine the Seebeck coefficient. Additionally, a van der Pauw measurement can be done to find the electrical conductivity of the sample. By this, the setup will enable the user to rapidly characterize samples by its TE power factor.

CPP 5.4 Tue 17:30 P

Tailoring the Optical Properties of Sputter-Deposited Gold Nanostructures on Nanostructured Titanium Dioxide Templates — •Suzhe Liang[1], Wei Chen[1], Shanshan Yin[1], Simon J. Schaper[1], Jonas Drewes[2], Niko Carstens[2], Thomas Strunskus[2], Franz Faupel[2], Marc Gensch[1,3], Matthias Schwartzkopf[3], Stenphan V. Roth[3,4], and Peter Müller-Buschbaum[1,5] — [1]TU München, Garching, Germany — [2]CAU,Kiel, Germany — [3]DESY, Hamburg, Germany — [4]KTH, Stockholm, Sweden — [5]MLZ, TU München, Garching, Germany

Au/TiO2 nanohybrid materials have attracted significant attention due to the outstanding optical, photocatalytic and photovoltaic performance. We use customized polymer templating to achieve TiO2 nanostructures with different morphologies. Au/TiO2 hybrid thin films are fabricated by sputter deposition. An in-depth understanding of the Au morphology on the TiO2 templates is achieved with in situ GISAXS during the sputter deposition. The resulting Au nanostructure is largely influenced by the TiO2 template morphology. Based on the detailed understanding of the Au growth process, characteristic distances can be selected to achieve tailored Au nanostructures at different Au loadings. For selected sputter-deposited Au/TiO2 hybrid thin films, the optical response with a tailored localized surface plasmon resonance is demonstrated.

CPP 5.5 Tue 17:30 P

Sputter-depostion vs. spraying: effect of doping technique on the structural and thermoelectric properties of P3HT-based thin films — •Benedikt Sochor[1], Constantin Harder[1], Anna-Lena Oechsle[2], Matthias Schwartzkopf[1], Alexei Vorobiev[3], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,4] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]Technical University Munich, Physics Department, James-Franck-Str. 1, 85748 Garching, Germany — [3]Institue Laue-Langevin, 71 Avenue des Martyrs, 38042 Grenoble Cedex 9, France — [4]KTH Royal Institute of Technology, Teknikringen 56-58, 100 44 Stockholm, Sweden

Poly(3-hexylthiophen-2,5-diyl) (P3HT) is one of the most prominent semiconducting, conjugated polymers in the fields of organic electronics and photovoltaics. This study aims for correlating process and fabrication parameters and the structural changes with the overall thermoelectric performance of P3HT and P3HT:PMMA films. Especially, we focus on two routes of gold (Au) doping, namely sputter and spray deposition techniques. The structure of the resulting polymer composites indicated distinct differences whether the gold is sprayed or grown on the surface as shown by AFM as well as neutrons and X-ray reflectivity measurements. During in situ GISAXS experiments, the growth and structure of the gold particles was mapped, which indicated the presence of sub-nanometer sized gold clusters in case of sputter deposition.

CPP 5.6 Tue 17:30 P

Hybrid energy harvester based on triboelectric nanogenerator and solar cell — •Tianxiao Xiao[1], Wei Chen[1], Wei Cao[1], and Peter Müller-Buschbaum[1,2] — [1]Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße. 1, 85748 Garching, Germany

Developing clean energy lies the heart of sustainable development of human society. Triboelectric nanogenerator (TENG) originating from Maxwell*s displacement current is a new type of energy harvester for harnessing ambient mechanical energy based on the coupling of triboelectrification and electrostatic induction effect. Compared with other counterparts, owing to the light-weight, low-cost, and easily fabricated, TENG has become one of the most promising candidates in replacement of conventional fossil fuels and attracted worldwide attention in the past years. However, to further increase the energy harvesting efficiency and broaden application fields, integrating the TENG with other kinds of energy harvesters in one device is a possible way to meet these needs. In the present work, a TENG based hybrid energy harvester is designed and fabricated on the flexible polyethylene terephthalate (PET) substrate. This hybrid device consists of a single-electrode mode TENG component and a PbS quantum dots based solar cell component, which can harness both mechanical and solar energy from ambient environment to directly generate electricity.

CPP 5.7 Tue 17:30 P

Colloidal photonic crystal slabs toward enhanced photoconductivity — •Swagato Sarkar[1], Vaibhav Gupta[2], and Tobias A. F. König[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V. (IPF), Institute for Physical Chemistry and Polymer Physics, Hohe Str. 6, 01069 Dresden, Germany — [2]Institute of Particle Technology, Friedrich-Alexander University Erlangen-Nürnberg, Cauerstrasse 4, 91058 Erlangen, Germany — [3]Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden 01062 Dresden, Germany

In the present work, a fusion of interference lithography (IL) and nanosphere imprint lithography [Gupta, König, Fery, ACS Appl. Mater. Interfaces 2019, 11, 28189.] on various target substrates ranging from carbon film on transmission electron microscope grid to inorganic and dopable polymer semiconductor is reported. 1D colloidal photonic crystals are printed with 75% yield on the centimeter scale using colloidal ink and an IL-produced polydimethylsiloxane stamp. Atomically smooth facet, single-crystalline, and monodisperse colloidal building blocks of gold (Au) nanoparticles can produce 1D plasmonic grating on top of a titanium dioxide (TiO2) slab waveguide, producing waveguide-plasmon polariton [Sarkar, Fery, König, Adv. Funct. Mater. 2021, 31, 2011099.] modes with superior 10 nm spectral line-width. Plasmon-induced hot electrons are confirmed via two-terminal current measurements resulting in increased photoresponsivity as well as enhanced photocatalytic degradation of methyl orange (MO) dye molecules.

CPP 5.8 Tue 17:30 P

Upscaling Perovskite: Optoelectronics and Morphology of Slot-Die Coated Solar cells — •Andrea Vitaloni[1], Lennart K. Reb[1], and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite solar cells (PSCs) have attracted increasing attention in research and industry due to their high efficiency, low material cost, and simple solution-based fabrication process. Additionally, the possibility to fabricate flexible and thin solar cells creates new opportunities compared to traditional solar modules.

In laboratory devices, the efficiency already exceeds 25% and is comparable with c-Si. However, one of the most important steps towards commercialization is the upscaling of the PSCs production to larger areas. Slot-die coating is considered to be one of the most promising technology, being a fast process with minimum material consumption and waste. Furthermore, the highly tuneable perovskite ink composition strongly determines kinetic processes during film formation and the final morphology.

We vary the composition of MAPI inks and analyze the printed perovskite thin-films and derived solar cells with spectroscopic and X-ray scattering methods. The focus is on developing a comprehensive understanding of the slot-die coating process for printed, flexible, and high-efficiency PSCs.

CPP 5.9 Tue 17:30 P

In-Operando study of humidity on the performance of perovskite solar cell — •Kun Sun[1] and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite solar cells (PSCs) are one of the most promising photovoltaic technologies and reached a certified 25.2% efficiency owing to their tuneable bandgap, high carrier mobility, long diffusion length and so on. The long-term operational stability of PSCs, however, has been not investigated. Herein, we probe the structure change with grazing-incidence small-angle scattering (GISAXS) under high humidity. Also, the solar cell parameters are obtained simultaneously during the device operation. We find that PSCs fabricated with and without caesium iodide (CsI) show differences in the device degradation and morphology change in the perovskite layer. The decrease of open-circuit voltage (VOC) can be attributed to the morphology changes and the evolution of crystallize grain size. With the additive of CsI, solar cells show slow decay of VOC, which is correlated to improved morphology of active layer and passivation of trap states. Our work presents a crucial step towards a fundamental understanding of morphology change combined with solar cell parameters during the device operation.

CPP 5.10 Tue 17:30 P

Tailoring the orientation of perovskite crystals via adding two-dimensional polymorphs for perovskite solar cells — •Renjun Guo[1], Ali Buyruk[2], Xinyu Jiang[1], Wei Chen[1], Lennart K. Reb[1], Manuel A. Scheel[1], Tayebeh Ameri[2], and Peter Müller-Buschbaum[1] — [1]Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany — [2]Chemie-Department, Ludwig-Maximilians-Universität München, Butenandtstr. 5-13 (E), 81377 München, Germany

Due to their outstanding properties, organic-inorganic perovskite materials are gaining increasing attention for their use in high-performance solar cells. Finding an effective method of defect passivation is thought to be a promising path for advancements toward narrowing the distribution of the power conversion efficiency (PCE) values, as measured by the spread in the PCE over different devices fabricated under identical conditions, for easier commercialization. We add 2*(4*fluoroph-enyl)ethyl ammonium iodide (p-f-PEAI) into the bulk of a mixed cation lead halide perovskite film in this study. The addition of the appropriate amount of p-f-PEAI affects the preference orientation of the perovskite crystals, increases the strength of the crystal texturing, and reduces non-radiative charge recombination. As a result, we achieve a tighter range of the PCE of perovskite solar cells (PSCs) without losing the PCE values obtained [1].

[1] Guo et al. J. Phys. Energy 2, 034005 (2020)

CPP 5.11 Tue 17:30 P

Fabrication and characterisation of slot-die coated formamidinium-cesium lead iodide perovskite solar cells — •Alexander Franz Weinzierl[1], Manuel A. Scheel[1], Lennart K. Reb[1], and Peter Müller-Buschbaum[1,2] — [1]Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite solar cells (PSC) are a promising candidate to evolve the solar energy market due to high energy conversion efficiencies and low cost material usage. However, many perovskite absorber compositions suffer from long-term stability problems. Perovskites, composited of formamidinium/caesium lead iodide/bromide (FACs), as the active layer of such solar cells are promising to overcome this issue. Crucial for FACs is the development of a solvent system together with an optimised printing process enabling to produce highly homogeneous layers and, as a result, cells with high performance and low degradation. To achieve this outcome, slot-die coating is examined for depositing the Perovskite ink, especially, since this printing technique is transferable to the scale-up of PSCs towards commercial sizes. In this work inverted slot-die coated FACs solar cells are produced with different solvents. Their film morphology is investigated by microscopy, X-ray diffraction and GIWAXS. Moreover, the cells are characterised and compared via their respective current-voltage characteristic, giving insight into the performance parameters.

CPP 5.12 Tue 17:30 P

The Influence of CsBr on Crystal Orientation and Optoelectronic Properties of MAPbI3-based Solar Cells — •Yuqin Zou and Peter Müller-Buschbaum — Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany.

Crystal orientations are closely related to the behavior of the photogenerated charge carrier and vital for controlling the optoelectronic properties of perovskite solar cells. Herein, we propose a facile approach to reveal the effect of lattice plane orientations on the charge carrier kinetics via constructing CsBr doped mixed-cation perovskite phases. Through GIWAXS measurements, we systematically investigate the crystallographic properties of mixed perovskite films in the microscopic scales and reveal the effect of the extrinsic CsBr doping on the stacking behavior of the lattice planes. And provides a unique insight into the underlying relationship among the stacking pattern of crystal planes, the photo-generated charge carrier transport and the optoelectronic properties of solar cells.

CPP 5.13 Tue 17:30 P

Self-assembled Hybrid Plasmonic Nanostructures for Perovskite Solar Cells — •Tianfu Guan, Renjun Guo, Lennart K. Reb, Suzhe Liang, Christian L. Weindl, Wei Cao, and Peter Müller-Buschbaum — Technische Universität

München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany

Plasmonic metal-dielectric composites have gained great interest in various fields, owning to surface plasmon resonance (SPR) induced by incident radiation. The utilization of plasmonic metal nanoparticles (NPs) is frequently proposed as a means to further enhance the light absorption in the broad wavelength range as well as to facilitate charge collection and transport in the Perovskite solar cells (PSCs). To regulate the plasmonic spectral of Au NPs for maximizing the enhancement in light-absorption of the photoactive layer, we assembly the metal NPs onto the electron collecting layer to broaden the absorption band of the photoactive layer of optoelectronic devices as well as enhance the device performance. To meet the optimal results, we put effort into the plasmonic structure regulation, since the size, density, and morphology of the Au NPs will influence the crystallinity of the perovskite film and charge transportation of the device. GISAXS is used to study the quality of the plasmonic structure interface in terms of contact area with the perovskite film. GIWAXS is used to probe the crystalline structure of the perovskite active layers.

CPP 5.14 Tue 17:30 P

Effect of chemical modification on crystal structure and thermal properties of Polydiketopyrrolopyrrole Copolymers — •Robert Kahl[1], Gert Krauss[2], Andreas Erhardt[2], Oleksandr Dolynchuk[1], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany — [2]Applied Functional Polymers, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany

Polydiketopyrrolopyrrole (PDPP) copolymers are second-generation semiconducting polymers that gained interest due to their superior performance in transistors and solar cells. Their chemical structure consisting of a DPP core with flanking units and/or co-monomers offers many opportunities to tune the optoelectronic properties by introducing chemical modifications. Here we investigated the thermal properties and crystal structure in bulk (DSC, TGA, WAXS) and in thin films (GIWAXS, AFM) of three PDPPs: PDPP$[T]_2\{2\text{-HD}\}_2$-T{DEG} (PDPP1) with thiophene flanking units and an additional OEG side chain, PDPP$[Py]_2\{2\text{-HD}\}_2$-T (PDPP2) with pyridine flanking units and PDPP$[T]_2\{2\text{-HD}\}_2$-T (PDPP3) with thiophene flanking units. PDPP3 shows only sanidic liquid crystalline order. PDPP1 shows crystalline order and a significantly lower melting temperature than PDPP2 and PDPP3. PDPP2 shows the most WAXS peaks, but has poor thermal stability. Our results demonstrate that thermal properties and ordering ability can be significantly influenced by introducing seemingly minor changes to the chemical structure of PDPPs.

CPP 5.15 Tue 17:30 P

Following the morphology formation of printed non-fullerene active layers for solar cells — •Xinyu Jiang[1], Suo Tu[1], Manuel A. Scheel[1], Shanshan Yin[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, Garching, Germany — [2]DESY, Notkestr. 85, 22607 Hamburg, Germany — [3]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — [4]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Bulk heterojunction (BHJ) organic solar cells have gained significant improvements in the past few years, however, traditional laboratory deposition methods like spin coating are limited to small-scale production. Encouragingly, the emergence of printing techniques and the development of in-situ observation technology open new windows for lager-area device manufacturing and inspection of the formation process of the printed active layer, respectively. We fabricate an active layer, which contains a donor polymer (PDTBT2T-FTBDT) and a non-fullerene acceptor (BTP-4F) with slot-die coating. The structure formation of the polymer domains is followed in-situ during the printing process with GIWAXS and UV-Vis spectroscopy measurements, respectively. Thus, structure evolution is coupled with optical properties during the printing process, thereby providing an understanding of the film formation kinetics of non-fullerene organic BHJ thin films.

CPP 5.16 Tue 17:30 P

Influence of non-halogenated solvents on the morphology and stability of PTQ10:BTP-4F organic solar cells — •Lukas Spanier[1], Renjun Guo[1], Julian Heger[1], Yuqin Zou[1], Matthias Nuber[2], Matthias Schwartzkopf[3], David Toth[4], Rachid Houssaini[4], Hristo Iglev[2], Reinhard Kienberger[2], Achim Hartschuh[4], Stephan Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Lehrstuhl für Funktionelle Materialien, Garching, Germany — [2]TU München, Lehrstuhl für Laser- und Röntgenphysik, Garching, Germany — [3]Deutsches Elektronen-Synchrotron (DESY), FS-PE, Hamburg, Germany — [4]Ludwig-Maximilians-Universität München, Department Chemie und CeNS, Munich, Germany

Organic solar cells (OSCs) have recently gained increasing attention due to their rapidly increasing efficiencies as well as the relatively easy scalability in their production. However, their manufacture relies heavily on the use of halogenated solvents, as organic solar cells made with environmentally friendly solvents often suffer from reduced performance. This can be partially reversed by raising the temperature of the solvents during formation of the bulk-heterojunction (BHJ). We investigate and compare the changes in morphology and performance stability of PTQ10:BTP-4F OSCs processed from various solvents, utilising operando grazing-incidence X-ray scattering during illumination and solar cell operation. We further show the impact of solvent composition on the charge carrier dynamics in the respective BHJs using time-resolved transient absorption spectroscopy.

CPP 5.17 Tue 17:30 P

Polarization Resolved Optical Spectroscopy of PEN:PFP Charge-Transfer Excitons — •Darius Günder[1], Ana M. Valencia[2,3], Michele Guerrini[2,3], Tobias Breuer[1], Caterina Cocchi[2,3], and Gregor Witte[1] — [1]Molekulare Festkörperphysik, Philipps-Universität Marburg — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [3]Physics Dept., Humboldt-Universität zu Berlin & IRIS Adlershof

Charge-transfer excitons (CTX) occurring at molecular donor/acceptor interfaces are considered important intermediates for charge separation in photovoltaic devices. Co-crystalline pentacene:perfluoro-pentacene (PEN:PFP) films can be prepared with different molecular orientation on SiO2 and graphene substrates [1] and thus are well-suited model systems for detailed structure-property investigations of such CTX states. In this study, such crystalline PEN:PFP films with different molecular orientations are used to perform polarization and angular resolved UV/Vis absorption spectroscopy, in order to determine the direction of the transition dipole moment (TDM) of the CTX state, which is found to be perpendicular to the aromatic ring planes i.e. along the stacking direction. Interestingly, this orientation is different than for the singlet excitons of unitary acene films, which can be well-described by the Kasha-model using the TDMs of the single molecule HOMO-LUMO excitations that are oriented along the M-axis and thus constitutes an important benchmark system for a refined theoretical analysis of such molecular donor/acceptor systems. [1] D'Avino et al. Chem. Mater. 32, 3, 1261-1271 (2020)

CPP 5.18 Tue 17:30 P

Charge-transfer excitons in pentacene:perfluoropentacene co-crystal — •Ana M. Valencia Garcia[1,2], Darius Günder[3], Michele Guerrini[1,2], Tobias Breuer[3], Gregor Witte[3], and Caterina Cocchi[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [2]Physics Dept., Humboldt-Universität zu Berlin & IRIS Adlershof — [3]Philipps-Universität Marburg, Molekulare Festkörperphysik, Marburg

Disclosing the nature of optical excitations in organic co-crystals is a challenge due to the complex interplay between the structural arrangement of the molecules and long-range electronic interactions in these systems. For these reasons, the application of isolated cluster models is highly questionable. By means of density functional theory and many-body perturbation theory, we investigate the electronic and optical properties of the triclinic pentacene:perfluoropentacene co-crystal. The band-structure analysis indicates that the highest-occupied and the lowest-unoccupied states are mainly localized on different molecules, suggesting the presence of a charge-transfer exciton at the lowest energy, which is indeed revealed in the dielectric tensor computed from the solution of the Bethe-Salpeter equation. We demonstrate that this feature cannot be reproduced by a molecular cluster model where the first excitation is unambiguously polarized along the short molecular axis. Comparison with corresponding measurements clarifies the importance of adequate periodic treatment of molecular co-crystals to correctly reproduce the character of their excitations [1]. [1] Günder, Valencia, et al., in preparation.

CPP 5.19 Tue 17:30 P

Towards an accurate calculation of excitation energies of Bacteriochlorophyll complexes with Green's function-based many-body perturbation theory — •Zohreh Hashemi[1] and Linn Leppert[1,2] — [1]Institute of Physics, University of Bayreuth, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, Netherlands

Bacteriochlorophylls (BCL) are a family of chromophores with key functions in the primary energy-converting processes of bacterial photosynthesis. *In vivo*, BCLs are embedded in densely packed pigment-protein complexes; an accurate prediction of their electronic structure and excited states is key to understanding their interactions with each other and with their protein environment. However, the sheer size of these complexes, is presently an insurmountable challenge for highly accurate quantum chemical calculations.

Here we present calculations of the optoelectronic properties of BCL monomers and dimers based on first principles Green's function-based many-body perturbation theory within the GW and Bethe-Salpeter equation (BSE) approach. We find that optical excitations calculated with GW+BSE are in excellent agreement with experimental data and state-of-the-art wavefunction-based approaches - but achieved at considerably lower computational cost than the latter. Our study provides accurate reference results and highlights the potential of the GW+BSE approach for the simulation of larger pigment complexes.

CPP 6: Poster Session II

Complex Fluids and Colloids, Micelles and Vesicles (1-6); Crystallization, Nucleation and Self-Assembly (7-9); Modeling and Simulation of Soft Matter (10-19); Polymer and Molecular Dynamics, Friction and Rheology (20-23); Polymer Networks and Elastomers (24-26).

Time: Tuesday 17:30–19:30 Location: P

CPP 6.1 Tue 17:30 P

Self-assembled micelles in aqueous diblock copolymer solution — •Yanan Li[1], Chia-Hsin Ko[1], Varvara Chrysostomou[2], Dmitry Molodenskiy[3], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]Physics Department, Technical University of Munich, Garching, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece — [3]EMBL at DESY, Hamburg, Germany

Micelles with stimuli-responsive behavior have attracted great interest as nanocarriers, especially for drug delivery. Here, we investigate the diblock copolymer poly(2-(dimethylamino) ethyl methacrylate)-*b*-poly(lauryl methacrylate) (PDMAEMA-*b*-PLMA), having both pH and thermoresponsive properties in aqueous solution [1]. The self-assembled micelles can be applied in gene transfer and drug delivery applications. We investigate both the pH-dependent micellar structures depending on concentration and the designable micellar shapes from two preparation methods by dynamic light scattering and synchrotron small-angle x-ray scattering. Depending on the preparation method, cylindrical or ellipsoidal micelles are formed. In addition, as the solution is brought from the basic to the acidic state, the micellar size increases, which we attribute to the expansion of the charged PDMAEMA blocks.

[1] V. Chrysostomou, S. Pispas, *J. Polym. Sci. A: Polym. Chem.* **2018**, *56*, 598.

CPP 6.2 Tue 17:30 P

Direct Measurement of the Forces Acting Between Colloidal Silica Particles — •Thomas Tilger, Michael Ludwig, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Natural colloidal dispersions have accompanied mankind in the form of blood or milk ever since. Besides this, artificial systems have gained a significant importance for our daily life during the last decades. From the production of many cosmetics or the water purification and sewage water treatment to the medical field, colloidal systems are widely used nowadays.

For all these applications, it is of special interest to gain an understanding of which interparticle forces govern the stability of colloidal dispersions and how this stability can be tailored. In electrolyte solutions, the classical DLVO theory describes these interactions as a superposition of van der Waals and electrostatic double layer forces. Complex fluids such as micellar dispersions show additional oscillatory contributions caused by a structuring of the micelles.

For a detailed examination of these two regimes, we directly measure the forces between two colloidal silica particles in aqueous solutions by the colloidal probe AFM (atomic force microscopy) technique. Varying the concentration of sodium chloride solutions allows us to compare the transition from the double layer to the van der Waals dominated regime with the predictions of the DLVO theory. Similar measurements for the anionic surfactant sodium dodecyl sulfate (SDS) reveal a structuring of the SDS micelles under confinement.

CPP 6.3 Tue 17:30 P

Aggregation of Gold Nanoparticles: Effects of Ion Type, Salt Concentration, and Aging — •Philipp Ritzert and Regine v. Klitzing — TU Darmstadt, Institute for Condensed Matter Physics, Soft Matter at Interfaces, Hochschulstr. 8, 64283, Darmstadt

The combination of inorganic nanoparticles (NPs) with (responsive) organic polymer matrices advances numerous scientific and technical applications, *e.g.* catalysis, nanoactuation, and medical engineering. Despite considerable progress of embedding NPs into a matrix, the process is often not well-controlled and the composite manufacturing relies on trial-and-error to augment the product quality. Better control over the product manufacturing (*i.e.* NP incorporation) enhances the applicability through more complex NP assemblies.

The project aims at the control of gold NP structuring in a polymer brush matrix. Gold NPs present a versatile model system as they are easily synthesized and stabilized. Furthermore, they exhibit a strong localized surface plasmon resonance in the visible range. Addition of salt triggers the re-ordering, thus, providing multiple adjusting parameters: salt concentration, ion type, and exposure time.

Preceeding composite manufacturing, characterizing the response of gold NPs is essential. The present contribution studies the time evolution of the optical absorption spectra of citrate-capped gold NP suspensions (diameter approx. 13 nm) containing different concentrations of various monovalent sodium salts along the Hofmeister series. In addition, the project exemplifies the influence of basic gold NP properties, namely size and capping molecule.

CPP 6.4 Tue 17:30 P

Mesoscale computer simulations of diffusion and sedimentation of colloidal suspensions — •Yashraj Wani[1], Penelope Grace Kovakas[2], Arash Nikoubashman[1], and Michael Howard[2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany — [2]Department of Chemical Engineering, Auburn University, Auburn, AL 36849, USA

The diffusive motion in colloidal suspensions is a central process in soft matter, and it also plays an essential role for a wide range of applications. Through simulations, we investigated the self- and collective diffusion in suspensions of spherical colloids at various solute concentrations. To this end, we tested several methods with and without hydrodynamic interactions (HI). We found reasonable agreement for the long-time self-diffusion coefficients between all methods, which is in agreement with previous theoretical considerations. There were, however, fundamental differences in the collective diffusivity (quantified via the sedimentation coefficients) between the various methods: When HI were neglected, the collective diffusivity was identical to the short-time self-diffusion, whereas in the simulations with HI, the sedimentation coefficients decreased with increasing solute concentration. Finally, we applied our methodology to study the equilibrium dynamics of cubic colloids.

CPP 6.5 Tue 17:30 P

Effects of polymer block length asymmetry and temperature on the nanoscale morphology of thermoresponsive double hydrophilic block copolymers in aqueous solutions — •Apostolos Vagias[1], Aris Papagiannopoulos[2], Lucas P. Kreuzer[1], Despoina Giaouzi[2], Sebastian Busch[3], Stergios Pispas[2], and Peter Müller-Buschbaum[1,4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece — [3]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon, Garching, Germany — [4]Technische Universität München, Physik- Department, Lehrstuhl für Funktionelle Materialien, James-Franck- Str. 1, Garching, Germany

We combine Fourier transform infrared (FTIR) spectroscopy and small angle neutron scattering (SANS) to identify block length asymmetry and temperature effects on the nanoscale assemblies of novel thermoresponsive double hydrophilic poly(N-isopropylacrylamide)-block-poly(oligo ethylene glycol methyl ether acrylate) (PNIPAM-b-POEGA) diblock copolymers. Morphological transformations from hierarchical assemblies to more well-defined spherical morphologies were identified upon heating. Alteration in the PNIPAM block length induces differences in the strength and/or amount of hydrogen bonding and hydrophobic interactions and molecular solvation.

CPP 6.6 Tue 17:30 P

Rotating spherical particle in a continuous viscoelastic medium — a microrheological example situation — •Sonja K. Richter, Claudius D. Deters, and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

We consider rigid spherical particles in a continuous one-component viscoelastic environment that are subject to an external dynamic torque. A dynamic relaxation parameter quantifies the deformational memory of the embedding material. Consequently we can interpolate between damped reversible deformation dynamics and net terminal flow of the viscoelastic surroundings using the same formalism [1]. On this basis, we determine the dynamic linear response function for particle rotations that are driven by the external torque under no-slip conditions on the particle surface [2]. Specifically, we derive explicit expressions for the induced deformation and flow fields in the surrounding viscoelastic medium. To link to magnetic microrheology, we address magnetically anisotropic particles that are driven by a dynamic external magnetic field. Corresponding magnetic susceptibility functions are evaluated [2]. Overall, we expect that our results will be important in the context of microrheological measurements on soft and biological visoelastic matter.

[1] M. Puljiz, A. M. Menzel, *Phys. Rev. E* **99**, 012601 (2019).
[2] S. K. Richter, C. D. Deters, A. M. Menzel, *EPL (Europhys. Lett.)*, accepted.

CPP 6.7 Tue 17:30 P

STM and DFT study of BF4 anion migration on a triazatriangulenium SAM on Au(111) — •Sergii Snegir[1], Yannick Dappe[2], Dmytro Sysoiev[3], Olivier Pluchery[4], Thomas Huhn[1], and Elke Scheer[1] — [1]University of Konstanz, Konstanz, Germany — [2]SPEC, University Paris-Saclay, France — [3]I. Org. Chem. & Biochem., Prague — [4]INSP, Sorbonne University, France

Chemical coupling of functional molecules with so-called platforms allows the formation of functional Self-Assembled Monolayer (SAM). An example is triazatriangulenium (TATA), with an extended aromatic core, allowing the formation of good electronic contact with the metal surface. Here we present studies on SAMs of TATA-BF4 molecules on Au(111) by means of Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT). In solution, these molecules exist as ion pairs of TATA+ and BF4-. However, under electrochemical deposition on Au(111), on the TATA+ cations formed SAMs the BF4- anions seemingly disappear. Our STM experiments reveal dissociation of the TATA-BF4 complex1. The TATA+ remains stable within the SAM while the BF4- spontaneously migrates through the TATA SAM on the surface. DFT calculations show a reduction of the TATA-BF4 binding energy after deposition. 1.S.Snegir, Y. J.Dappe, D.Sysoiev, O.Pluchery, T.Huhn, E.Scheer, PCCP 2021, 23, 9930 - 9937.

CPP 6.8 Tue 17:30 P

Ordering of small polymer systems through the prism of partition function zeros. — •Timur Shakirov and Wolfgang Paul — Institute of Physics, University of Halle, Halle, Germany

Typical low temperature conformations of small alkane systems (single chains and few chain aggregates) differ frequently from the melt ones: even relatively short chains are folded in non-trivial structures at low temperatures [1]. The ordering of a system is related to change of thermodynamic and conformational characteristics of chains. In the case of big systems, the changes occur at one the same transition temperature, whereas for small systems the typical temperatures of the changes can be shifted relative to each other. The sensitivity of thermodynamic functions to the shift differs and can be hidden because of a widening of the transition region of the small system. We present here the results of an analysis of the partition function zeros, which helps to identify a two stage conformational reorganization of small alkane systems. Our calculations are based on Wang-Landau-type Monte Carlo simulations [2,3] of a chemically realistic united atom model [4].

[1] T. Shakirov, and W. Paul, J. Chem. Phys. 2019, 150, 084903.
[2] F. Liang, C. Liu, R. J Carroll, J. Am. Stat. Assoc. 2007, 102, 305-320.
[3] T. Shakirov, Comp. Phys. Commun. 228 (2018): 38-43.
[4] W. Paul, D. Y. Yoon, and G. D. Smith, J. Chem. Phys. 103 (1995) 1702-1709.

CPP 6.9 Tue 17:30 P

Alteration of self-assembly monolayers and their interactions with zinc oxide surfaces: A DFT study — •Azade YazdanYar[1], Petia Atanasova[2], and Maria Fyta[1] — [1]Institute for Computational Physics, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institute for Materials Science, Bioinspired Materials, Heisenbergstr. 3, 70569 Stuttgart, Germany

Self-assembled monolayers (SAMs) have gained profound interest due to their broad range of applicability such as in molecular electronics, bio-sensing and heterogeneous catalysis. One of the advantages of SAMs is the feasibility they provide in altering and controlling the properties of the substrate. Here, we use Density Functional Theory (DFT) to study the influence of various variations on the SAM-zinc oxide surface interactions. Specifically, we study the effect of several head groups (thiol, silane, phosphonate) and various crystallographic planes. We limit our work to SAMs of three methylene groups (CH2) in the chain with an azide functional group. The energetics of the system will be determined and compared in order to understand the strength of the SAM-surface interaction, which we expect to be greatly impacted by the type of the head group of the SAMs. We will also provide details on the specific interaction sites of the head group with the surface and the electronic structure. We discuss the relevance of these materials as functionalized templates for novel applications in catalysis and sensing.

CPP 6.10 Tue 17:30 P

Dissipative Self-Organization of Interfaces and Membranes — •Gregor Ibbeken and Marcus Müller — Frierich-Hund-Platz 1, 37075 Göttingen

Coupling a self-assembling system to a reaction cycle, we go beyond equilibrium self-assembly toward systems that dissipate energy and thus exhibit new, unique features of dynamic self-organization. We consider the general case of a precursor reacting with a fuel to a product, which itself can decay back to the precursor. To do so, a continuum model is utilized that treats concentrations as order parameters. Within the model, the free energy is given as a functional of the concentrations and the dynamics are computed via the chemical potentials. We show that under the assumption that the fuel diffuses faster than the reacting polymers, reactions introduce an effective connectivity between precursor and product. This way the systems show entirely different features than their respective equilibrium counterpart. For instance, a homopolymer melt can form lamellae, cylinders, spheres, as well as networks, similar to a diblock copolymer melt, and a solution with two reacting homopolymers can form bilayers. The length scale of emergent structures depends on the reaction rates. This way, one can control the size of micelles and vesicles in solution, by coupling an amphiphilic diblock copolymer to a hydrophilic precursor, giving rise to an interplay between the architecture- and the reaction-rate-determined length scales.

CPP 6.11 Tue 17:30 P

Measuring the line tension of a hemifusion diaphragm — •Yu-Jung Su, Yuliya Smirnova, and Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität, 37077 Göttingen, Deutschland

Changes of membrane topology are essential to cellular transport processes, such as e.g., synaptic release. The molecular pathways, however, are only incompletely understood. The hemifusion diaphragm (HD) is a putative intermediate, where two apposing membranes are locally fused into a single-membrane patch. The line tension of the three-bilayer junction at the rim of the HD controls the size and stability of the HD, and it is an important parameter for phenomenological free-energy models of fusion and fission processes. In the canonical ensemble, where the number of lipids is fixed, the line tension, λ, of the HD, which tends to decrease the area of the HD, is balanced by the membrane tension, π, resulting in a two-dimensional analog of the Laplace equation between λ, π, and the radius, R, of the HD. Using molecular dynamics simulation of the coarse-grained MARTINI model, we study this free-energy balance and calculate the line tension as a function of the membrane tension or the distance between the flat membranes in apposition. The results are compared to alternate estimates, e.g., obtained from the shape fluctuations of the rim of the HD.

CPP 6.12 Tue 17:30 P

Stability of the hemifusion diaphragm and the rim pore — •Yuliya Smirnova and Marcus Müller — Institute for Theoretical Physics, Georg-August University, Göttingen, Germany

Synapic transmission is a fundamental biophysical process that involves the exocytosis (neurotransmitter release) and endocytosis (vesicle recovery) of small synaptic vesicles at the presynaptic plasma membrane. Whereas the molecular mechanisms of these topology-altering membrane processes are only incompletely understood, it is hypothesized that a hemifusion diaphragm (HD), i.e., an extended single-membrane-thick, lipidic connection between the two apposing membranes, is an important intermediate state. We develop a phenomenological model to investigate the free-energy landscape of a HD with a (rim) pore (RP) that is formed inside the HD and borders the three-bilayer junction at the HD's rim. In the limit that the RP attains the size of the HD, a complete fusion pore is formed. In the absence of the RP, HDs of different sizes are (meta)stable in the canonical ensemble. It appears, however, to be difficult to stabilize a HD+RP complex in the canonical ensemble. Membrane tension, intermembrane distance, and the line tensions of a membrane pore, a HD, and a fusion pore, as well as external control of the HD's size are important parameters that dictate the (meta)stability of the HD+RP complex and, thereby, the pathway of synaptic transmission.

CPP 6.13 Tue 17:30 P

Analytical and computational study of advection-diffusion-reaction processes in catalytic fibrous membranes — •Gabriel Sitaru and Stephan Gekle — Biofluid Simulation and Modeling, Theoretische Physik VI, Universität Bayreuth

We investigate the efficiency of multi-step catalytic systems where a reactant species is flown through a set of fibrous catalytic membranes. The complexity of such systems arises from the interplay of three different time scales: advection, diffusion and reaction. A theory based on infinitely long cylindrical catalytic sites is developed for the steady-state of an advection-diffusion limited reaction. Additionally, the time-dependent concentration profiles are computed using a Lattice-Boltzmann based solver for both the advection-diffusion-reaction and the Navier-Stokes equations. The comparison shows a good agreement between the theory and the numerical results in the intermediate and high Péclet regimes. Both methods can be easily used to predict the efficiency of a multi-step catalysis in fibrous membranes with various geometries.

CPP 6.14 Tue 17:30 P

BoltzmaNN: Predicting effective pair potentials and equations of state using neural networks — •Fabian Berressem and Arash Nikoubashman — Johannes Gutenberg University, Mainz

Neural networks (NNs) are employed to predict equations of state from a given isotropic pair potential using the virial expansion of the pressure. The NNs are trained with data from molecular dynamics simulations of monoatomic gases and liquids, sampled in the NVT ensemble at various densities. We find that the NNs provide much more accurate results compared to the analytic low-density limit estimate of the second virial coefficient and the Carnahan-Starling equation of state for hard sphere liquids. Furthermore, we design and train NNs for computing (effective) pair potentials from radial pair distribution functions, g(r), a task that is often performed for inverse design and coarse-graining. Providing the NNs with additional information on the forces greatly improves the accuracy of the predictions since more correlations are taken into account; the predicted potentials become smoother, are significantly closer to the target potentials, and are more transferable as a result.

CPP 6.15 Tue 17:30 P

Establishment of a workflow and comparison of scattering data driven molecular dynamics simulations for two water models — •Veronika Reich[1], Sebastian Busch[1], and Martin Müller[2] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon, Lichtenbergstr. 1, 85748 Garching bei München, Germany — [2]Institute of Materials Physics, Helmholtz-Zentrum Hereon, German Engineering Materials Science Centre (GEMS) and Heinz Maier-Leibnitz Zentrum (MLZ)

Molecular dynamics simulations are increasingly used to evaluate scattering data. For many systems, reliable force fields are available that yield simulations which are compatible with the measured data. For many other systems, however, the agreement between simulation and experiment is not satisfactory yet. In this work, we aim to couple measured and simulated data on the example of different liquid water models in order to optimize force fields.

Two water models, TIP3P and TIP4P/2005, were first simulated by molecular dynamics simulations with the program LAMMPS and further the program SASSENA was used to calculate the corresponding scattering signals. The outcomes were compared to already existing experimental data and changes in the underlying force fields where evaluated in terms of their impact on the behaviour of the simulation.

CPP 6.16 Tue 17:30 P

Ground- and excited-state properties of tetraphenyl compounds from first-principles calculations — •Kevin Eberheim, Christof Dues, and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Tetraphenyl compounds with formula $X(C_6H_5)_4$ (X being a tetravalent atom of the 14_{th} group such as C, Si, Ge, Sn, Pb), crystallize either in a tetragonal crystalline structure or in an amorph phase [1]. Depending on their habitus, the compounds are characterized by very different optical properties. The molecular crystals are known for their second harmonic generation (SHG) properties, while the amorph phase is a white light emitter. Tetraphenyl molecules feature indeed the delocalized π-orbitals, which have been proposed as a prerequisite for the white-light generation [2]. In an attempt to understand the mechanisms related to the white light emission, we model the structural, electronic and vibrational properties of different $X(C_6H_5)_4$ structures within density functional theory. The calculated structural parameters closely reproduce the measured values, however vdW corrections are crucial for a correct description of the structural properties. This confirms that dispersion forces are responsible for the intermolecular bonds in the compound. Different implementations of the vdW forces lead to very similar results. Calculated vibrational properties are in agreement with measured Raman spectra. [1] A Kitaigorodsky, Molecular crystals and Molecules, Acad. Press (1973). [2] Nils W. Rosemann et al., J. Am. Chem. Soc. 138, 16224 (2016), Science 352, 1301 (2016).

CPP 6.17 Tue 17:30 P

Polymer Architectures by Chain Walking Catalysis - Topological Transition From Linear Chains to Dendrimers — •Ron Dockhorn[1], Laura Plüschke[1], Albena Lederer[1], Jan Merna[3], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany — [3]University of Chemistry and Technology Prague, CZ-16628 Praha, Czech Republic

Chain walking (CW) catalysis is a unique approach to synthesize dendritic polyethylenes by a "walking" Pd-α-diimine catalyst into a variety of complex branch-on-branch architectures. Coarse-grained Monte Carlo simulations utilizing the bond fluctuation model of the CW process are performed to investigate the influence of the walking mechanism on the polymer topology. Two distinct regimes can be identified: For low walking rates the structure growths with linear chain extension and low amounts of side chains, whereas high walking rates promote random and isotropic dendritic growth of the molecule. The transition regime is characterized by large amount of branched side chains reflecting a cross-over regime with characteristics of disordered dendronized bottle-brushes controllable by the walking rate of the catalyst. SANS experiments of the CW-polymerized ethylenes are compared to simulation data verifying the observed macro-conformational transitions. The CW one-pot preparation setup tunable by external parameters provides a powerful synthesis route to create dendrigrafts / dendronized polymers.

CPP 6.18 Tue 17:30 P

Aggregation of several flexible-semiflexible block-copolymer chains: flat histogram Monte Carlo simulation — •Viktor Ivanov[1,2], Ekaterina Kruglova[2], Julia Martemyanova[2], Timur Shakirov[1], and Wolfgang Paul[1] — [1]Martin-Luther-University Halle-Wittenberg, Institute of Physics, 06099, Halle, Germany — [2]Lomonosov Moscow State University, Faculty of Physics, 119992 Moscow, Russia

We study conformational properties of a single multi-block copolymer chain consisting of flexible (F) and semi-flexible (S) blocks with equal composition of F- and S-units and with different affinity to a solvent, as well as the aggregation of several such chains. We perform flat histogram Monte Carlo simulations based on the stochastic approximation Monte Carlo (SAMC) algorithm. We use the two-dimensional density of states, which depends on the energy of intramolecular stiffness and on the energy of non-valence interactions. We present data on different non-trivial globular morphologies, including several structures with high orientational ordering of bonds. Pseudo-phase diagrams in variables temperature vs. stiffness parameter are presented for different values of the block length. We also present our recent results on the aggregation behaviour of several FS-block-copolymer chains and discuss the possibility of shape-persistent aggregation of globules. We acknowledge the financial support from RFBR (grant 19-53-12006-NNIO-a) and DFG (project PA 473/18-1) and thank Moscow State University Supercomputer Center for providing the computational resources.

CPP 6.19 Tue 17:30 P

Crystallization of oligomers in melts between two hard walls: flat histogram Monte Carlo simulation — •Evgeniia Filimonova, Timur Shakirov, and Viktor Ivanov — Martin-Luther-University Halle-Wittenberg, Institute of Physics, 06099, Halle, Germany

We study conformational properties of short polymer chains in melts between two hard walls. Our final goal is to reveal physical factors which are responsible for a particular scenario of surface-induced polymer crystallization (e.g., the nucleation and growth or the 1st order prefreezing). We use a coarse-grained model and perform flat histogram Monte Carlo (MC) simulations based on the stochastic approximation Monte Carlo (SAMC) algorithm. We analyse different order parameters: nematic orientational order parameter, bond orientation order parameters (Steinhardt parameters), hexagonal order parameter (which shows a quasi-two-dimensional stacking of chain cross sections in a plane perpendicular to the director). We see the nematic transition (formation of rotator phase) upon cooling, followed by a crystallization transition. We are able to observe a coexistence of an isotopic structure in the center of the film with ordered structures at the walls at intermediate values of energies (in microcanonical analysis). We are able to localise the transition points between different pseudo-phases quite precisely. Financial support of the International Graduate School AGRIPOLY supported by the European Social Fund (ESF) and the Federal State Saxony-Anhalt is acknowledged.

CPP 6.20 Tue 17:30 P

Pressure and temperature-dependent changes in the microstructure of linear mono-ols — •Jennifer Bolle[1], Alexander Faulstich[1], Martina Požar[2], Aurélien Perera[3], Michael Paulus[1], Metin Tolan[1], and Christian Sternemann[1] — [1]Fakultät für Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]University of Split, Faculty of Science, Rudera Boškovića 33, 21000, Split, Croatia — [3]Sorbonne Université, Laboratoire de Physique Théorique de la Matière Condensée, 4 Place Jussieu, F75252, Paris. cedex 05, France

Hydrogen bonds are essential for understanding the microscopic structure of water, aqueous solutions and associated fluids in general. They stabilize the structure of peptides and proteins and are the driving force for association in molecular fluids. In this study, the evolution of the microstructure of a series of linear monohydroxy alcohols (mono-ols) with temperature and pressure was investigated by X-ray diffraction at beamlines BL2 and BL9 of the synchrotron radiation source DELTA (TU-Dortmund, Germany). Comparing the behavior of the so-called pre-peak in the diffraction patterns of the mono-ols with increasing chain length, the influence of steric hindrance on the charge order of these liquids was systematically studied. The results are compared with calculated diffraction intensities based on molecular dynamics simulations and interpreted on the basis of changes in their microstructure. We observe that the charge order for all the studied alcohols is significantly affected by pressure and temperature and strongly depends on chain length.

CPP 6.21 Tue 17:30 P

Systematic derivation of hydrodynamic equations for viscoelastic phase separation — •Burkhard Duenweg[1], Dominic Spiller[1], Maria Lukacova[2], Aaron Brunk[2], Herbert Egger[3], and Oliver Habrich[3] — [1]MPI for Polymer Research Mainz — [2]Mathematics, JGU Mainz — [3]Mathematics, TU Darmstadt

We present a simple hydrodynamic two-fluid model aiming at the description of the phase separation of polymer solutions with viscoelastic effects. It is directly based upon the coarse-graining of a molecular model (such that all degrees of freedom have a clear molecular interpretation), and a free-energy functional. The dynamics is split into a conservative and a dissipative part, following the GENERIC formalism. In a first step, we derive an extended model where inertial dynamics of the macromolecules and of the relative motion of the two fluids is taken into account. In the second step, we eliminate these inertial contributions and, as a replacement, introduce phenomenological dissipative terms. The final simplified model is similar, though not identical, to models that have been discussed previously. In contrast to the traditional two-scale description that is used to derive rheological equations of motion, we here treat the hydrodynamic and the macromolecular degrees of freedom on the same basis. Notably, we find a rheological constitutive equation that differs from the standard Oldroyd-B model. This difference may be traced back to a different underlying statistical-mechanical ensemble that is used for averaging the stress.

CPP 6.22 Tue 17:30 P

Controlling the dynamics of soft, coarse-grained polymer fluids at surfaces — •Pritam Kumar Jana[1], Petra Bacova[2], Ludwig Schneider[1], Vangelis Harmandaris[2], Patrycja Polinska[3], Craig Burkhard[4], and Marcus Müller[1] — [1]Institute for Theoretical Physics, University of Goettingen — [2]Institute of Applied and Computational Mathematics, Foundation for Research and Technology-Hellas, Heraklion, Greece — [3]Goodyear S.A., Colmar-Berg L-7750, Luxembourg — [4]The Goodyear Tire and Rubber Company, Akron, Ohio 44305, United States

The rheological properties of composites derived from fillers in a polymer matrix depend on particle size, filler loading, and dispersion, as well as the interfacial interaction between the fillers and polymer matrix. For the coarse-grained modeling of such systems, it is crucial to pay attention to the fluid flow past the solid filler surface because the classical no-slip hydrodynamic boundary condition does not hold on the micro-and nanoscopic length scale. Instead, the flow is characterized by a microscopically small but finite slip length. To explore the dynamics and slippage, we perform both atomistic and highly coarse-grained (hCG) simulations. In the atomistic simulations, we study the dynamics of polybutadiene close to a silica surface. In the hCG scale, since the solid surface appears smooth, special simulation techniques are required to generate friction at the solid-fluid contact and control slippage. We devise a simulation strategy that can reproduce the dynamics of the polymers close to the wall as seen in the atomistic simulations. The parametrized hCG model, which is devised by comparison with the atomistic simulations, allows the exploration of the dynamics and slippage of polymers with a wide range of molecular weights.

CPP 6.23 Tue 17:30 P

Molecular origins of shear-thinning in polymer melts — •Ranajay Datta, Friederike Schmid, and Peter Virnau — Institute of Physics, Johannes Gutenberg University, Staudingerweg 9, 55128 Mainz, Germany

We investigate the molecular origin of shear-thinning in melts of flexible, semiflexible and rigid oligomers with coarse-grained simulations of a sheared melt [1]. Emergence of entanglements and nematic phases in equilibrium, alignment, stretching and tumbling modes or suppression of the latter all contribute to understanding how macroscopic flow properties emerge from the molecular level. By performing simulations of single chains in shear flow, we identify which of these phenomena are of collective nature and arise through interchain interactions and which are already present in dilute systems.

Reference:
[1] https://arxiv.org/abs/2101.03645v2

CPP 6.24 Tue 17:30 P

Phase behavior of randomly crosslinked diblock copolymers — •Gaoyuan Wang, Annette Zippelius, and Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Deutschland

We have investigated the structure and the phase behavior of randomly crosslinked polymer networks formed by connecting symmetric diblock copolymers via covalent bonds. Particle-base Monte-Carlo simulation is applied to study the order-disorder transition, controlled by the Flory-Huggins parameter χ. We provide an accurate phase diagram, in which the $\chi_c N$ of the ODT is shown as a function of the crosslink density p and Flory-Huggins parameter of the preparation state $\chi_p N$. Depending on $\chi_p N$, the random crosslinks support the disordered or periodically ordered state over a larger range of incompatibilities (χN), because the irreversible bonds impart a memory of the structure that existed at their formation. Knowing the amount of crosslinking required to retain a microphase-separated or disordered structure at a χN that considerably differs from the preparation state is helpful for generating desired states, which may only be metastable without crosslinks.

CPP 6.25 Tue 17:30 P

Understanding the structure of reversible networks made of star polymers — •Kiran Suresh Kumar[1,2], Toni Müller[1,2], Jens-Uwe Sommer[1,2], and Michael Lang[1] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Hohe Strasse 6, 01069 Dresden, Germany — [2]Institute für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden, Germany

Bonds in reversible networks break and form continuously allowing the material to flow and self-heal on long time scales while being a solid on short times. Recent work utilized a regular star branched architecture in combination with a controlled pairwise association of reversible groups to reveal the impact of network defects on the material properties [1-4]. We develop a model for network structure by combining previous work on network defects in irreversible networks [5] with the method of balance equations [6] for reversible systems. The model predictions for the frequency of different star types are tested by Monte Carlo simulations of network structure.

[1] Rossow, T.; Habicht, A.; Seiffert, S. Macromolecules 2014, 51, 6473-6482. [2] Tang, S.; Wang, M.; Olsen , B. D. J. Am. Chem. Soc. 2015, 137, 3946-3957. [3] Tang, S.; Habicht, A.; Li, S.; Seiffert, S.; Olsen, B. D. Macromolecules 2016, 49, 5599-5608. [4] Ramirez, J.; Dursch, T. J.; Olsen , B. D. Macromolecules 2018, 51, 2517-2525. [5] Lang, M.; Schwenke, K.; Sommer, J.-U. Macromolecules 2012, 45, 4886- 4895. [6] Lang, M.; Kumar, K. S. Macromolecules 2021, 10.1021/acs.macromol.1c00718.

CPP 6.26 Tue 17:30 P

Thermal transport of epoxy networks: Bond engineering and network microstructures — •Manjesh Kumar Singh[1] and Debashish Mukherji[2] — [1]Department of Mechanical Engineering, Indian Institute of Technology Kanpur, Kanpur: 208016, Uttar Pradesh, India — [2]Quantum Matter Institute, University of British Columbia, Vancouver BC V6T 1Z4, Canada

Thermal transport coefficient (k) is a central property of condensed matter systems, where establishing the molecular level understanding is extremely important to tailor the materials properties for their possible uses under extreme environmental and practical conditions. Here polymers are an important class of materials because they provide different pathways for the energy transfer. For example, the heat flow between the two covalently bonded monomers is over 100 times faster than between the two non-bonded monomers [1]. Therefore, the delicate balance between these two contributions often provides a guiding tool for the design of tailor made polymeric materials with extraordinary thermal properties. Traditionally most studies have investigated k in the linear polymeric materials, the recent interests have also been directed towards the epoxy network. Using molecular dynamics simulations, we investigate the factors effecting k of epoxy networks. We emphasize on the importance of the bond types and their influence on the network microstructures, with a goal to provide a guiding principle for the tunability in k [2].

[1] Bhardwaj et al., ACS Nano 15, 1826 (2021). [2] Mukherji et al., Physical Review Materials 5, 025602 (2021).

CPP 7: Soft Matter (joint session CPP/DY)

Time: Wednesday 10:00–12:45 Location: H3

Invited Talk CPP 7.1 Wed 10:00 H3

Chemically Fueled Out-Of-Equilibrium Self-Assemblies and Autonomous Material Systems — •Andreas Walther — Department of Chemistry, University of Mainz

Living self-organizing systems operate far-from-equilibrium and maintain functions by constant energy dissipation in feedback-regulated adaptive steady states. In stark contrast, man made self-assemblies are typically oriented towards equilibrium or deep metastable states.

Some of the next steps in self-assembling systems are to approach multicomponent co-assembling systems, and to master temporal behavior as well as complex adaptation mechanisms. The latter require new types of internal control mechanisms, such as kinetic control over opposing reactions (built-up/destruction), the integration of feedback mechanisms, or the use of energy dissipation to sustain structures only as long as a chemical fuel is available. This ultimately goes along with a transition towards out-of-equilibrium complex systems, in which multiple components self-assemble dynamically in a non-linear and adaptive fashion.

In this talk I will present two conceptual pathways towards out-of-equilibrium systems, (i) driven environments and (ii) driven structures, which allow to program self-assemblies and materials with lifetimes and programmable steady state dynamics using feedback mechanisms and conversion dynamics of chemical fuels. This will be showcased for different self-assembling systems (polymers, peptides, DNA), and the connection to hydrogels and photonic materials demonstrates possibilities for new horizons in materials science.

CPP 7.2 Wed 10:30 H3

UV-light printing on APTES functionalized SiO2 surfaces: New approach for nanoparticle assembly — •Sergii Snegir[1], Olivier Plichery[2], Thomas Huhn[1], and Elke Scheer[1] — [1]University of Konstanz, Konstanz, Germany — [2]INSP, Sorbonne University, France

The 3-Aminopropyl)trimethoxysilane (APTES) terminated SiO2 surface allows creating self-assembled monolayers (SAMs) of gold nanoparticles (AuNPs). However, further functionalization of AuNPs with thiol-containing molecules leads to their strong aggregation due to the appearance of uncompensated dipole moments on the AuNP. Therefore, we developed a UV-light fixation method, which anchors AuNPs on their initial positions on the APTES surface prior to the process of AuNP functionalization. Herein, we present detailed studies of the passivation efficiency as the function of UV light wavelength, time of exposure, the concentration of O2, N2, O3 gases (1). We have found that the combination of O3 and UV light under ambient atmospheric conditions lead to complete passivation of APTES terminated glass already after 2 min of UV exposure (26.1 mW/cm2). We have tested also the possibility to use the UV-light passivation for printing on APTES terminated surfaces by using different chromium masks. With this method, we can create SAMs of AuNP with different geometry and size (resolution limit several um) on a SiO2 surface (glass/quartz/silicon). 1. S.Snegir, T.Huhn,J. Boneberg, S.Haus, O.Pluchery, E.Scheer, J.Phys.Chem.C, 2020,124(35), 19259-19266.

CPP 7.3 Wed 10:45 H3

In situ GISAXS analysis of printed hybrid diblock copolymer thin films containing mixed magnetic nanoparticles — •Christopher Everett[1], Xinyu Jiang[1], Manuel Scheel[1], Huaying Zhong[1], Martin Bitsch[2], Martina Plank[3], Markus Gallei[2], Matthias Schwartzkopf[4], Stephan V. Roth[4,5], and Peter Müller-Buschbaum[1,6] — [1]TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — [2]Saarland University, LS Polymer Chemistry, Saarbrücken, Germany — [3]TU Darmstadt, Ernst-Berl-Institut, Darmstadt, Germany — [4]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [5]KTH Royal Institute of Technology, Stockholm, Sweden — [6]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany

Diblock copolymer (DBC) thin films that form periodic nanostructures are appropriate scaffolds for magnetic nanoparticles (NPs) and have potential for a variety of applications such as highly functional magnetic sensors and in high-density magnetic data storage. In this investigation, ultra-high molecular weight PS-b-PMMA films are used as templates for both ferrimagnetic magnetite NP and ferromagnetic Ni NPs. The thin films, containing up to 6 wt% NPs, are fabricated by a slot-die coating technique and the morphological evolution of the films during the deposition and drying process is monitored in situ with grazing incidence small-angle X-ray scattering (GISAXS). The dry thin films are subjected to solvent vapor annealing and ordered nanostructured hybrid films are obtained. Using a SQUID magnetometer, the resulting magnetic properties are measured.

15 min. break

Invited Talk CPP 7.4 Wed 11:15 H3

The quest for robust superhydrophobic surfaces — •Robin Ras — Department of Applied Physics, Aalto University, Espoo, Finland

Nature offers various examples of extreme water-repellency, such as the leaves of Lotus plant and wings of cicada. The water repellency allows plants for efficient photosynthesis even in dusty environments, and allows large-wing insects to fly even in humid conditions. Likewise, our technological society could benefit from surfaces that stay clean and dry in challenging conditions. For example, solar cells on roof tops loose efficiency when they are covered with sand and dust.

The extreme water-repellency, also called superhydrophobicity, is attributed to the combination of micro/nanoscale topography and hydrophobic surface chemistry that allows trapping of a thin air film between the water and the solid substrate. The air film effectively shields the water from the solid by reducing the contact area, leading to very high contact angle and very low adhesion and friction. The required topography, however, also makes these surfaces very fragile.

Here I will present the progress made during previous decade, including different strategies for enhancing the mechanical durability. Recently, in collaboration with the group of Xu Deng, we developed an extremely durable superhydrophobic surface, by making use of a microstructured armor that protects the otherwise fragile nanostructures. I will present the concept, and steps that we are taking towards commercialization.

CPP 7.5 Wed 11:45 H3

Calculating Magnetization Fields in Magnetoactive Elastomers: A Cascading Mean-Field Approach — •Dirk Romeis and Marina Saphiannikova — Leibniz Institute of Polymer Research Dresden, Germany

We consider the application of an external magnetic field to a composite of a non-magnetizable elastomer matrix with embedded magnetizable particle inclusions. The resulting interactions are determined by the magnetization field which is generated not only by the external magnetic field but also by the magnetic fields arising due to surrounding inclusions. A comprehensive description requires knowledge about the magnetization of individual particles and of macroscopic portions of the composite. Accordingly, a precise calculation becomes elaborate for a specimen comprising billions of particles. We present a greatly simplified, but accurate approximation for the computation of magnetization fields in such composites. Based on the dipole model, we introduce the cascading mean-field description [1] by separating the magnetization field into three contributions on the micro-, meso-, and macroscale. It is revealed that the contributions are nested into each other, as in the Matryoshka's toy. Our description allows for an efficient and transparent analysis of such composite materials under rather general conditions.

Financial support by DFG, SPP 1713, is gratefully acknowledged.

[1] D. Romeis and M. Saphiannikova: A cascading mean-field approach to the calculation of magnetization fields in magnetoactive elastomers. Polymers, 13(9):1372, 2021.

CPP 7.6 Wed 12:00 H3

Magnetostrictive effects in soft magnetic gels and elastomers — •Lukas Fischer and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

Our work focuses on magnetic gels and elastomers, also known as magnetorheological elastomers or ferrogels, that feature a soft elastic matrix enclosing magnetizable particles. These materials react to an applied external magnetic field mainly in a twofold manner: by changing their overall mechanical properties (magnetorheological effect) and by overall macroscopic deformations (magnetostriction).

We have developed a mesoscopic theory to describe the latter effect. For this purpose, we analytically solve the linear elastic problem, linking the particle scale to the scale of overall deformation. To adjust the deformational response, we modify the initial positioning of the particles inside the material, relative to the magnetic field direction [1].

Specific spatial arrangements of the magnetizable particles inside the elastic medium favor specific magnetostrictive modes of deformation, for example torsion [2]. Targeted modification of the particle size can likewise serve to adjust the magnetostrictive response [3]. Our work supports the construction of magnetically controlled soft actuators that are tailored to requested deformational tasks.

[1] L. Fischer, A. M. Menzel, *J. Chem. Phys.* **151**, 114906 (2019).
[2] L. Fischer, A. M. Menzel, *Phys. Rev. Research* **2**, 023383 (2020).
[3] L. Fischer, A. M. Menzel, *Smart Mater. Struct.* **30**, 014003 (2021).

CPP 7.7 Wed 12:15 H3

Perturbed Jamming transitions — Moumita Maiti[1] and •Michael Schmiedeberg[2] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

By minimizing the interaction energy in a soft sphere system without crossing energy barriers the discontinuous athermal jamming transion can be observed at a packing fraction of about 0.64 in 3D [1]. However, if perturbations like thermal fluctuations [2] or an active self-propulsion [3] are added, the transition becomes continuous and the transition packing fraction might occur at a different density. For example, in case of thermal fluctuations, the transition packing fraction approaches 0.55 in case of small thermal fluctuations [2]. We show that the thermal jamming transition lies within the universality class of directed percolation. As a consequence, athermal jamming is a (singular) limit of a much wider class of perturbed jamming transitions that can also be understood as dynamical transitions [2,4]. Therefore, perturbed jamming transitions open up a large variety of amorphous packings and insights how these packings are related to glassy dynamics.

[1] C.S. O'Hern et al., Phys. Rev. Lett. 88, 075507 (2002), Phys. Rev. E 68, 011306 (2003).
[2] M. Maiti and M. Schmiedeberg, Scientific Reports 8, 1837 (2018).
[3] M. Maiti and M. Schmiedeberg, EPL 126, 46002 (2019).
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CPP 7.8 Wed 12:30 H3

Fluidity models for amorphous glassy materials — •Robin Lautenschlager and Thomas Voigtmann — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

Different rheological models are proposed to describe the complex flow properties of amorphous glassy materials, such as granular materials or colloidal glasses, intermediate between a solid and liquid behavior. These systems show a strong non-linearity due to stresses and strain rates, as well as time-dependent ageing effects. The materials are hence described by a time-dependent local fluidity as a main rheological quantity. Spatial non-localities are quantified by a characteristic cooperativity length that describes the extent over which neighboring material regions influence their flow behavior.

We compare three different approaches of such fluidity models and discuss their key features regarding the complex flow properties and how they try to reproduce the time-dependent effects of such a flow. We probe the models in a pressure driven two-dimensional-channel-flow and compare their long-time numerical results to analytically estimated steady state solutions for this test case. We will discuss how the models respond to different flow properties to evaluate their usability in applications.

CPP 8: Poster Session III

Active Matter (1-2); 2D Materials (3); Biopolymers, Biomaterials and Bioinspired Functional Materials (4-7); Charged Soft Matter, Polyelectrolytes and Ionic Liquids (8-12); Composites and Functional Polymer Hybrids (13); Hydrogels and Microgels (14); Interfaces and Thin Films (15-27); Nanostructures, Nanostructuring and Nanosized Soft Matter (28); Responsive and Adaptive Systems (29-32).

Time: Wednesday 17:30–19:30 Location: P

CPP 8.1 Wed 17:30 P

Janus Particles Self-Assembly: Magnetic and Catalytic Propulsion of Clustered Janus Particles — •Yara Alsaadawi[1], Anna Eichler-Volf[1], Michael Heigl[2], Peter Zahn[1], Manfred Albrecht[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Janus particles are one type of artificial microswimmers consisting of two asymmetrically functionalized surfaces. With proper manipulation, one can control their movement from one point to another at certain velocities, as well as clustering, and orientations. In this work, we prepared Janus particles with caps consisting of Co/Pd, providing magnetic and H2O2 catalytic activity for particle propulsion. Due to their magnetic properties, individual particles undergo self-assembly by cap-cap interactions, forming clusters with varying sizes and shapes. Here, we observed clusters of two- and three-janus particles with standard video microscopy. Furthermore, the influence of external magnetic field on a cluster propulsion was studied, as well as the effect of propulsion next to a wall. We reported varying propulsion trajectories, which in turn depend on the number of particles and the cap-cap arrangement within a cluster.

CPP 8.2 Wed 17:30 P

Analytical study of active semiflexible ring polymer — •Christian Anton Philipps, Roland Georg Winkler, and Gerhard Gompper — Forschungszentrum Jülich Institute of Biological Information Processing, Jülich, Germany

Nature provides a variety of active matter systems, with self-propelled agents consuming internal energy or extracting it from their vicinity for locomotion [1]. Examples on the cellular level are self-propelled semiflexible actomyosin ring-like filaments driven by myosin motors in the cytoskeleton. We present a theoretical study of an active ring polymer [2] with tangential propulsion, applying the continuous Gaussian semiflexible polymer model [3] and introducing periodic boundary conditions. By a normal-mode expansion, the ring polymer conformational and dynamical properties, emerging by the homogeneous active force and its interplay with rigidity, are determined. Remarkably, the ring conformations are unaffected by activity for any stiffness. In contrast to linear filaments, the center-of-mass motion is independent of propulsion. However, activity strongly influences the internal dynamics with a dominant rotational mode over several orders of magnitude in time for high activities. This corresponds to a rotational motion of the entire ring polymer. [1] R. G. Winkler, J. Elgeti, G. Gompper, J. Phys. Soc. Jpn. 86, 101014 (2017); [2] M. Mousavi, R. G. Winkler, G. Gompper, J. Chem. Phys. 150, 064913 (2019); [3] T. Eisenstecken, G. Gompper, R. G. Winkler, Polymers 8, 304 (2016).

CPP 8.3 Wed 17:30 P

Predicting the bulk modulus of single-layer 2D COFs from their molecular building-blocks properties — •Antonios Raptakis[1,2], Alexander Croy[1], Arezoo Dianat[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str.

Two-dimensional Covalent Organic Frameworks (2D COFs) have attracted a lot of interest due to their large range of potential applications. Bottom-up engineering of their molecular building-blocks can lead to novel structures with fine-tuned physical and chemical properties. We have carried out a computational investigation of the elastic properties of different 2D COFs with square and hexagonal lattices. Specifically, the 2D bulk modulus and equivalent spring constants of the respective molecular building-blocks were calculated. Considering the material as a spring network, an analytical model for each topology was derived, which can be used to predict the 2D bulk modulus based on the properties of the monomeric units.

CPP 8.4 Wed 17:30 P

The possibilty of spray coating of lignin and characterization of the thin film — •Sophie Snoke[1,2,3], Constantin Harder[1,4], Wienke Reynolds[2], and Stephan V. Roth[1,5] — [1]Deutsches Elektronen-Synchrotron DESY, 22607, Hamburg, Germany — [2]Lignopure GmbH, 21073 Hamburg — [3]Institute of Thermal Separation Processes, Technische Universität Hamburg-Harburg, 21073, Hamburg, Germany — [4]Lehrstuhl f. Funktionelle Materialien, Physik-Department, Technische Universität München, 85748 Garching, Germany — [5]KTH Royal Institute of Technology, 100 44 Stockholm, Sweden

Lignin is a binding agent in wood and very promissing regarding the sustainable development of new bio-based applications. Therefore, three different lignins were tested for spray coating. The lignin was dissolved in two different solvent mainly in Aceton and Tetrahydrofuran. The structure and morphology as well as the crystallinity of the lignin thin films were investigated by using grazing incidence small-angle and wide-angle X-ray scattering (GISAXS/GIWAXS). Through atomic force microscopy (AFM) the surface morphology and film thickness were characterized. The first goal is to discover possible applications of lignin in thin film applications by the usage of spray coating. The second one is to characterize the moleculare and nonoscale arrangment of lignin in thin films.

CPP 8.5 Wed 17:30 P

Inorganic-organic hybrid nanostructures based on biopolymer templating — •Linus Fidelis Huber and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Inorganic-organic hybrid nanostructures are researched for many different applications. This work is focused on energy conversion through the thermoelectric effect, where electrical current can be generated from a temperature difference. However, the state of the art thermoelectric generators (TEG) often use materials like bismuth (Bi), tellurium (Te), antimony (Sb) or lead (Pb). These materials are toxic and expensive, giving rise to a need for a cleaner and more abundant alternative that still produces good conversion efficiencies. The efficiency of materials to produce thermoelectric power is mainly governed by three factors. The Seebeck coefficient, the electrical conductivity and the thermal conductivity. These parameters can be improved by changing the material morphology. For example, a sufficient percolation network can increase electrical conductivity. Beta-lactoglobulin is a bovine whey bio-polymer, that is known to form different aggregates under different environmental conditions. This material is used to structure and improve the performance of titania films. The differently structured beta-lactoglobulin-titania thin-films are studied with AFM and SEM as well as the Seebeck coefficient, thermal conductivity and electrical conductivity are measured using a 4-point probe setup.

CPP 8.6 Wed 17:30 P

Protein-polysaccharide nanoparticles stabilized by thermal treatment — •Johannes Allwang[1], Yanan Li[1], Stefano Da Vela[2], Dimitris Selianitis[3], Angeliki Chroni[3], Aristeidis Papagiannopoulos[3], and Christine M. Papadakis[1] — [1]Physics Department, Technica University Munich, Garching, Germany — [2]EMBL, DESY, Hamburg, Germany — [3]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

Protein complexes appear in healthy and diseased life forms as well as in food systems and medical applications. Their study can, therefore, give vital insights into biological mechanisms and help understand and treat diseases. Thermal treatment of protein-polysaccharide complexes was shown to create tunable nanoparticles with potential applications as carriers for nutriens and drugs [1].

Here, we investigate nanoparticles from trypsin; a proteolytic enzyme from the small intestine [2]. We use two different polysaccharides: hyaluronic acid and chondroitin sulfate. Synchrotron small-angle x-ray scattering is combined with light scattering methods to get insight into both the internal structure of the particles and their overall size.

[1] A. Papagiannopoulos, E. Vlassi, A. Radulescu, *Carbohydr. Polym.* **2019**, 218, 218

[2] S. Trampari, A. Papagiannopoulos, S. Pispas, *Biochem. Biophys. Res. Commun.* **2019**, 515, 282

CPP 8.7 Wed 17:30 P

Colloidal layer formation and imbibition of colloidal inks on and in thin cellulose films — •Constantin Harder[1,2], Marie Betker[1,3], Alexakis E. Alexakis[3], Andrei Chumakov[1], Benedikt Sochor[1], Elisabeth Erbes[1,4], Marc Gensch[1,2], Qing Chen[1], Julian Heger[2], Jan Rubeck[1], Calvin Brett[1,3], Matthias Schwartzkopf[1], Eva Malmström[3], Daniel Söderberg[3], Peter Müller-Buschbaum[2], and Stephan Roth[1,3] — [1]DESY, Hamburg, Germany — [2]Lehrstuhl für Funktionelle Materialien, TUM, Garching, Germany — [3]KTH, Stockholm, Sweden — [4]Institute for X-ray Physics, Goettingen University, Goettingen, Germany

Layer formation and annealing of nanoparticles especially colloidal inks applied to porous materials is very relevant for functional coatings and printing. The goal is to distinguish and quantify the differences in structure formation during annealing of deposited colloidal inks on a porous material. Therefore, we use layers of cellulose nano fibers (CNF) as porous media. We use novel colloidal inks consisting of poly-butylmethacrylate (PBMA) and poly-sobrerolmethacrylate (PSobMA) in aqueous solution. We studied the deposition and the subsequent structural and morphological changes during annealing of the colloidal layers in real-time. During deposition part of the liquid enters the CNF layer while part of the solvent and the colloids remain on top of the nanopaper surface, leading to a complex drying process. Our results show that the CNF- and colloidal layer will change if the glass transition temperature of the colloids is exceeded.

CPP 8.8 Wed 17:30 P

Conformation and packing of polyanions in polelyectrolyte complexes - a combined PFG and solid-state NMR study — Benjamin Kohn, Carolin Naas, Uwe Lappan, and •Ulrich Scheler — Leibniiz-Institut für Polymerforschung Dresden e.V, Dresden, Germany

Polyelectrolyte complexes find wide applications in surface modificationand controlled drug delivery. In the highly charged states direct ion pairing between polycation and polyanion is expected. The conformation of a weak polyanion depends on pH and ionic strength. The effective charge is determined from electrophoresis NMR, PFG NMR yields the hydrodynamic size as a measure for the conformation. Separating 1H MAS spectra in two-dimensional single-quantum-double-quantum correlation spectra identifies acid protons hydrogen bonded to other acid protons and thus and polyanion-rich regions in the complexes. At low pH this are reduced by a factor of three in the complexes compared to the pure polyanion. At higher pH (high nominal charge) with a more stretched conformation almost none acid-acid contacts are found in the complexes. In the 22Na spectra signals from NaCl and sodium maleate are distinguished and quantified. Even at the highest pH when all of the polyanion is dissociated about one quarter of the sodium is detected in maleate in the complexes. This extrinsic charge compensation shows that in any case there is no straight ion pairing between the polycation and polyanion, phases of pure polyanion remain.

CPP 8.9 Wed 17:30 P

Dielectric spectroscopy on lithium-salt-based deep eutectic solvents — •Arthur Schulz, Peter Lunkenheimer, and Alois Loidl — University Augsburg, Experimental Physics V

Lithium-salt-based deep eutectic solvents, where the only cation is Li+, are promising candidates as electrolytes in electrochemical energy-storage devices like batteries. We have performed broadband dielectric spectroscopy on three such systems, covering a broad temperature and frequency range that extends from the low-viscosity liquid around room temperature down to the glassy state approaching the glass-transition temperature. We observe a relaxational process that can be ascribed to dipolar reorientational dynamics and exhibits the clear signatures of glassy freezing. We find that the temperature dependence of the ionic dc conductivity and its room-temperature value also are governed by the glassy dynamics of these systems, depending, e.g., on the glass-transition temperature and fragility. Compared to previously investigated systems, containing the same hydrogen-bond donors and choline chloride instead of a lithium salt, both the reorientational and ionic dynamics are significantly reduced due to variations of the glass-transition temperature and the higher ionic potential of the lithium ions. These lithium-based deep eutectic solvents partly exhibit significant decoupling of the dipolar reorientational and the ionic translational dynamics and approximately follow a fractional Debye-Stokes-Einstein relation, leading to an enhancement of the dc conductivity, especially at low temperatures.

CPP 8.10 Wed 17:30 P

Poly((trifluoromethane)sulfonimide lithium styrene) as solid polymer electrolyte for lithium-ion batteries — •Fabian Alexander Christian Apfelbeck[1] and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, Physik Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany — [2]Heinz Maier-Leibniz Zentrum (MLZ), Technische Universität München, Garching, Germany

Lithium-ion batteries turned out as an indispensable energy supplier in modern society which however suffers from safety concerns due to the flammability of the liquid electrolyte. Solid polymer electrolytes (SPEs) can bypass this obstacle and therefore represent a serious alternative to conventional electrolytes. Especially single-ion conducting polymers (SICPs), which have the anion covalently bonded to the backbone of the polymer and thus exhibit a theoretical transference number of unity, are of great interest in battery research. This property is especially interesting for lithium metal batteries due to the ability of supressing dendritic growth. In addition to that, these polymers show reasonable high ionic conductivities (10^{-4} S cm^{-1} at room temperature) compared to common electrolytes, what makes commercialization possible. Here, the SICP Poly((trifluoromethane)sulfonimide lithium styrene) (PSTFSILi) with Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) is used as SPE and capillary battery cells are fabricated and tested. This special cell type allows the observation of the structural evolution of the polymer electrolyte during cycling of the battery with small/wide angle x-ray scattering (SAXS/WAXS).

CPP 8.11 Wed 17:30 P

Influence of Mg on the structure and electrolyte/electrode interface in all-solid-state lithium battery — •Yuxin Liang and Peter Müller-Buschbaum — Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany

The interest in all-solid-state lithium battery mainly stems from its high safety and energy density compared with conventional Li-ion batteries. Solid polymer electrolytes (SPEs) as an essential component with high durability, long shelf life, high energy density, great flexibility for cell design and light in weight are considered as the most promising material for the next generation batteries. However, as the most common SPE, poly(ethylene oxide) (PEO) electrolytes have limited electrochemical windows and can react with lithium metal to form a solid electrolyte interphase (SEI), meaning that such SPE is more instable in high-energy-density batteries. Moreover, inhomogeneity at the electrolyte/electrode interface, with or without a SEI, can elicit an irregular lithium plating that leads to dendrite formation, resulting in the cycle life reduction and total cell resistance increase. As a modifying strategy, adding inorganic particles can alter the degree of non-conducting crystalline polymer volume within the electrolyte, promote the dissociation of Li+-TFSI- ion pairs and increase the amount of mobility Li+ ions. Herein, Mg(ClO4)2 is introduced to the PEO electrolyte to modify the structure of SPE and increase the ionic conductivity. Besides, the additive can also assist in constructing a Li+ conducting SEI at the electrolyte/electrode interface.

CPP 8.12 Wed 17:30 P

Poly(propylene carbonate) as a solid polymer electrolyte — •Thien An Pham[1,2], Ralph Gilles[1], and Peter Müller-Buschbaum[1,2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [2]Technische Universität München, Physik- Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany

Li dendrite growth was identified as one of the main obstacles preventing Li metal as anode material in commercial batteries with liquid electrolytes since it can cause short circuits, and, ultimately, generate safety concerns. By using solid polymer electrolytes (SPE), the safety of the lithium-ion battery cell can be increased since they offer higher mechanical stability impeding Li dendrite growth. There has been a lot research on poly(ethylene oxide) (PEO) based SPE for the use with Li metal anodes since it offers high ionic conductivity. However, PEO is only stable up to potentials of 4V and thus, cannot be used with state of the art cathode materials like $LiNi_{1-x-y}Mn_xCo_yO_2$ that normally are operated at voltages above 4V. Aliphatic polycarbonates such as poly(ethylene carbonate) (PEC) or poly(propylene carbonate) (PPC) have intrinsically higher oxidation voltages than PEO making them suitable for high energy cathodes. Here, thin PPC films with different amount of Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) as Li salt are prepared via drop casting method and studied with electrochemical impedance spectroscopy in order to determine the ionic conductivity.

CPP 8.13 Wed 17:30 P

Multi-dimensional morphology control for PS-b-P4VP templated mesoporous iron (III) oxide thin films — •Shanshan Yin[1], Wei Cao[1], Qing Ji[2], Yajun Cheng[2], Lin Song[3], Nian Li[1], Christian L. Weindl[1], Matthias Schartzkopf[4], Stephan V. Roth[4,5], and Peter Müller-Buschbaum[1,6] — [1]Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, 85748 Garching, Germany — [2]Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, 315201, P. R. China — [3]Northwestern Polytechnical University, Xi'an 710072, China. — [4]DESY, Notkestr. 85, 22603 Hamburg, Germany — [5]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden — [6]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany

We systematically investigate the synthesis of polystyrene-block-poly(4-vinylpyridine) templated *-Fe2O3 thin films by changing the solvent category (DMF or 1,4-dioxane) and the polymer-to-FeCl3 ratios. DMF/1,4-dioxane mixtures with different component ratios are also prepared for revealing the effect of the solvent selectivity on the thin film morphology. The structure transition mechanism of the thin films is explained by the preferential affinity and the small-molecule surfactant micelles theory.

CPP 8.14 Wed 17:30 P

Magnetic response of $CoFe_2O_4$ nanoparticles confined in PNIPAM-microgel networks — •Joachim Landers[1], Marcus Witt[2], Juri Kopp[1], Stephan Hinrichs[3], Soma Salamon[1], Birgit Hankiewicz[3], Regine von Klitzing[2], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]Department of Physics, TU Darmstadt — [3]Institute of Physical Chemistry, Hamburg University

Magnetic microgels of $CoFe_2O_4$ nanoparticles embedded in N-isopropylacrylamid (NIPAM) hydrogel exhibit versatile response behavior to external stimuli, combining the characteristic NIPAM volume phase transition (VPT) with tunable response to external magnetic fields determined by the local surrounding of the magnetic nanoparticles. In addition to conventional magnetic microgels, samples modified with allyl mercaptan affecting their swelling behavior were examined regarding their internal structure and magnetization dynamics. For an in-depth analysis of the nanoparticle confinement governing the microgels' magnetic response, detailed mappings of frequency- and temperature-dependence of the microgels' magnetic AC-susceptibility were recorded, enabling the precise resolution of Néel-type and Brownian dynamics as well as the extraction of nanoparticle confinement parameters. We observe a distinct reaction of nanoparticle dynamics across the VPT, showing characteristic differences when comparing conventional and allyl mercaptan - modified microgels. Funding by the DFG via SPP 1681 (project WE 2623/7-3, FI 1235/2-2 and KL 1165/18-1) is gratefully acknowledged.

CPP 8.15 Wed 17:30 P

2D covalent organic frameworks on monolayer MoS2 — •Wenbo Lu[1], Davor Čačpeta[2], Mihaela Enache[1], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Center of Excellence for Advanced Materials and Sensing Devices, Institute of Physics, Bijenička 46, 10000 Zagreb, Croatia

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have received increasing attention as promising materials for different applications. One possibility to precisely tune the electronic and optical properties to the desired applications is based on adsorbing well-ordered organic assemblies on TMDs. Here, a study of on-surface synthesis of 2D covalent organic frameworks (COFs) on monolayer molybdenum disulfide (MoS2) on highly oriented pyrolytic graphite (HOPG) will be presented. Monolayer MoS2 films were synthesized by chemical vapor deposition and transferred to HOPG. The transferred MoS2 was characterized by atomic force microscopy and scanning tunneling microscopy (STM), from which we conclude that the transferred MoS2 is of high-quality with micrometer sized domains. For 2D COF formation, 1,4-benzenediboronic acid (BDBA) was deposited onto the MoS2/HOPG. The structure of the formed 2D COFs was studied via STM. The dehydration of BDBA results in the formation of a long-range ordered honeycomb molecular network on MoS2. Our results show the possibility of using 2D COFs to build up ordered organic/2D TMDs interfaces, which is promising for the fabrication of hybrid organic-inorganic devices possessing tailored properties.

CPP 8.16 Wed 17:30 P

PbS quantum dot solar cells via hybrid interfacial architecture — Huaying Zhong[1], Wei Chen[1,2], and •Peter Müller-Buschbaum[1,3] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]Southern University of Science and Technology (SUSTech), Department of Electrical and Electronic Engineering, 1088 Xueyuan Avenue, 518055 Shenzhen, P.R. China — [3]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Colloidal quantum dots (CQDs) have generated great interest in various optoelectronic devices because of their size-tunable bandgap, low-temperature solution processability. Lead sulfide (PbS) CQDs, with a strong absorption coefficient and large Bohr radius, enable solar cells to harvest infrared photons of the solar spectrum beyond the absorption edge of crystalline silicon and perovskites. There have been many strategies to improve device performance, among which interface engineering is a promising method. Excellent interface engineering is designed to form an energy cascade to enable an efficient charge transfer and promote exciton dissociation. Moreover, it can also offer good interfacial contact and improve device air stability by selecting appropriate materials. Here, we use phenyl-C61-butyric acid methyl ester (PCBM) as the interlayer between QDs and electron transport layer, and additive into PbS CQD solution to fabricate PbS QD solar cells and study the trap densities and charge transport process at QDs interfaces.

CPP 8.17 Wed 17:30 P

Mesoporous ZnO thin films templated by diblock copolymer for photovoltaic applications — •Ting Tian and Peter Müller-Buschbaum — Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

Mesoporous ZnO thin films have received tremendous attention in photovoltaic applications in view of their high electron mobility, high transparency, high surface area, and the superior ability to host the light-harvesting dyes and the organic molecular hole-transporters. Considering the morphology-dependent device performance, a precise control over the ZnO nanostructures is indispensable. Among the existing synthesis routes, the diblock copolymer assisted sol-gel approach has been corroborated to be powerful and promising in morphology tunability. Benefiting from the solution processability, this wet chemical method can be integrated into industry-based processes and thus achieve large-scale, high-throughput production. In the present work, an amphiphilic diblock copolymer is used as the structure-directing agent and slot-die coating is applied as the deposition technique to fabricate the mesoporous ZnO films. Effects of ZnO precursor variables on morphological evolution of mesoporous ZnO films are systematically investigated. The tailored nanostructures on the film surface are detected by surface-sensitive scanning electron microscope (SEM), and the inner morphologies are probed by GISAXS.

CPP 8.18 Wed 17:30 P

Sol-gel based tailored lithium-ion battery electrodes — •Ivana Pivarníková[1,2], Ralph Gilles[1], and Peter Müller-Buschbaum[1,2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany — [2]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Silicon (Si) based materials have been considered one of the most promising candidates for the next-generation lithium-ion battery anodes. The aim of this work is the usage of copolymer assisted sol-gel synthesis of mesoporous silica thin films for anode application. This wet chemical method consists of the formation of the organic-inorganic composites by a self-assembly mechanism, where the organic phase (PEO-b-PPO-b-PEO non-ionic triblock copolymer) serves as a template for the inorganic structure (SiOx). The tetraethoxysilane (TEOS) is used as a Si precursor. The solution mix is coated onto the cleaned Si substrates and the template removal is done by calcination at high temperature (400 °C). The properties of the thin films can be tuned by adjusting the synthesis conditions such as concentration of reaction compounds, choice of the deposition technique or choice of the final calcination step. The aim is to reach the desired thickness, porosity, conductivity and mechanical stability for the successful Li-ion battery anode application. Thin films are characterized by scanning electron microscopy (SEM), grazing incidence small-angle X-ray scattering (GISAXS), profilometry and ellipsometry measurements.

CPP 8.19 Wed 17:30 P

The influence of toluene in an Si/Ge sol-gel approach — •Christian L. Weindl[1], Christian Fajman[2], Michael A. Giebel[2], Matthias Schwarzkopf[3], Stephan V. Roth[3,4], Thomas F. Fässler[2], and Peter Müller-Buschbaum[1,5] — [1]Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]Lehrstuhl für Anorganische Chemie mit Schwerpunkt Neue Materialien, Chemie Department, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Notkestr.85, 22607 Hamburg, Germany — [4]Royal Institute of Technology KTH, Teknikringen 34-35, 10044 Stockholm, Sweden — [5]Heinz Maier-Leibniz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The latest research has revealed promising results for Silicon (Si) and Germanium (Ge) as anode materials for lithium-ion batteries (LIBs). Owing to their high energy capacity these two group 14 semiconductors are considered as auspicious alternatives to graphite anodes in LIBs. In this study, we set the goal of synthesizing a porous silicon-germanium structure over a well-known wet chemical sol-gel approach. Here, the amphiphilic diblock copolymer polystyrene-block-polyethylene oxide (PS-b-PEO) is used as the structuring agent. In the experiment, we investigate the structural difference that occurs when toluene is used as an additive. Real-space data as SEM and EDX spectroscopy will be discussed with reciprocal-space analysis methods as GISAXS.

CPP 8.20 Wed 17:30 P

Investigation of Au(100) and Au(110) surfaces in electrolyte by Reflection Anisotropy Spectroscopy (RAS) — •Mario Löw[1], Margot Guidat[1], Timothée Gômes[1,2], Jongmin Kim[1], and Matthias M. May[1] — [1]Ulm University, Institute of Theoretical Chemistry, D-89081 Ulm — [2]Chimie Paristech - PSL, F-75005 Paris

Rechargeable magnesium batteries will probably play a huge role in the future of the battery market. However, there is until now no standard cathode material, like for lithium ion batteries. One possible material could be the porphyrin molecule CuDEPP.[1]

To get a deeper knowledge on how the structure of this molecule changes while applying a voltage, its adsorption on the well-ordered Au-surfaces is studied by Reflection Anisotropy Spectroscopy (RAS). This technique allows to investigate the structure of the interface while applying potentials in the electrolyte.

As a starting point for this investigation, we first establish the surface of the well-ordered Au-surface with RAS (in electrolyte) as a reference. Then we relate this spectra to electronic structure models via computational spectroscopy to understand chemical and physical processes that occur at the electrochemical double layer. Here, we show first results employing the approach.

[1] Abouzari-Lotf, Ebrahim, et al. ChemSusChem 14.8 (2021): 1840-1846.

CPP 8.21 Wed 17:30 P

Tuning the electronic and magnetic properties of graphene with periodically arranged metal-organic coordination networks — •Qiankun Wang, Brian D. Baker Cortés, Joris de la Rie, Mihaela Enache, and Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

Here, we investigated by means of scanning tunneling microscopy and photoelectron spectroscopy how the electronic properties of graphene are modified upon deposition of 5,10,15,20-tetra(4-pyridyl)porphyrin (H2TPyP) with and without coordination to Co atoms. Graphene was prepared on Cu(111) via chemical vapor deposition, and it is known to be n-type doped. We will discuss (i) the transition of the H-bonded self-assembled H2TPyP network into a long-range ordered metal-organic coordination network (MOCN) upon Co deposition and (ii) the electronic level alignment at the graphene/MOCN interface and how this is influenced by the underlying substrate. Our study provides a viable possibility for the usage of graphene as a charge and spin transport material in future electronic and spintronic applications.

CPP 8.22 Wed 17:30 P

bias- and concentration-dependent switching of supramolecular nanostructures at the solid-liquid interface — •Baoxin Jia[1], Mihaela Enache[1], Sandra Miguez-Lago[2], Milan Kivala[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Institute of Organic Chemistry, University of Heidelberg, Germany

Research into the controlled switching between different molecular phases at the solid-liquid interface induced by an external electric field has gained increasing attention over the past years. Here we discuss the bias- and concentration-dependent switching of a carboxy-functionalized triarylamine derivative at the nonanoic-HOPG interface studied by scanning tunneling microscopy. For a fully saturated solution, a porous phase (chickenwire) was observed for negative sample bias and a close-packed phase for positive sample bias. For a 50% saturated solution, a second porous phase (flower) coexisted with the chickenwire phase at negative sample bias, while the close-packed phase was still observed at positive sample bias. For a 20% saturated solution, the two porous phases and the close-packed phase coexisted at positive sample bias because of the low molecule concentration in the solution, while the two porous phases were observed at negative bias. For all concentrations investigated, by changing the polarity of bias voltage, a reversible phase transformation between the porous phases to the close-packed phase was accomplished. Our study demonstrates that controlled structural changes can be accomplished by changing the polarity of the applied external field.

CPP 8.23 Wed 17:30 P

Phase Transitions in Disordered Mesoporous Solids: Effect of Geometric Disorder — •Henry R. N. B. Enninful, Dirk Enke, and Rustem Valiullin — Leipzig University, Leipzig, Germany

Majority of porous solids used in industrial processes such as energy storage, separations and catalysis possess structural disorder over varying length scales. These disorder effects strongly affect the properties of the confining fluids in the pores. Hence, detailed quantification of structural disorder with correlation to fluid phase behavior is a necessary step towards optimization for practical applications.

Employing the serially connected pore model, (SCPM), we have determined the impact of a number of disorder-related parameters, including effect of pore chain length, *powder effect* and interconnectivity effect on phase transitions in disordered mesopore spaces. Additionally, we have showed experimental results from solid-liquid phase transitions obtained by NMR cryoporometry and gas-liquid transitions observed from nitrogen sorption experiments to corroborate the theoretical predictions from the SCPM.

We conclude that, the SCPM has the potential of explaining many features of experimentally observed phase transitions in disordered mesoporous solids.

References [1] Enninful et 2020, Microporous and Mesoporous Materials 309, 110534. [2] Enninful et 2021, Langmuir 37, 12, 3521*3537.

CPP 8.24 Wed 17:30 P

Real-time observations of alkali metal doped 6-Phenacene films — •Matthias Zwadlo[1], Jakub Hagara[2], Giuliano Duva[1], Jan Hagenlocher[1], Alexander Gerlach[1], Martin Hodas[1], Alexander Hinderhofer[1], Peter Siffalovic[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Institute of Physics, Slovak Academy of Sciences Bratislava, Slovakia

The characterization of growth and structure formation in molecular und hybrid e.g. doped systems is an important topic in fundamental organic semiconductor research. In order to study and influence this process different real-time methods have to be used [1]. The growth and structure formation of pure 6-Phenacene as well as the effects of potassium, caesium and rubidium doping were investigated. Thin films of pure 6-Phenacene have been grown in ultra-high vacuum (UHV) and investigated with x-ray, AFM and optical methods. Furthermore, in-situ GIWAXS measurements were performed at PETRA 3 P03. Results on 6-Phenacene as well as preliminary doping results have been published [2]. Doping shows small distortions in crystal structure as well as optical spectra which are yet under investigation and will allow us to get a better understanding on the structural behavior and growth process in theory and experiment.

[1] Hosokai, T., et al., Appl. Phy. Lett. , 97(6), 9 (2010) doi:10.1063/1.3478450
[2] Zwadlo, M., et al., Adv. Optical Mater. (2021), 9, 2002193. doi:/10.1002/adom.202002193

CPP 8.25 Wed 17:30 P

Spray-deposited anisotropic ferromagnetic hybrid polymer films of PS-b-PMMA and strontium hexaferrite magnetic nanoplatelets — •Wei Cao[1], Shanshan Yin[1], Andrei Chumakov[2], Matthias Opel[3], Markus Gallei[4], Matthias Schwartzkopf[2], Stephan V. Roth[2,5], and Peter Müller-Buschbaum[1,6] — [1]TU München, Physik-Department, 85748 Garching — [2]DESY, 22607 Hamburg — [3]WMI, Bayerische Akademie der Wissenschaften, 85748 Garching — [4]Saarland University, Chair in Polymer Chemistry, 66123 Saarbrücken — [5]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, 44 Stockholm, Sweden — [6]TU München, MLZ, 85748 Garching

Spray deposition is applied to fabricate anisotropic ferromagnetic hybrid polymer films by controlling the orientation of strontium hexaferrite nanoplatelets inside ultrahigh molecular weight diblock copolymer (DBC) polystyrene-block-poly(methyl methacrylate) films. During spray deposition, the kinetics of structure evolution of the hybrid film is monitored in situ with grazing-incidence small-angle X-ray scattering. The obtained final hybrid film is then solvent annealed inside a closed chamber with tetrahydrofuran to study the influence of solvent vapor annealing (SVA). Due to the rearrangement of the nanoplatelets inside the DBC during SVA, an obvious change in the magnetic behavior of the hybrid film is observed. The hybrid film shows a perpendicular ferromagnetic anisotropy before SVA, which is strongly weakened after SVA. The spray deposited hybrid film appears highly promising for potential applications in magnetic data storage and sensors.

CPP 8.26 Wed 17:30 P

Influence of Chaotropic NaBr on the Swelling Behavior of PNIPMAM Thin Films — •Julija Reitenbach[1], Christina Geiger[1], Peixi Wang[1], Lucas P. Kreuzer[1], Robert Cubitt[2], Viet Hildebrand[3], André Laschewsky[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck- Str. 1, 85748 Garching — [2]Institut Laue-Langevin, 71 Avenue des Martyrs, CS 20156, 38042 Grenoble Cedex 9, France — [3]Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm

Thermoresponsive polymer thin films have gained a lot of attention in the past decades due to their attractiveness for a wide range of applications. A variety of polymer showing LCST- or UCST-type behavior are known, and their transition temperatures can be influenced by various factors such as molar mass, end groups, copolymerization or by the addition of salts. For polymers in aqueous solution, it was found that the folding of polymers can be strongly influenced by the type of salt and this ability follows a trend called the Hofmeister series. While this effect is well known in solution, the influence on the swelling behavior of PNIPMAM thin films has yet to be investigated thoroughly. We aim to elucidate the underlying mechanism by spectral reflectance and time-of-flight neutron reflectometry on a macroscopic scale and by in situ Fourier-transform infrared spectroscopy on a molecular level.

CPP 8.27 Wed 17:30 P

Made2Reflect: A tool for joint analysis of neutron reflectometry data and Molecular Dynamics Simulations of interfaces — •Nebojša Zec[1], Gaetano Mangiapia[1], Hanh Vi Lê[2], Muriel Rovira Esteva[1], Sebastian Busch[1], and Jean-François Moulin[1] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ) Helmholtz-Zentrum Hereon Lichtenbergstr. 1, 85747 Garching bei München, Germany — [2]SMIS beamline, synchrotron Soleil, L'orme des Merisiers Saint-Aubin, BP 48 91192 Gif-sur-Yvette Cedex

Neutron and X-Ray reflectometry are standard methods for the investigation of thin films and interfaces. Data inversion leading to a structural model is rendered difficult by the well known phase problem. Molecular Dynamics Simulations (MD) are another tool used to study interfaces. MD however has problems of its own: convergence issues and validity of the force fields, to name a few. We show here how jointly using MD and reflectometry can help elucidate details of interfacial structures such as those typically encountered in cell membranes, thin polymer films or electrochemistry. We have developed a Python software tool (Made2Reflect) which makes it easy to extract a scattering length density profile from atomistic MD and compute the corresponding reflectivity curve, thereby taking into account all aspects of the sample as well as the experimental effects such as the instrumental resolution. Actual examples will be shown illustrating that this joint method allows to (in)validate structural hypotheses which cannot be tested by means of any one of the techniques used alone.

CPP 8.28 Wed 17:30 P

Fabricating high resolution nanostructures using polymethyl methacrylate and isopropanol water mixtures — •Stephanie Lake[1], Frank Heyroth[2], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, MartinLuther-Universität Halle-Wittenberg, 06120 Halle, Germany

Electron beam lithography (EBL) can produce high resolution structures but has its drawbacks. Compared to photolithography, it takes more time and has lower throughput. An ideal EBL procedure would require lower exposure dose and withstand environmental fluctuations. Establishing a "process window" (PW) quantifies such requirements.

In this poster, we define a primary PW for polymethyl methacrylate (PMMA) during the developer stage. The area dose is varied and the range where there is sufficient development is subsequently identified. Isopropanol (IPA) and water mixtures can decrease the exposure dose needed for full development compared to other standard PMMA developers[1]. Thus, we defined yet another PW by varying the IPA concentration and measuring the aforementioned, primary PW.

From this work, we discovered mixtures of 69% to 77% IPA can require lower exposure doses than pure IPA. With 73% IPA, the required dose can be up to 82.9% less than that for pure IPA. We show it is feasible to use this developer for high resolution structures without compromising reproducibility.

[1]Mohsin, M. A. & Cowie, J. M. G. *Polymer (Guildf).* **29**, 2130-2135 (1988).

CPP 8.29 Wed 17:30 P

A thermoresponsive poly(2-oxazoline)-based molecular brush in aqueous solution: effect of a cosolvent — •Bahar Yazdanshenas[1], Clemens Sachse[2], Stefano Da Vela[3], Rainer Jordan[2], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Garching, Germany — [2]Technische Universität Dresden, Fakultät Chemie und Lebensmittelchemie, Dresden, Germany — [3]EMBL c/o DESY, Hamburg, Germany

Poly(2-oxazoline)s are well-known for their easy and direct synthesis, providing access to well-defined structures, with tunable properties [1]. In this study, a 1 wt% P*i*POx$_{100}$-g-PEtOx$_{17}$ molecular brush with a poly(2-isopropenyl-2-oxazoline) (P*i*POx) thermoresponsive backbone grafted with thermoresponsive poly(2-ethyl-2-oxazoline) (PEtOx) side chains is investigated in water-ethanol solvent mixtures. This densely grafted polymer with functional and biocompatible segments can be attractive for many applications, such as biomaterials.

In aqueous solution of 3 wt% of this molecular brush, lower critical solution temperature (LCST) behavior has been observed with an increase of the brush length upon heating from room temperature to T_{cp} [2]. In water-ethanol solvent mixtures of 1 wt% concentration, Tcp increases with the ethanol fraction. The temperature-dependent structural evolution is investigated using dynamic light scattering and synchrotron small-angle X-ray scattering.

[1] R. Hoogenboom, Angewandte Chemie International Edition, 2009, 48, 7978 [2] J.-J. Kang, C. M. Papadakis et al., Colloid Polym. Sci. 2021, 299, 193

CPP 8.30 Wed 17:30 P

Highly Metastable Switchable Surfaces Based on Polymer Brushes Containing End-Adsorbing Chains — •Markus Koch[1], Dirk Romeis[1], and Jens-Uwe Sommer[1,2] — [1]Institute Theory of Polymers, IPF Dresden, Germany — [2]Institute Theory of Physics, TU Dresden, Germany

We investigate a switchable polymer brush system that responds to external stimuli by adsorbing (hiding) or exposing specific functional groups. Our design enables targeted changes to the properties of a surface, e.g. to change the interactions with the environment or increase the density of functional groups below the brush. The system consists of a monodisperse polymer brush containing a small fraction of end-modified minority chains. The length of these chains differs from the brush and their end groups can adsorb at the grafting surface. We study this system using Scheutjens-Fleer SCF calculations, MD simulations, and analytical theory [1]. The conformational changes of the admixed chains depend on their relative length and the attraction of their end groups to the surface. Based on the free energy profiles of the adsorption transition, we extract free energy barriers, that are in good agreement with our theoretical predictions. The barriers are strongly reduced when the brush is collapsed, for instance, via a solvent change. Thus, the system can be tuned to obtain a reversible or irreversible end-adsorption behavior. Financial support by the DFG, project SO 277/17-1, is gratefully acknowledged.

[1] Koch, M., Romeis, D., Sommer, J.-U., Macromolecules 53 (17), 7356-7368 (2020)

CPP 8.31 Wed 17:30 P

Effect of pressure on the micellar structures of PMMA-b-PNIPAM in aqueous solution — •Pablo A. Álvarez Herrera[1], Geethu P. Meledam[1], Chia-Hsin Ko[1], Bart-Jan Niebuur[1], Shu-Hsien Huang[1], Leonardo Chiappisi[2], Cristiane Henschel[3], André Laschewsky[3], Alfons Schulte[4], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]Universität Potsdam, Institut für Chemie, Potsdam-Golm, Germany — [4]University of Central Florida, Orlando, USA

Amphiphilic diblock copolymers feature self-assembly behavior in aqueous solution. In particular, poly(methyl methacrylate)-b-poly(N-isopropylacrylamide) (PMMA-b-PNIPAM) forms core-shell micelles upon heating above the cloud point (T_{CP}). In aqueous solutions of PNIPAM homopolymers, it was previously found that the dehydration behavior is strongly altered by pressure [1]. We study the effect of pressure on the micellar structure of PMMA-b-PNIPAM in aqueous solution by small-angle neutron scattering (SANS). In temperature-resolved experiments at 0.1 and 75 MPa, we find that the micelles dehydrate and collapse above T_{CP} at low pressure, while the PNIPAM shells remain hydrated, and the micelles form large clusters at higher pressure.

1.B.-J. Niebuur, C. M. Papadakis et al., ACS Macro Lett. 2017, 6, 1180 and Macromolecules 2019, 52, 1942.

CPP 8.32 Wed 17:30 P

Co-nonsolvency behavior of responsive polymers in thin film/vapor systems — •Christina Geiger[1], Morgan Le Dû[1], Anna Lena Oechsle[1], Peixi Wang[1], Suo Tu[1], Robert Cubitt[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Institut Laue-Langevin, 38000 Grenoble, France

After exposure to mixed water/cosolvent vapor, hydrated thin films of stimuli-responsive block copolymers with PNIPAM or PNIPMAM blocks exhibit a co-nonsolvency behavior. In a rapid film contraction, in either system, both water and cosolvent are expelled. Film swelling and contraction kinetics from saturated vapor are investigated in time-of-flight neutron reflectometry (ToF-NR) with simultaneous spectral reflectance (SR). Molecular interactions of the solvent with the respective polymer chains are analyzed with Fourier-transform infrared (FTIR) spectroscopy. In our latest study with PNIPAM, we focus on the swelling behavior in mixed vapors starting not from the hydrated, but from the dry film state. A minimum in reached thickness due to the co-nonsolvency effect is found, which is reversely related to the interaction strength of polymer chains facilitated by the present water/cosolvent ratio.

CPP 9: Active Matter (joint session DY/BP/CPP)

Time: Thursday 11:45–13:00 Location: H2

See DY 12 for details of this session.

CPP 10: Organic Electronics and Photovoltaics, Electrical and Optical Properties (joint session CPP/KFM)

Time: Thursday 13:30–16:15 Location: H3

Invited Talk CPP 10.1 Thu 13:30 H3

Nanophotonic structures by inkjet printing — Yidenekachew J. Donie[1], Qiaoshuang Zhang[1], Guillaume Gomard[1,2,3], and •Uli Lemmer[1,2] — [1]Light Technology Institute, Karlsruhe Institute of Technology (KIT), Germany — [2]Institute of Microstructure Technology (KIT), Karlsruhe Institute of Technology, Germany — [3]present address: Carl Zeiss AG, Eggenstein-Leopoldshafen, Germany

Inkjet printing (IJP) is a versatile method for additive manufacturing of electronic and optoelectronic devices with a typical spatial resolution on the order of 30 microns. For realizing photonic nanostructures using this approach, the deposited materials have to be controlled on a subwavelength length scale. Here, we demonstrate that this can be realized, both, in vertical and in lateral direction. Using the spontaneous phase-separation of two polymers from a common ink, we realize quasi-periodic and disordered assemblies of light scatterers. The phase separated nanostructures feature sizes that can be tuned from a few microns down to the sub-100 nm level. Applications are in the field of photonic sensors and organic optoelectronic devices. An even more precise control is necessary for realizing one-dimensional photonic crystals (dielectric mirrors) by IJP. Such an approach enables digitally controlled dielectric mirror pixels for various opto-electronic applications.

CPP 10.2 Thu 14:00 H3

On the role of interfaces in controlling the molecular orientation in thin films of polythiophenes — •Oleksandr Dolynchuk[1], Philip Schmode[2], Matthias Fischer[1], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Experimental Polymer Physics, Martin Luther University Halle-

Wittenberg, Germany — [2]Applied Functional Polymers, University of Bayreuth, Germany

Directed crystallization on a substrate is a superior method for inducing crystal orientation in many ordered materials. Although a preferred face-one molecular orientation was evidenced in monolayers of poly(3-hexylthiophene) (P3HT) on graphite, a full face-one orientation in thicker P3HT films has not been realized so far. By using surface-sensitive GIWAXS, here we show that thin films of P3HT crystallized on graphene exhibit a double-layered face-on and edge-on crystal orientation with the latter formed on the top surface [1]. We assume that it is a result of two competing interfacial orientations initiated at the interfaces to graphene and vacuum. By increasing the side-chain polarity in poly[3-(6-bromohexyl)]thiophene, the influence of the interface to vacuum can be reduced, resulting in full face-on orientation in films with a thickness of up to 26 nm [1]. Our findings evidence that directed crystallization can be used to control the orientation of semicrystalline conjugated polymers in thin films if interactions with both interfaces are properly taken into account.

[1] Dolynchuk et al. Macromolecules 2021, 54, 5429-5439.

CPP 10.3 Thu 14:15 H3

Molecular Charge Transfer Effects on Perylene Diimide Acceptor and DNTT / DIP Donor Systems — •Nadine Russegger, Alexander Hinderhofer, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

A very important and fundamental process for organic semiconductors is the charge transfer effect between electron donor and electron acceptor molecules in the ground and in the excited state.

In this work, we present a comprehensive investigation on co-crystal formation and charge transfer effects in weakly interacting organic semiconductor mixtures. We choose dinaphthothienothiophene (DNTT) and diindenoperylene (DIP) as donor and several perylene-diimide derivatives with different side chains in the imide position as acceptor molecules (PDIF-CN_2, PDIC3 and PDIC8-CN_2).

For a full structural overview of the resulting mixed co-crystals, the bulk-heterojunction films were evaluated by surface X-ray scattering. The optical and electronic properties of the intermolecular interactions were characterized by optical absorption and photoluminescence. For the various equimolar mixed systems of DNTT as well as DIP and the different perylene-diimide derivatives different charge transfer effects were determined [1].

The results allow us to correlate the structural morphology and the charge transfer effects depending on the side chains and to evaluate the energy levels of the CT complexes in the different mixed systems.

[1] V. Belova et al., *J. Phys. Chem. C*, **2020**, 124, 11639-22651.

CPP 10.4 Thu 14:30 H3

Dynamics in polymer-fullerene blends for photovoltaic applications and the influence of performance enhancing measures — •Dominik M. Schwaiger[1], Wiebke Lohstroh[2], and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien James-Franck-Straße 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active layer due to their superior performance compared to e.g. planar structured devices. In this optically active polymer layer, photons are absorbed, excitons are created, subsequently dissipated at a material interface and hence free charges are provided. A promising low-bandgap electron donor material is the conjugated polymer PTB7. Besides a large number of studies on structure and electrical properties, the level of knowledge about dynamics in this system is very limited. We investigated films of PTB7, the fullerene derivate PCBM and different blends of these two, prepared out of chlorobenzene solutions. Quasielastic neutron scattering experiments were done at the cold neutron time of flight spectrometer TOFTOF (MLZ, Garching) to determine hydrogen dynamics on a pico- to nanosecond timescale. In addition, two well established techniques for performance enhancement in organic photovoltaics, namely the addition of DIO to the casting solution and a methanol posttreatment of the active layer, are applied and their influence on the polymer dynamics is investigated.

CPP 10.5 Thu 14:45 H3

Thermally Evaporated Donor Molecules Well-Suited for Low-Voltage Loss Organic Solar Cells — •Pascal Kaienburg[1], Helen Bristow[2], Anna Jungbluth[1], Irfan Habib[1], David Beljonne[3], and Moritz Riede[1] — [1]Clarendon Laboratory, Department of Physics, University of Oxford, UK — [2]Department of Chemistry, University of Oxford, UK — [3]Laboratory for Chemistry of Novel Materials, University of Mons, Belgium

Novel molecules are key drivers in the development of efficient organic solar cells (OSCs). Device fabrication via solution-casting, mostly of polymer-blends, and thermal evaporation of small molecule blends in vacuum have proven successful. The advent of non-fullerene acceptors (NFAs) in solution processing pushed OSC efficiency by 50%, outpacing the development of vacuum-deposited OSCs.

We take an important first step towards efficient NFA-based evaporated OSCs by demonstrating that donors commonly used in vacuum deposition benefit from being combined with NFAs. We do so by evaporating donors onto solution-cast NFAs and performing in-depth analysis of voltage losses via sensitive EQE and electroluminescence on the resulting bilayer devices. We find that voltage losses of donor/NFA systems are reduced by up to 400mV compared to corresponding donor/C60 systems, without compromising photocurrent.

Together with evaporated OSCs' advantages such as industrial scalability as proven by OLEDs, our findings highlight the technology's potential and stress the need for evaporable non-fullerene acceptors, which - once available - will significantly increase OSC efficiency.

15 min. break

CPP 10.6 Thu 15:15 H3

Cellulose-silver nanoparticle composites for optical applications — Calvin J. Brett[1,2], Björn Fricke[1], Alexandros E. Alexakis[2], Tim Laarmann[1,3], Volker Körstgens[4], Peter Müller-Buschbaum[4,5], Daniel Söderberg[2], and •Stephan V. Roth[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]KTH Royal Institute of Technology, 100 44 Stockholm, Sweden — [3]The Hamburg Centre for Ultrafast Imaging CUI, 22761 Hamburg, Germany — [4]Lehrstuhl f. Funktionelle Materialien, Physik-Department, Technische Universität Muenchen, 85748 Garching, Germany — [5]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität Muenchen, 85748 Garching, Germany

Cellulose nanofibrils (CNF) provide biocompatibility and are emerging candidates for functional composites and for templating organic optoelectronics. Here we present a facile fabrication of biocompatible hybrid thin films with tunable optical responses by establishing a thin film composite of silver nitrate precursor and CNF films. Subsequent thermal annealing induces the transformation of the silver nitrate into metallic silver nanoparticles and their CNF-template assisted growth. Correlating nanoparticle morphology and optical spectroscopy, our results show the ability to tailor the electronic band gap of the silver nanoparticles and thus of the hybrid material by adjusting the time scale of the thermal transformation.

[1] Brett et al., ACS Appl. Mater. Interfaces 13, 27696 (2021)

CPP 10.7 Thu 15:30 H3

Tunability of the Circular Dichroism through Photoluminescent Moiré Patterns — •Olha Aftenieva[1] and Tobias A.F. König[1,2] — [1]Leibniz Institute for Polymer Research Dresden e.V. Hohe Straße 6, 01069 Dresden, Germany — [2]Center for Advancing Electronics Dresden (cfaed) Technische Universität Dresden 01062 Dresden, Germany

In nanophotonics, there is a current demand for ultrathin, flexible nanostructures that are simultaneously easily tunable, demonstrate a high contrast, and have a strong response in photoluminescent polarization. In this work, the template-assisted self-assembly of water-dispersed colloidal core-shell quantum dots into 1D light-emitting sub-micrometer gratings on a flexible substrate is demonstrated. Combining such structures with a light-absorbing metallic counterpart by simple stacking at various angles results in a tunable Moiré pattern with strong lateral contrast. Furthermore, a combination with an identical emitter-based grating leads to a chiroptical effect with a remarkably high degree of polarization of 0.72. Such a structure demonstrates direct circular polarized photoluminescence, for the first time, without a need for an additional chiral template as an intermediary. The suggested approach allows for reproducible, large-area manufacturing at reasonable costs and is of potential use for chiroptical sensors, photonic circuit applications, or preventing counterfeit.

CPP 10.8 Thu 15:45 H3

Ultrafast Energy Conversion in Organic Photovoltaic Materials: First-principles modelling of the prototypical P3HT-PCBM blend heterojunction — •Elisa Palacino-González and Thomas la Cour Jansen — University of Groningen, Faculty of Science and Engineering, Nijenborgh 4, 9747 AG Groningen

One of the reasons behind the low energy conversion efficiency of organic photovoltaic cells has been ascribed to electronic-vibrational dynamics affecting the ultrafast charge separation material upon light absorption. The absence of a comprehensive theoretical description of this process has restrained further advancements in this direction. Here the first step towards this is presented by introducing a first-principles modelling of the key prototype P3HT-PCBM heterojunction system with a realistic description of the blend environment. MD simulations with the GROMOS 53A6 force field are performed to determine structural and dynamical properties of the blend. Representative strongly coupled subsystems of donor-acceptor pairs with a few P3HT-PCBM moieties are selected from the MD structures, with the bright donor state localised on the P3HT molecule and the charge transfer state with a hole on P3HT and the electron on PCBM. Using an electronic basis, the Hamiltonian includes localised excitons and charge transfer states. Excitation energies fluctuating along the MD trajectory are determined using TDDFT and an electrostatic mapping scheme, which are used to define the spectral densities of the system-bath coupling. The resultant molecular Hamiltonian will be used in the quantum dynamical and spectral simulations in the following step.

CPP 10.9 Thu 16:00 H3

Understanding directional charge transfer in a bacterial reaction center: effect of molecular vibrations — •Mario Marques[1] and Linn Leppert[2,1] — [1]Institute of Physics, University of Bayreuth, Bayreuth 95440, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

The primary energy conversion reactions of photosynthesis in purple bacteria occur in the reaction center (RC), a complex structure in which photo-active pigments arranged along two pseudo-symmetric branches mediate excitation and charge transfer. Our previous first-principles calculations of optical excitations in the RC of *Rhodobacter sphaeroides* indicated that charge transfer occurs along both pigment branches, in contradiction with well-established experimental observations that show charge transfer along only one branch. In this work, we use (time-dependent) density functional theory to investigate the influence of molecular vibrations on the excited states of the main RC pigments of purple bacteria, to unravel their role in the directional charge transfer.

CPP 11: Thin Oxides and Organic Thin Films (joint session DS/CPP)

Time: Thursday 15:15–16:15 Location: H5

See DS 7 for details of this session.

CPP 12: Annual General Meeting of the CPP Division (CPP Mitgliederversammlung)

Virtual Zoom Meeting - Report of the current speaker team - Election of the second deputy speaker - Miscellaneous (Link will be available via the CPP newsletter)

Time: Thursday 17:30–18:30 Location: MVCPP

Virtual Zoom Meeting

CPP 13: Molecular Electronics, Hybrid and Perovskite Photovoltaics

Time: Friday 10:00–12:45 Location: H3

Invited Talk CPP 13.1 Fri 10:00 H3

Electron-lattice relaxation effects in halide perovskites — •David A. Egger — Technichal University of Munich, Germany

Halide perovskites (HaPs) have shown great promise as materials for applications in energy and optoelectronic devices owing to their fascinating microscopic properties. Of particular scientific interest is the coupling of electronic to lattice-dynamical properties of HaPs, because a comprehensive understanding of it is key to predicting and further improving charge-carrier and optical transport characteristics. In this talk, I will present our recent theoretical findings on electron-lattice relaxation effects in HaPs. Specifically, using molecular dynamics in conjunction with electronic-structure theory, it will be shown that the soft, polar lattice of paradigmatic HaPs leads to a variety of very interesting electron-lattice relaxation phenomena. These include structural anharmonicities, nonlinear electron-phonon couplings and short-range correlated disorder potentials. It will be demonstrated that these mechanisms are key to a microscopic picture of charge-carrier mobilities and optical absorption properties of HaPs.

CPP 13.2 Fri 10:30 H3

In situ GIXS study on the crystallization and mesoscale film formation of lead-free MBI perovskite on mesoporous titania during spray deposition from a green solvent — •Julian E. Heger[1], Marie Betker[2,3], Constantin Harder[1,3], Benedikt Sochor[3], Christian L. Weindl[1], Matthias Schwartzkopf[3], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany — [2]Royal Institute of Technology KTH, Teknikringen 34-35, 100 44 Stockholm, Sweden — [3]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [4]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Hybrid halide perovskites are highly promising materials in photovoltaics, due to high efficiencies and industrial favorable processability. However, most of the studied systems are based on water-soluble lead and toxic solvents, which lower the broad application within European standards of hazardous materials. Bismuth-based alternatives like methylammonium bismuth iodide (MBI) can offer a green route to lead-free perovskite solar cells on a large scale when synthesized in the comparably non-toxic solvent methyl acetate and processed by industrially applicable spray deposition. In this work, we investigate with in situ synchrotron GIXS the crystallization and mesoscale film formation of MBI perovskite on mesoporous titania during spray deposition, to understand MBI formation on a typical solar cell interface.

CPP 13.3 Fri 10:45 H3

In situ GIWAXS phase and texture tracking of 2-step slot-die coated perovskite — •Manuel Andree Scheel[1], Lennart Klaus Reb[1], Renjun Guo[1], Matthias Schwartzkopf[2], Stephan Volkher Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]DESY, 22607 Hamburg, Germany — [3]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — [4]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite slot-die coating is a promising thin-film deposition technique for organic-inorganic perovskite materials and might lead the way towards commercial high efficient solar cells. Roll-to-roll compatible deposition techniques offer the possibility to combine high production throughput with minimal waste, and offer high customizability at the same time. We investigate the conversion of slot-die coated lead iodide and slot-die coated methylammonium iodide to perovskite by in situ grazing-incidence wide-angle X-ray scattering (GIWAXS). Here, we study the thin-film morphology and texture of the resulting thin film during the annealing process. We track the phase evolution and their respective crystal orientations over time. We find, that the precursor-solvent phase influences the final crystal orientation in the thin-film by acting as a precursor source that controls the level of available precursor material. We also investigate deposition-technique depending differences that can influence thin-film characteristics.

15 min. break

CPP 13.4 Fri 11:15 H3

Perovskite and Organic Solar Cells Generate Power in Space — •Lennart Klaus Reb[1], Michael Böhmer[1], Benjamin Predeschly[1], Sebastian Grott[1], Christian Ludwig Weindl[1], Goran Ivkovic Ivandekic[1], Renjun Guo[1], Christoph Dreissigacker[2], Jörg Drescher[2], Roman Gernhäuser[1], Andreas Meyer[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Garching, DE — [2]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, DE — [3]Heinz Maier-Leibnitz-Zentrum, Garching, DE

Perovskite and organic solar cells have become a hot research topic in the last few years. The lightweight thin-film solar cells are of particular interest for space applications due to their exceptional power per mass, exceeding their inorganic counterparts by magnitudes.

Here, we present the Organic and Hybrid Solar Cells In Space experiment (OHSCIS) and the launch of perovskite and organic solar cells to space for the first time [1, 2]. The mechanical and electronic design of the experiment aims at maximizing the data collection rate and precise measurements. We show that the solar cells operate in space conditions and produce reasonable power per area of up to 14 and 7 mW cm-2, respectively. Also, during a phase being turned away from the Sun, the solar cells produce power from collecting faint Sun-light scattered from Earth. Our results highlight the potential for near-Earth applications and deep space missions of these technologies.

[1] L. Reb et al., Joule 4,1880-1892 (2020), doi.org/10.1016/j.joule.2020.07.004.
[2] L. Reb et al., Rev. Sci. Instrum. 92 (2021), doi.org/10.1063/5.0047346.

CPP 13.5 Fri 11:30 H3

Optimally-tuned range-separated hybrid functionals for accurate molecular excited-state geometries — •Bernhard Kretz and David A. Egger — Technical University of Munich, Germany

Molecular excited-state (ES) potential energy surfaces (PES) obtained by computational methods can shed light on reaction mechanisms and pathways in photocatalytic reactions. These ES PES can be calculated using either time-dependent density functional theory (TD-DFT) or high-level wave-function methods. TD-DFT based calculations are computationally very efficient, but often lack the accuracy achieved by computationally more expensive wave-function methods[1]. Recently, the class of optimally-tuned range-separated hybrid (OT-RSH) functionals[2] was developed which promises to reduce the gap in accuracy.

In our recent work[3], by comparison with high accuracy wave-function data from literature, we assessed the accuracy of TD-DFT and OT-RSH for the excited-state geometries for a selection of organic molecules with varying complexity of their ES PES. We mainly focused on the structural parameters of the lowest-excited singlet states. Our results show that OT-RSH maintains the accuracy of conventional functionals for small molecules, while it improves the description of more complex ES PESs involving charge-transfer states.

[1] C. Azarias, J. Phys. Chem. A, 121, 32, 6122 (2017)
[2] L. Kronik et al., J. Chem. Theory Comput., 8, 5, 1515 (2012)
[3] B. Kretz and D. A. Egger, J. Chem. Theory Comput., 17, 1, 357 (2021)

Invited Talk CPP 13.6 Fri 11:45 H3

Light-actuated colloidal nano- and microparticles — •Cornelia Denz[1], Matthias Rueschenbaum[1], Valeria Bobkova[1], Julian Jeggle[2], and Raphael Wittkowski[2] — [1]Institute of Applied Physics, University of Muenster — [2]Institute of Theoretical Physics, University of Muenster

Propelled colloidal particles constitute biomimetic analogues to natural microswimmers and represent ideal agents for responsive and adaptive soft matter. Among the numerous propulsion mechanisms developed recently to self-propel such nano- and microparticles, light is a most promising stimulus, since it enables a natural spatio-temporal control of the motion, especially for large numbers of the particles, leading to swarming-like behaviour or novel active materials with exceptional properties.

We introduce on the one hand a novel class of such particles that are light-actuated based on symmetry-broken refraction, fabricated by 3d laser printing based on two-photon polymerization. By numerical simulations, we will discuss collective, light-actuated effects including unexpected patterns and transport effects.

On the other hand, we demonstrate that light actuation of a large number of colloidal particles in optical feedback leads to self-organized pattern formation including the superposition of symmetric patterns as hexagons, rolls and squares. We discuss the stability of these patterns and their control.

CPP 13.7 Fri 12:15 H3

Laser-Induced Electronic and Vibronic Dynamics in the Pyrene Molecule and its Cation — •Katherine R. Herperger[1,2], Jannis Krumland[2], and Caterina Cocchi[2,3] — [1]Department of Physics, University of Ottawa, Ottawa, Ontario K1N 6N5, Canada — [2]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin, Germany — [3]Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg, Germany

Among polycyclic aromatic hydrocarbons (PAHs), pyrene ($C_{16}H_{10}$) is widely used as an optical probe thanks to its unique ultraviolet absorption and infrared emission features. In this first-principles study based on real-time time-dependent density-functional theory coupled with the Ehrenfest molecular dynamics scheme, we investigate the sub-picosecond electronic and vibronic response of a pyrene molecule and its cation excited by a coherent ultraviolet Gaussian pulse. The response of both the species is analyzed in terms of electronic population, absorption spectra, and vibrational activity. Combining this knowledge with the symmetry properties of pyrene, we gain insight into the transient response of this molecule to laser perturbation, setting the stage for future studies on larger and more complex PAHs.

CPP 13.8 Fri 12:30 H3

Charge transfer dynamics across the Au/Ferrocene (aq) interface studied by a two photon pump - photovoltage probe scheme — •Manuel Bridger, Zhipeng Huang, Yujin Tong, Oscar Naranjo, Alexander Tarasevitch, Richard Kramer Campen, and Uwe Bovensiepen — University Duisburg/Essen

Photo-excitation at interfaces redistributes electrons between bulk phases on microscopic spatial and ultrafast time scales. Here we employ a two photon pump - photovoltage probe scheme to quantify the relationship of particular resonant optical transitions to interfacial charge redistribution for the case of charge transfer between a gold electrode and ferrocene self assembled monolayer in an electrochemical cell. We access vibrational and electronic excited states of ferrocene with femtosecond pulses of center wavelength 3 μm and 400 nm respectively. Two signals are apparent: a large amplitude voltage transient at 120 ± 80 fs and a small at 4.0 ± 2.7 ps. Control experiments and comparison to similar systems probed in vacuum by 2PPE spectroscopy suggest the former is the result of charge transfer via vibronically coupled ferrocene CH vibration and hybrid ferrocene/Au electronic states and the later charge transfer via vibrationally mediated interfacial polarization. These results imply that stabilising such vibronically coupled states is a useful target for devices that rely on efficient charge transfer at solid/liquid interfaces.

CPP 14: Condensed-Matter Simulations augmented by Advanced Statistical Methodologies (joint session DY/CPP)

Time: Friday 10:00–11:00 Location: H2

See DY 15 for details of this session.

CPP 15: Theory and Simulation (joint session CPP/DY)

Time: Friday 13:30–15:00 Location: H3

Invited Talk CPP 15.1 Fri 13:30 H3

Data-driven protein design and simulation — •Andrew Ferguson — University of Chicago, Chicago, IL, USA

Data-driven modeling and deep learning present powerful tools that are opening up new paradigms and opportunities in the understanding, discovery, and design of soft and biological materials. In this talk, I will first describe an approach integrating ideas from dynamical systems theory, nonlinear manifold learning, and deep learning to reconstruct protein folding funnels and molecular structures from one-dimensional time series in experimentally measurable observables obtainable by single molecule FRET. I will then describe our recent development and application of deep representational learning to expose the sequence-function relationship within homologous protein families and to use these principles for data-driven design of synthetic proteins with new and/or elevated function.

CPP 15.2 Fri 14:00 H3

Are there knots in chromatin? — •Peter Virnau — Institut für Physik, Staudingerweg 9, Johannes Gutenberg-Universität Mainz, 55128 Mainz

The rise of HiC chromosome capture methods has recently enabled low-resolution structures of interphase chromatin [1]. In this presentation I will explain how structures based on single cell contact matrices are obtained from simulations of coarse-grained bead-spring polymer Go models [2]. The role of self-entanglements which naturally occur in this process [2,3] will be critically assessed in the light of theoretical arguments and recent experiments [4].

[1] T.J. Stevens et al, Nature 544, 59-64 (2017). [2] S. Wettermann et al, Comp. Mat. Sci 173, 109178 (2020). [3] J.T. Siebert et al, Polymers 9, 317 (2017). [4] D. Goundaroulis, Biophys. J. 118, 2268-2279 (2020).

CPP 15.3 Fri 14:15 H3

Surface Segregation in Athermal Polymer Blends due to Conformational Asymmetry — •Russell Spencer[1] and Mark Matsen[2] — [1]Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany — [2]University of Waterloo, Waterloo, Ontario, Canada

Monte Carlo simulations are used to investigate the surfaces of athermal blends of stiff and flexible polymers. We vary the bending modulus of the stiff polymers, κ, from zero to the point where the bulk undergoes an isotropic-to-nematic transition. For hard walls characteristic of polymer/solid surfaces, the flexible polymers generally segregate to the surface. However, prior to the bulk transition, there is a surface ordering transition, where a thin nematic layer rich in stiff polymers forms at the surface. On increasing κ further, the thickness of the nematic layer rapidly increases as the bulk isotropic-to-nematic transition is approached. For soft boundaries representative of polymer/air surfaces, a thin layer rich in stiff polymers but without nematic order forms on the outer edge of the surface with a more significant layer rich in the flexible chains beneath. In this case, the nematic layer never appears, and the surface profile evolves continuously with increasing κ.

CPP 15.4 Fri 14:30 H3

Ultra-coarse-graining of homopolymers in inhomogeneous systems — •Fabian Berressem[1], Christoph Scherer[2], Denis Andrienko[2], and Arash Nikoubashman[1] — [1]Johannes Gutenberg University, Mainz — [2]Max Planck Institute for Polymer Research, Mainz

We develop coarse-grained (CG) models for simulating homopolymers in inhomogeneous systems, focusing on polymer films and droplets. If the CG polymers interact solely through two-body potentials, then the films and droplets either dissolve or collapse into small aggregates, depending on whether the effective polymer-polymer interactions have been determined from reference simulations in the bulk or at infinite dilution. To address this shortcoming, we include higher order interactions either through an additional three-body potential or a local density-dependent potential (LDP). We parameterize the two- and three-body potentials via force matching, and the LDP through relative entropy minimization. While the CG models with three-body interactions fail at reproducing stable polymer films and droplets, CG simulations with an LDP are able to do so. Minor quantitative differences between the reference and the CG simulations, namely a slight broadening of interfaces accompanied by a smaller surface tension in the CG simulations, can be attributed to the deformation of polymers near the interfaces, which cannot be resolved in the CG representation, where the polymers are mapped to spherical beads.

CPP 15.5 Fri 14:45 H3

How to accurately estimate the specific heat of liquid polymers? — •Debashish Mukherji[1], Hongyu Gao[2], Tobias P. W. Menzel[2], and Martin H. Mueser[2] — [1]Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada — [2]Department of Materials Science and Engineering, Saarland University, 66123 Saarbruecken, Germany

The field of atomistic simulations of polymers is in a mature stage, yet predictions of specific heat from molecular simulations and successful comparisons with experimental data are scarce if existing at all. One reason for this may be that the internal energy and thus the specific heat cannot be coarse-grained so that they defy their rigorous computation with united-atom models. Moreover, many modes in a polymer barely contribute to the specific heat because of their quantum mechanical nature. Here, we adopt an existing method [1], which defines a specific heat for a harmonic reference, to estimate the specific heat difference between classical and quantum-mechanical systems and use this as a correction factor. Thereby, we predominantly correct the stiff, high-frequency harmonic modes, while leaving the specific-heat contributions of the slow (anharmonic) modes intact [2]. We show how to construct corrections for both all-atom and united-atom descriptions of chain molecules. Corrections computed for a set of hydrocarbon oligomers and commodity polymers deviate by less than kB/10 per particle. The results compare well with experimental data.

[1] Horbach, Kob, and Binder, JPCB 103, 4104 (1999). [2] Gao, Menzel, Mueser, and Mukherji, PRM 5, 065605 (2021).

Thin Films Division
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Overview of Invited Talks and Sessions

(Lecture halls H1, H3, and H5; Poster P)

Topical Talks

DS 5.1	Tue	13:30–14:00	H3	**Single crystal diamond grown by CVD: state of the art, current challenges and applications** — •Jean-Charles Arnault, Samuel Saada, Victor Ralchenko
DS 5.2	Tue	14:00–14:30	H3	**Tuning Semiconductor Mode-Locked Laser Frequency Combs by Gain and Cavity Design** — Stefan Meinecke, •Kathy Lüdge
DS 5.3	Tue	14:30–15:00	H3	**Monolayer-thick GaN/AlN heterostructures for UVB & UVC ranges: technology, design and properties** — Valentin Jmerik, Alexey Toropov, Valery Davydov, •Sergey Ivanov
DS 5.4	Tue	15:15–15:45	H3	**Optical and vibrational properties of layered 2D materials** — •Janina Maultzsch
DS 5.5	Tue	15:45–16:15	H3	**Organic/inorganic low dimensional material systems: Fundamental aspects and device applications** — •Emil List-Kratochvil
DS 6.1	Thu	13:30–14:00	H1	**Exceptional Topology of Non-Hermitian Systems: from Theoretical Foundations to Novel Quantum Sensors** — •Jan Carl Budich
DS 6.2	Thu	14:00–14:30	H1	**In situ fabrication of (Bi,Sb)-based topological insulator - superconductor hybrid devices** — •Peter Schüffelgen
DS 6.3	Thu	14:30–15:00	H1	**Atomic monolayers as two-dimensional topological insulators** — •Ralph Claessen
DS 6.4	Thu	15:15–15:45	H1	**Topological Insulator Lasers** — •Mordechai Segev
DS 6.5	Thu	15:45–16:15	H1	**TBA** — •Morais Smith

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium Advanced neuromorphic computing hardware: Towards efficient machine learning (SYNC)

See SYNC for the full program of the symposium.

SYNC 1.1	Wed	10:00–10:30	Audimax 1	**Equilibrium Propagation: a Road for Physics-Based Learning** — •Damien Querlioz
SYNC 1.2	Wed	10:30–11:00	Audimax 1	**Machine Learning and Neuromorphic Computing: Why Physics and Complex Systems are Indispensable** — •Ingo Fischer
SYNC 1.3	Wed	11:00–11:30	Audimax 1	**Photonic Tensor Core Processor and Photonic Memristor for Machine Intelligence** — •Volker Sorger

SYNC 1.4	Wed	11:45–12:15	Audimax 1	**Material learning with disordered dopant networks** — •Wilfred van der Wiel
SYNC 1.5	Wed	12:15–12:45	Audimax 1	**In-memory computing with non-volatile analog devices for machine learning applications** — •John Paul Strachan

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Attosecond and coherent spins: New frontiers (SYAS)

See SYAS for the full program of the symposium.

SYAS 1.1	Thu	10:00–10:30	Audimax 2	**Ultrafast Coherent Spin-Lattice Interactions in Iron Films** — •Steven Johnson
SYAS 1.2	Thu	10:30–11:00	Audimax 2	**Ultrafast spin, charge and nuclear dynamics: ab-initio description** — •Sangeeta Sharma, John Kay Dewhurst
SYAS 1.3	Thu	11:15–11:45	Audimax 2	**Light-wave driven Spin Dynamics** — •Martin Schultze, Markus Münzenberg, Sangeeta Sharma
SYAS 1.4	Thu	11:45–12:15	Audimax 2	**All-coherent subcycle switching of spins by THz near fields** — •Christoph Lange, Stefan Schlauderer, Sebastian Baierl, Thomas Ebnet, Christoph Schmid, Darren Valovcin, Anatoly Zvezdin, Alexey Kimel, Rostislav Mikhaylovskiy, Rupert Huber
SYAS 1.5	Thu	12:15–12:45	Audimax 2	**Ultrafast optically-induced spin transfer in ferromagnetic alloys** — •Stefan Mathias

Invited talks of the joint symposium Physics of van der Waals 2D heterostructures (SYWH)

See SYWH for the full program of the symposium.

SYWH 1.1	Thu	13:30–14:00	Audimax 2	**Spin interactions in van der Waals topological materials and magnets** — •Saroj Dash
SYWH 1.2	Thu	14:00–14:30	Audimax 2	**Exciton optics, dynamics and transport in atomically thin materials** — •Ermin Malic, Samuel Brem, Raul Perea-Causin, Daniel Erkensten, Roberto Rosati
SYWH 1.3	Thu	14:30–15:00	Audimax 2	**Correlated Electrons in van der Waals Superlattices: Control and Understanding** — •Tim Wehling
SYWH 1.4	Thu	15:15–15:45	Audimax 2	**Exciton manipulation and transport in 2D semiconductor heterostructures** — •Andras Kis
SYWH 1.5	Thu	15:45–16:15	Audimax 2	**Chern Insulators, van Hove singularities and Topological Flat-bands in Magic-angle Twisted Bilayer Graphene*** — •Eva Andrei, Shuang Wu, Zhenyuan Zhang

Sessions

DS 1.1–1.4	Mon	10:00–11:00	H3	**Thin Film Properties**
DS 2.1–2.7	Mon	11:15–13:00	H3	**2D materials and their heterostructures (joint session DS/HL/CPP)**
DS 3.1–3.9	Mon	13:30–16:15	H4	**2D semiconductors and van der Waals heterostructures I (joint session HL/DS)**
DS 4.1–4.27	Tue	10:00–13:00	P	**Poster**
DS 5.1–5.5	Tue	13:30–16:15	H3	**Focus Session: Highlights of Materials Science and Applied Physics I (joint session DS/HL)**
DS 6.1–6.5	Thu	13:30–16:15	H1	**Focus Session: Topological Phenomena in Synthetic Matter (joint session DS/HL)**
DS 7.1–7.4	Thu	15:15–16:15	H5	**Thin Oxides and Organic Thin Films (joint session DS/CPP)**
DS 8	Thu	18:00–19:00	MVDS	**Annual General Meeting of the Thin Films Division**
DS 9.1–9.4	Fri	10:00–11:00	H1	**Focus Session: Highlights of Materials Science and Applied Physics II (joint session DS/HL)**
DS 10.1–10.7	Fri	11:15–13:00	H1	**Focus Session: Highlights of Materials Science and Applied Physics III (joint session DS/HL)**
DS 11.1–11.5	Fri	13:30–14:45	H4	**2D semiconductors and van der Waals heterostructures II (joint session HL/DS)**

Annual General Meeting of the Thin Films Division

Donnerstag 18:00–19:00 MVDS

- Bericht
- Wahl
- Verschiedenes

Sessions

– Invited Talks, Topical Talks, Contributed Talks, and Posters –

DS 1: Thin Film Properties

Time: Monday 10:00–11:00 Location: H3

DS 1.1 Mon 10:00 H3

Ultra-thin lithium fluoride on Ag(100): growth and morphology — •Vladyslav Romankov and Jan Dreiser — Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

Thin films of lithium fluoride (LiF) are of high interest for spintronic applications [1], and they can be potentially used as decoupling layers for single-molecule magnets [2] and other molecules. In the present work we show that two strikingly different morphologies of LiF/Ag(100) can be achieved by keeping the Ag substrate at two different temperatures during the deposition of LiF.

Polarized X-ray absorption spectroscopy, scanning tunneling microscopy and low energy electron diffraction reveal that LiF grows epitaxially, preferring a vertical growth over the layer-by-layer growth. At room temperature LiF forms anisotropic strained dendrites with branches parallel to the [011] and [0$\bar{1}$1] directions of the substrate. Conversely, at a substrate temperature of 500 K LiF assembles into more relaxed square islands displaying a Moiré pattern. The strong qualitative difference between the two morphologies makes LiF/Ag(100) an interesting model system to study the dependence of the growth kinetics on the temperature.

References: [1] A. J. Drew et al., Nature Materials, **8**, 109, (2009); [2] C. Wäckerlin et al., Advanced Materials, **28**, 5142, (2016).

DS 1.2 Mon 10:15 H3

Stacking fault fold and step junctions as nucleation sites of threading dislocations in III-nitride films — •Georgios Dimitrakopulos[1], Isaak Vasileiadis[1], Joanna Moneta[2], Polyxeni Chatzopoulou[1], Philomela Komninou[1], and Julita Smalc-Koziorowska[2] — [1]Physics Department, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece — [2]Institute of High Pressure Physics, Polish Academy of Sciences, Sokołowska 29/37, 01-142 Warsaw, Poland

III-nitride semiconductor heterostructures have been employed with great success in optoelectronic and electronic devices despite the high densities of threading dislocations (TDs) that they contain. In order to unlock the full potential of these materials, it is imperative to diminish the TD nucleation sites. We present a mechanism of TD nucleation taking place at folds and steps of basal stacking faults (BSFs), particularly intrinsic I1 BSFs, that are frequent in (0001) epilayers due to their low self-energy. In-depth analysis by transmission electron microscopy (TEM) revealed that TD introduction is geometrically necessary at nodes of Shockley-like partial dislocations (PDs) at such BSFs. These PDs have the same Burgers vectors as normal Shockley PDs but exist only at junctions of the two variants of the BSF stacking sequence. In I1 BSF overlaps, the introduction of Frank-Shockley PDs is avoided, thus eliminating the elastic strain along the growth direction. Overlapped BSFs were observed to form hexagonal closed domains in which the coexistence of PD segments makes TD nucleation energetically favorable.

DS 1.3 Mon 10:30 H3

Cellulose nanofibrils as sustainable template material for thin silver nanowire electrodes fabricated via spray deposition — •Marie Betker[1,2], Constantin Harder[1,3], Elisabeth Erbes[1,4], Matthias Schwartzkopf[1], Andrei Chumakov[1], Daniel L. Söderberg[2], and Stephan V. Roth[1,2] — [1]Deutsches Elektronen Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany — [2]KTH Royal Institute of Technology, Teknikringen 8, 10044 Stockholm, Sweden — [3]Physik-Department E13, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [4]Institute for X-ray Physics, Goettingen University, Friedrich Hund Platz 1, 37077 Goettingen, Germany

Cellulose nanofibrils (CNFs) are wood-based, lightweight, and flexible, making them suitable for the fabrication of sustainable composite materials. With spray deposition the preparation of thin, homogenous CNF films of large scale and with an low roughness as well as their functionalization with e.g. nanoparticles is possible. We use CNF as a sustainable template material for the fabrication of two different types of thin silver nanowire (AgNW) electrodes via spray deposition: (I) A layered structure of a AgNW-network on top of a thin CNF layer and (II) a thin layer consisting of a mixture of CNF and AgNW. We compare the structural and electrical properties of both types using SEM, AFM, grazing incidence small angle X-ray scattering (GISAXS), and four-point measurements. The results demonstrate that type (II) is more conductive, leading to the conclusion that CNF has beneficial templating effects on the electronic properties of the AgNW network.

DS 1.4 Mon 10:45 H3

Epitaxial growth of $(Cr_{1-x}Fe_x)_2AlC$ MAX Phase thin films by pulsed laser deposition — •Hanna Pazniak[1], Marc Stevens[1], Martin Dahlqvist[2], Benjamin Zingsem[1,3], Johanna Rosen[2], Michael Farle[1,4], and Ulf Wiedwald[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Germany — [2]Thin Film Physics Division, Department of Physics, Chemistry, and Biology (IFM), Linköping University, Sweden — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, Germany — [4]Kirensky Institute of Physics, Federal Research Center KSC SB RAS, Russian Federation

MAX phase epitaxial thin films attract increasing attention with respect to high-temperature applications [1]. The partial substitution of M atoms in their nanolaminated structure is a promising way to tailor magnetic properties. In this study, we synthesized $(Cr_{1-x}Fe_x)_2AlC$ ($0<x<0.2$) epitaxial thin films by Pulsed Laser Deposition on MgO(111) and Al_2O_3(0001) at 600°C using pure elemental targets. By combining structural characterization and density functional theory, we explored the phase composition of synthesized $(Cr_{1-x}Fe_x)_2AlC$ solid solutions, finding a Fe solubility limit of 4 at.%. Excess Fe leads to the formation of the $(Cr,Fe)_5Al_8$ intermetallic secondary phase.

[1] M. Stevens, H. Pazniak, et al., MRL 9, 343 (2021).

Funding by the DFG within CRC/TRR 270, project B02 (Project-ID 405553726) is acknowledged.

DS 2: 2D materials and their heterostructures (joint session DS/HL/CPP)

Time: Monday 11:15–13:00 Location: H3

DS 2.1 Mon 11:15 H3

Tunable phases of Moire excitons in van der Waals heterostructures — •Samuel Brem[1], Christopher Linderälv[2], Paul Erhart[2], and Ermin Malic[1,2] — [1]Philipps University, Marburg, Germany — [2]Chalmers University of Technology, Göteborg, Sweden

Two monolayers of Transition Metal Dichalogenides can be vertically stacked to form a type-II heterostructure, hosting spatially indirect interlayer excitons. Recent studies have shown that moire superlattices can be created by stacking monolayers with a finite twist-angle, giving rise to a tunable modification of exciton features in optical spectra. The moire patterns lead to a spatially varying band gap and consequently, excitons experience a periodic potential modifying their transport properties.

We have combined first-principles calculations with the excitonic density matrix formalism to develop an exciton model for small-angle twisted MoSe2/WSe2 heterostructures. Based on a microscopic approach, we calculate the band structure and wave functions of intra- and interlayer excitons within a twist-tunable moire lattice as well as the resulting optical response. For a range of small twist-angles, we predict completely flat exciton bands corresponding to moire trapped, localized quantum emitters. However, we reveal that this moire exciton phase quickly changes with increasing twist-angle, and at 3°, there are only delocalized excitons. We find the emergence of multiple moire exciton peaks in the absorption, whose spectral shifts with varying twist-angle are characteristic for the trapped or delocalized phase.

DS 2.2 Mon 11:30 H3

Electrical control of spin-orbit coupling-induced spin precession and spin-to-charge conversion in graphene proximitized by WSe2 — •Franz Herling[1], Josep Ingla-Aynes[1], C. K. Safeer[1], Nerea Ontoso[1], Jaroslav Fabian[2], Luis E. Hueso[1,3], and Felix Casanova[1,3] — [1]CIC nanoGUNE BRTA, Spain — [2]University of Regensburg, Germany — [3]IKERBASQUE, Basque Foundation for Science, Spain

When combined with WSe2, a large spin-orbit coupling gets imprinted by proximity effect into graphene. Here, we use this effect to achieve the strong SOC regime in bilayer graphene. Together with the long, gate tunable spin diffusion, this provides unique control knobs to manipulate coherent spin precession in the absence of an external magnetic field. Remarkably, we observe in these devices that the sign of the precessing spin polarization can be tuned electrically by a back gate voltage and by a drift current. This realization of a spin field-effect transistor at room temperature in a diffusive system, a long-awaited goal of spintronics, could be a cornerstone for the implementation of energy efficient spin-based logic.

In accordance with the large proximity-induced SOC, we also observe spin Hall effect in similar heterostructures with an unprecedented spin-to-charge conversion length of up to 41 nm. Such highly efficient conversion up to room temperature will play a crucial role for the future integration of spintronic devices into existing electronic infrastructure.

DS 2.3 Mon 11:45 H3

Gate-Switchable Arrays of Quantum Light Emitters in Contacted Monolayer MoS_2 van der Waals Heterodevices — •Alexander Hötger[1,2], Julian Klein[1,2,3,4], Katja Barthelmi[1,3], Lukas Sigl[1,2], Samuel Gyger[5], Takashi Taniguchi[6], Kenji Watanabe[6], Val Zwiller[5], Klaus D. Jöns[5], Ursula Wurstbauer[2,7], Jonathan Finley[1,2,3], and Alexander Holleitner[1,2,3] — [1]Walter Schottky Institut, TU Munich — [2]Exzellenzcluster e-conversion — [3]Munich Center for Quantum Science and Technology — [4]Massachusetts Institute of Technology, Cambridge — [5]KTH Royal Institute of Technology, Dept. of Applied Physics — [6]National Institute for Materials Science, Tsukuba — [7]Institute of Physics, Westfälische Wilhelms-Universität Münster

Controlling single-photon emission on a few nanometers plays an important role for the scalability of future quantum photonic circuits. Moreover, it is highly relevant to facilitate a gate-switchable emission for quantum information schemes. By irradiating MoS_2 with helium ions, we generate single-photon sources at ~1.75 eV with a lateral position accuracy of only a few nanometers. [1] Second-order correlation measurements unambiguously proof the nature of single-photon emission. Charge doping of the monolayer MoS_2 can be used for switching the quantum emission on and off. [2] This deterministic control of light emission in spatial and temporal means paves the way for new integrated quantum photonic technologies.

[1] J. Klein, L. Sigl et al., ACS Photonics 8, 2 (2021).
[2] A. Hötger et al., Nano Lett. 21, 2 (2021).

DS 2.4 Mon 12:00 H3

Tunnelling transport in bilayer graphene nanostructures with quantum dots — •Angelika Knothe[1], Vladimir Fal'ko[1], and Leonid Glazman[2] — [1]National Graphene Institute, University of Manchester, Manchester M13 9PL, United Kingdom — [2]Department of Physics, Yale University, New Haven, CT 06520, USA

Quantum nanostructures, e.g., quantum wires and quantum dots, are needed for applications in quantum information processing devices, e.g., transistors or qubits. In gapped bilayer graphene (BLG), one can confine charge carriers electrostatically, inducing smooth confinement potentials while allowing gate-defined control of the confined structure. I will discuss charge transport in BLG nanostructures with electrostatically confined quantum dots. We investigate both theoretically and in collaboration with experiments how the BLG dots' highly degenerate single- and two-electron spin and valley multiplets, which depend on, e.g., the displacement field and the electron-electron interactions, manifest in tunnelling transport. This way, we shed light on BLG material parameters while opening the field for using the dots' rich spin and valley multiplets for quantum information.

1) Theory of tunneling spectra for a few-electron bilayer graphene quantum dot, A. Knothe, L. Glazman, V. Fal'ko, arXiv:2104.03399 2) Probing two-electron multiplets in bilayer graphene quantum dots, S. Möller, L. Banszerus, A. Knothe, L. Glazman, V. Fal'ko, C. Stampfer, et. al, arXiv:2106.08405 3) Quartet states in two-electron quantum dots in bilayer graphene, A. Knothe, V. Fal'ko, PRB 101, 235423 (2020)

DS 2.5 Mon 12:15 H3

Unconventional Superconductivity in Magic-Angle Twisted Trilayer Graphene — •Ammon Fischer — Institute for Theory of Statistical Physics, RWTH Aachen University

Magic-angle twisted trilayer graphene (MATTG) recently emerged as a highly tunable platform for studying correlated phases of matter, such as correlated insulators and superconductivity. Superconductivity occurs in a range of doping levels that is bounded by van Hove singularities which stimulates the debate of the origin and nature of superconductivity in this material. In this work, we discuss the role of spin-fluctuations arising from atomic-scale correlations in MATTG for the superconducting state. We show that in a phase diagram as function of doping (ν) and temperature, nematic superconducting regions are surrounded by ferromagnetic states and that a superconducting dome with $T_c \approx 2$ K appears between the integer fillings $\nu = -2$ and $\nu = -3$. Applying a perpendicular electric field enhances superconductivity on the electron-doped side which we relate to changes in the spin-fluctuation spectrum. We show that the nematic unconventional superconductivity leads to pronounced signatures in the local density of states detectable by scanning tunneling spectroscopy measurements.

DS 2.6 Mon 12:30 H3

Twist angle dependent proximity induced spin-orbit coupling in graphene/transition-metal dichalcogenide heterostructures — •Thomas Naimer[1], Klaus Zollner[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Physics, P. J. Šafárik University in Košice, 04001 Košice, Slovakia

We investigate proximity-induced spin-orbit coupling (SOC) in graphene on the four transition-metal dichalcogenides (TMDCs) MoS_2, WS_2, $MoSe_2$ and WSe_2 from first principles. By using different supercells of graphene/TMDC heterostructures we provide systematic insight on the effect of twist angles on the low energy Dirac spectrum. We find that the exact position of the Dirac cone within the TMDC band gap depends linearly on the biaxial strain applied to the graphene. From this relation we extrapolate the zero-strain band offset and correct the band offsets of all calculations by employing a transverse electric field across the heterostructure. The corrected results reveal massive twist angle tunability of both the magnitude and flavor of proximity induced SOC: We observe a peak in SOC at approximately 19° twist angle and vanishing SOC at 30°. This work was supported by ENB "Topologische Isolatoren" and SFB 1277.

DS 2.7 Mon 12:45 H3

Predicting the adsorption of alkali metals on 2D materials — Maofeng Dou and •Maria Fyta — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

The adsorption of alkali metal atoms on two-dimensional transition metal dichalcogenides (2D TMDCs) is investigated using quantum-mechanical calculations. Specifically, we evaluate the adsorption characteristics of Li on 2D TMDCs through the respective adsorption energies. We decompose these energies into separate components in order to fundamentally understand the adsorption process. The adsorption energies of lithium on 2D TMDCs were found to strongly and linearly correlate with the energy of the lowest unoccupied states of the materials. Accordingly, we propose and demonstrate the use of this energy as a descriptor for predicting adsorption energies. We further proceed with additional 2D TMDCs and adsorbed alkali atoms in order to generate a database that allows us to learn and make predictions. Our results strongly support the use of the energy of the lowest unoccupied states as a novel efficient descriptor for a data-driven design of materials with pre-selected properties and functions for target applications.

DS 3: 2D semiconductors and van der Waals heterostructures I (joint session HL/DS)

Time: Monday 13:30–16:15 Location: H4

See HL 5 for details of this session.

DS 4: Poster

Time: Tuesday 10:00–13:00 Location: P

DS 4.1 Tue 10:00 P

Two-color time-resolved Kerr rotation measurements of twisted MoS_2/WS_2 heterostructures — •Michael Kempf[1], Alina Schubert[1], Annika Bergmann[1], Mustafa Hemeid[1], Antony George[2], Andrey Turchanin[2], Rico Schwartz[1], and Tobias Korn[1] — [1]University of Rostock, Rostock, Germany — [2]University of Jena, Jena, Germany

Transition metal dichalcogenides (TMDC) have revealed many intriguing properties in recent years. For valleytronics especially, the coupling of spin and valley degrees of freedom shows great promise. Using valley-selective optical selection rules, a coupled spin-valley polarization can easily be introduced in these systems. Keeping possible future applications in mind, the dynamics of this polarization, especially its lifetime, is of great importance. Yet in pristine monolayer

TMDCs this is strongly limited due to ultrafast optical exciton recombination and electron-hole exchange interaction. By contrast, in TMDC heterostructures, ultrafast interlayer charge transfer may circumvent these limits on valley polarization lifetimes.
We use two-color time-resolved Kerr rotation measurements to study the spin-valley dynamics in disulfide-based TMDCs and their heterostructures. The independent tunability of our coupled laser systems allows to selectively pump and probe their excitonic transitions resonantly. We present low-temperature valley dynamics studies on TMDC monolayers and twisted MoS2-WS2 heterostructures fabricated by combining CVD-grown and exfoliated monolayers.

DS 4.2 Tue 10:00 P

Revealing in plane g factors in multilayer WSe2 via time-resolved Faraday experiments — •Simon Raiber, Dennis Falter, and Christian Schüller — Universtiät Regensburg

With the increasing investigation of two-dimensional heterostructures, the question arises how far the layer-intrinsic properties are imparted to multilayer van der Waals structures. While the effects of external magnetic fields on transition metal dicalcogenides monolayers have been studied intensively during the last years, the interaction of multiple layers remained largely disregarded.

We demonstrate a non-zero effective g factor for in plane magnetic fields in few-layer WSe2 making use of time-resolved Faraday rotation experiments. The found values commensurate to the established out of plane effective g factors. This indicates an isotropic effective in plane g factor for multilayer WSe2, which stands in contrast to monolayer samples. Up to now no standard theoretical approach can model an non-zero in plane g factor.

DS 4.3 Tue 10:00 P

Controlled moirè potentials of MoSe2/WSe2 heterostructures for time resolved kerr measurments — •Andreas Beer, Philipp Parzefall, Laura Zinkl, Anna Weindl, and Christian Schüller — Universität Regensburg

In heterostructures the twist angle serves as an degree of freedom to severly manipulate exciton dynamics.

We fabricate heterostructures with advanced twist angle control by staking CVD-grown triangulars of TMDCs.

To track the excitons dynamics on the femtosecond timescale we use two color pump probe measurements.

DS 4.4 Tue 10:00 P

Strong coupling of Bloch Surface Waves and excitons in ZnO up to 430 K — •Sebastian Henn, Marius Grundmann, and Chris Sturm — 1Universität Leipzig, Faculty of Physics and Earth Sciences, Felix-Bloch institute for solid state physics, Linnéstr. 5, 04103 Leipzig, Germany

Exciton-polaritons are bosonic quasi-particles consisting of a cavity photon and an electron-hole pair, exhibiting interesting physical phenomena like Bose-Einstein condensation [1]. Of special interest are exciton-polaritons in semiconductors with large exciton binding energies, where the strong coupling is observable above room temperature [2]. We report here on the experimental observation of the strong coupling between ZnO excitons and Bloch Surface Waves (BSW) up to 430 K. The sample consists of a Bragg reflector and a thin ZnO top layer. This system holds several advantages compared to exciton-polaritons in conventional microcavities: high propagation lengths due to the low loss BSW with large in-plane wave vector, a reduced complexity of production and direct access to the mode-supporting surface layer. In combination with a stable operation at high temperatures, this is of interest for the development of integrated optics devices. By means of a prism coupler in reflection geometry the polariton dispersion was observed and analyzed. We determined the temperature dependent coupling strength, exciton energy and dielectric background.

[1] J. Klaers *et al.*, Nature **468**, 545-548 (2010)
[2] C. Sturm *et al.*, New J. Phys. **11**, 073044 (2009)

DS 4.5 Tue 10:00 P

Novel 2D surface alloys on Pt(111): electronic and structural properties — •Marta Przychodnia[1], Tomasz Grzela[1], Roland Wiesendanger[2], and Maciej Bazarnik[1,2] — [1]Institute of Physics, Poznan University of Technology, Poznan, Poland — [2]Department of Physics, Hamburg University, Hamburg, Germany

Lately, a new class of 2D magnetic films has been discovered, namely rare earth (RE) metals - transition metals (TM) surface alloys. Limiting the dimensionality of RE-TM alloys to 2D (so-called surface alloys) influences their properties in surprising ways. For example, a $GdAu_2$ and $GdAg_2$ surface alloys are ferromagnetic while in bulk they are antiferromagnetic. Small change of Au to Ag in this system raise the Curie temperature from 19°C to 85°C showing potential for tuneability.

Here, I will present the comparison study of Dy-Pt and Gd-Pt mono- and double-layers of surface alloys grown on Pt(111). Structural and electronic properties in atomic scale of both systems were investigated using scanning tunneling microscopy (STM) and spectroscopy (STS).

DS 4.6 Tue 10:00 P

Measuring Material-Specific Properties with Ultra-High Vacuum Atomic Force Microscopy — •Frederic Luis Condin, Jesús Sánchez Lacasa, and Baran Eren — Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot, Israel

The real-space imaging capabilities provided by scanning probe microscopy techniques have undoubtedly revolutionized the scientific study of surfaces and processes happening thereon. Whereas scanning tunneling microscopy is limited to conductive samples, atomic force microscopy can be used for any surface. A general problem of scanning probe microscopy is its lack of element specificity, i.e., it cannot be used for the identification of materials or adsorbed surface species without additional information or prior knowledge about the sample. We address this problem and present contributions towards the chemical identification of surface materials. To this end, we calculate Hamaker constants on different points of a sample from bias voltage and tip-sample distance dependent measurements of the frequency shift in amplitude and frequency modulation atomic force microscopy.

DS 4.7 Tue 10:00 P

Coordinated Development of Tubes and Optics: New possibilities for X-ray Analytics — •Jörg Wiesmann, Moritz Schlie, Jürgen Graf, Frank Hertlein, and Paul Radcliffe — Incoatec GmbH, Max-Planck-Strasse 2, 21502 Geesthacht

At Incoatec, we have a long history of offering solutions driven by the needs of the customers. As a specialist for multilayer optics we penetrated the crystallography market with our complete IμS Microfocus Solutions in 2006. Optics can only evolve their whole strength when the source is also matched to it. Due to this fact, we started in 2011 with the in-house development of X-ray sources. The aim was to offer the best combination of optics and sources for certain applications in small and macromolecular structure analysis. We were able to launch new solutions like the IμS3.0 and the IμS DIAMOND that offers a flux density of more than $5*10^{10}$ ph/s/mm^2 within a spot of less than 100μm. This high flux density is achieved with a low power air-cooled source that doesn't need maintenance during the typical life time of more than 6 years. We will summarize the key parameters for combining multilayer optics and microfocus tubes to achieve collimated or focused X-ray sources with high brilliance. The main part of the talk will explain the application-dependent design of our metal-ceramic tubes and how to match them with our multilayer optics. Applications include crystallography, nanotechnology and thin film research.

DS 4.8 Tue 10:00 P

Persistent response in ultra-strongly driven mechanical membrane resonators — •Fan Yang[1], Felicitas Hellbach[1], Felix Rochau[1], Wolfgang Belzig[1], Eva Weig[1,2], Gianluca Rastelli[3], and Elke Scheer[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Fakultät für Elektrotechnik und Informationstechnik, Technische Universität München, 80333 München, Germany — [3]INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento, 38123 Povo, Italy

We study experimentally and theoretically the phenomenon of *persistent response* in ultrastrongly driven membrane resonators. The term persistent response denotes the development of a vibrating state with nearly constant amplitude over an extreme wide frequency range of more than 50% of the eigenfrequency. This phenomenon is unusual and is key to avoid breakdown, since it imposes a self-limitation of the maximum amplitude. We reveal the underlying mechanism by directly imaging the vibrational state using advanced optical interferometry. We argue that this state is related to the nonlinear interaction between higher-order flexural modes and higher-order overtones of the driven mode. Finally, we propose a stability diagram for the different vibrational states that the membrane can adopt.

DS 4.9 Tue 10:00 P

Tunable frequency comb in flexural-mode-coupling regime in nonlinear mechanical membrane resonators — •Mengqi Fu, Fan Yang, and Elke Scheer — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Multimode coupling in mechanical systems has attracted broad interest in many realms of physics[1,2]. Recently, the research on the multimode coupling has been extended to strong nonlinear systems and novel phenomena have been observed caused by the strong nonlinearity of the coupled flexural modes[2]. Here, we demonstrate a novel tunable frequency comb generated by driving the mechanical system into the strongly nonlinear regime, i.e. the flexural-mode-coupling regime, by one-tone excitation. The studied system is based on a suspended SiN membrane (~ 500 nm thickness) with a quality factor of ~ 19000. The frequency separation between neighboring sidebands of the frequency comb strongly depends on the damping factor, nonlinearity, vibration amplitude and the detuning frequency of the two coupled flexural modes. The frequency separation is tunable by varying the detuning frequency and the strength of the drive power. By systematically investigating the frequency response of the fluctuations close to the coupled flexural modes, we show that the observed frequency comb is generated when the "very states"[3] produced by the nonlinearity of the coupled flexural modes are crossed experimentally.

1. A. Ganesan et al., Phys. Rev. Lett. 118, 033903 (2017).
2. F. Yang et al., Phys. Rev. Lett. 127, 014304 (2021).
3. J.S. Huber et al., Phys. Rev. X, 10, 021066 (2020).

DS 4.10 Tue 10:00 P

Forming-free resistive switching in amorphous gallium oxide device — •Aman Baunthiyal[1], Jon-Olaf Krisponeit[1], Christian Habben[1], Alexander Karg[1], Martin Eickhoff[1], Sandra Pérez Domínguez[2], Manfred Radmacher[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Institute of Biophysics, University of Bremen, Germany

Currently, semiconductor based devices are reaching their limitations in terms of scalability and long time storage capability. To overcome this problem, inorganic and organic materials which show resistive switching (utilized in ReRAMs), magnetic switching (MRAMs), and phase change switching (PCRAMs) have been studied over the past 40 years. In ReRAMs, a repeatable switching between high resistive state (HRS) and low resistive state (LRS) can be observed when a voltage sweep is applied across an active layer sandwiched between two metal electrodes.

In this study, the forming-free bipolar resistive switching was observed in a Al/GaO_x(76 nm)/Ru devices. The observed switching was proposed to be connected to the formation and rupture of conductive filaments constituted by oxygen vacancies in the GaO_x film. X-ray photoelectron spectroscopy (XPS) analysis confirmed the high amount of oxygen vacancies in the GaO_x film. The LRS was found to be of ohmic nature, while the HRS followed Poole-Frenkel emission model. Due to their stable endurance cycle and long retention time with more than 10^3 order resistance ratio ,the devices can be regarded as promising prototypes for future non-volatile ReRAMs.

DS 4.11 Tue 10:00 P

Adsorption of fluids on hydrophobic surfaces under sub- and supercritical conditions — •Mike Moron, Göran Surmeier, Marc Moron, Jennifer Bolle, Susanne Dogan, Julia Nase, Michael Paulus, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

Adsorption at interfaces is crucial for many industrial applications, e. g. adsorption-based separation, regeneration of adsorbents in purification processes as well as for natural gas storage. In subcritical systems the adsorption layers of different fluids had been successfully described as molecular thin layers. The layer thickness diverges when the pressure reaches the condensation pressure of the corresponding fluid, meaning that the adsorption layer transforms into a macroscopic condensate. Supercritical adsorption, however, is far less understood on a molecular scale because of the complex requirements to the experimental environment, although the phenomenon is of outstanding importance for many applications. For example, the use of supercritical CO_2 is a gentle method to dry porous materials without damaging the frameworks. We investigated the pressure dependent adsorption of the fluids argon, carbon dioxide, hexafluoroethane, octafluoropropane, and decafluoropropane on a hydrophobic silicon wafer coated with octadecyltrichlorsilane by means of X-ray reflectivity (XRR), where we could access the supercritical regime for hexafluoroethane and argon. The XRR studies were carried out at PETRA III Beamline P08 (DESY, Hamburg) at a photon energy of 25 keV and Beamline BL9 (DELTA, Dortmund) at 27 keV, repsectively.

DS 4.12 Tue 10:00 P

Simulation Based Conductivity Tensor Determination of Sintered Nanosilver — •Lennart Schwan[1,2], Michael Feige[1], Andreas Hütten[2], and Sonja Schöning[1] — [1]Bielefeld Institute for Applied Materials Research (BIfAM), Bielefeld University of Applied Sciences, Department of Engineering Sciences and Mathematics, Interaktion 1, 33619 Bielefeld — [2]Thin Films & Physics of Nanostructures, Bielefeld University, Department of Physics, Universitätsstrasse 25, 33615 Bielefeld, Germany

3D-printing of conductive and dielectric materials in one process is an emerging technology. In addition to the printing of planar structures like circuit boards, the modern Multi Material Jetting process allows to realize three dimensional structures such as antennas, coils or cooling elements.

In the present case the conductive material consists of small silver particles which are sintered with infrared light. The conductivity reaches up to 70 % of the conductivity of copper but is highly anisotropic due to the print and sinter process.

In order to optimize the printed structures with regard to the anisotropic conductivity, it is necessary to determine reliable value of the conductivity tensor. Here we propose an approach based on a coupling of FEM simulation with mathematical optimization to determine the conductivity tensor. The simulation with the conductivity tensor as free parameter is fitted to experimental data of meander shaped test structures which are orientated in different directions to consider all components of the conductivity tensor.

DS 4.13 Tue 10:00 P

Molecular dynamics simulations of carbon nanomembranes (CNMs) — •Julian Ehrens, Levin Mihlan, and Jürgen Schnack — Universität Bielefeld, Universitätsstrasse 25, D-33615 Bielefeld

CNMs are made by electron-induced crosslinking of aromatic self-assembled monolayers (SAMs) [1,2]. Their supposedly irregular internal structure can not be adequately investigated by standard techniques, e.g. X-ray diffraction, which requires a characterization through physical quantities like solvent permeability and the Young's modulus. In order to propose possible internal molecular structures obtained from various initial configurations of the SAM and irradiation processes, we investigate the monolayers with respect to the Young's modulus in terms of classical molecular dynamics calculations using LAMMPS and use the experimental value of around 10 GPa for comparison. We present three distinct methods to calculate the Young's modulus: Global scaling of all coordinates (curvature of energy), stress-strain response from clamped straining and barostatted dynamics. Discrepancies among the methods with regard to vastly different outcomes of the Young's modulus will be discussed considering finite size effects and suitability of each method for this particular system.

[1] Dementyev, Petr, et al. "Carbon Nanomembranes from Aromatic Carboxylate Precursors" ChemPhysChem 21.10 (2020): 1006 [2] Ehrens, Julian, et al. "Theoretical formation of carbon nanomembranes under realistic conditions using classical molecular dynamics" Phys. Rev. B 103, 115416

DS 4.14 Tue 10:00 P

Influence of processing parameters on the electrical conductivity of 3D printed silver structures — •Michael Feige, Lennart Schwan, and Sonja Schöning — Bielefeld Institute for Applied Materials Research (BIfAM), Bielefeld University of Applied Sciences, Department of Engineering Sciences and Mathematics

3D-printing of conductive and dielectric materials in one process is an emerging technology. The Multi Material Jetting technique allows to realize three dimensional structures such as antennas, coils or cooling elements.

The deployed method is very similar to that used by a conventional inkjet printer. Small ink drops are deposited layer by layer through fine nozzles in the print heads. The stacking of those layers finally forms the 3D buildup. Multiple materials are introduced by two or more print heads.

In the considered case the dielectric material, a polymer, is cured with UV-light. The conductive material consists of small silver particles and is sintered with IR-light.

The electrical conductivity can reach up to 70 % of the conductivity of copper but it is anisotropic with regard to the print direction and it depends on several production parameters. We are identifying these contributing key factors, like layer thicknesses, drop placement patterns, environmental conditions during the print stage and temperature patterns used for heat treatment during postprocessing. In addition we investigate how the determined influence of the parameters can be used to optimize the conductivity.

DS 4.15 Tue 10:00 P

Selective Area Epitaxy of Bi-based 3D Topological Insulators on Sapphire — •Christoph Ringkamp, Michael Schleenvoigt, Peter Schüffelgen, Gregor Mussler, and Detlev Grützmacher — Peter-Grünberg-Institut 9, Forschungszentrum Jülich, 52428 Jülich, Germany

Topological insulators (TI) possess topologically protected, conducting surface states, which – in conjunction with superconductors (SC), are predicted to show Majorana signatures. A prerequisite for this is a high transparency between the TI and the SC, and that is why an in-situ fabrication of the TI/SC heterostructures is crucial. On Si(111) substrates, we have already established the selective area growth and a shadow mask technique to fabricate such heterostructures via molecular-beam epitaxy (MBE). However, one major problem in transport experiments still poses the impact of the Si substrate, as the Si/TI interface may serve as an additional conducting channel. Hence, we intend to grow the TI/SC heterostructures on sapphire, as it is a purely insulating substrate, which may allow to investigate the topological properties of the TI films in transport experiments in more detail.

We will report on the selective area epitaxy via MBE of Bi-based TI like Bi_2Te_3 and Bi_2Se_3 on sapphire substrates that are prepared with a combination of lithographically defined SiO_2 and Si_3N_4 structures as a growth mask and their application as a shadow mask for TI/SC heterostructures. Additionally, I will show a substantial improvement of the carrier mobility in the TI films on sapphire compared to Si(111).

DS 4.16 Tue 10:00 P

Area-selective deposition on 3D granular PtC scaffolds — •Fabrizio Porrati, Sven Barth, and Michael Huth — Goethe Uni Frankfurt

We present a novel fabrication method to prepare 3d metallic nanostructures by area-selective chemical vapor deposition (CVD). The method is based on the fabrication of 3d PtC granular scaffolds by focused electron beam induced deposition (FEBID). These nanostructures are written between two electrods and biased by an electrical current in order to increase their temperature to several hundreds degrees. This is possible since the 3d PtC scaffolds are high ohmic resistors with low thermal coupling to the substrate. Here we show that CoFe and NbNC metallic layers form on the 3d biased scaffolds by decomposition of the HFeCo3(CO)12 and Nb(NMe2)3(N-t-Bu) precursor gas when injected in the SEM preparation chamber.

DS 4.17 Tue 10:00 P

Characterizing ALD printed structures by imaging ellipsometry — •Peter H. Thiesen[1], Ivan Kundrata[2,3], Maksym Plakhotnyuk[3], and Julien Bachmann[2,3] — [1]Accurion GmbH, Göttingen, Germany — [2]FAU, Erlangen, Germany — [3]ATLANT 3D, Lyngby, Dänemark

ATLANT 3D Nanosystems develops a disruptive 3D printing technology for micro and nano device rapid prototyping. The initial 3D printer prototype will be able to process oxides such as SiO2, TiO2, Al2O3, ZnO, and platinum with line width of 400 um. Later on, we will add processing of other materials, such as metals, sulfides, nitrides etc., also with a better selection of resolution down to 10 um. Thin film metrology of printed structures requires a fast measurement technique that is sensitive to thinnest films and offers a high lateral resolution also suited for the next development steps. Imaging Ellipsometry is an all-optical, non-contact metrology technique. It combines microscopic imaging with the measurement principles of spectroscopic ellipsometry and reaches a spatial resolution of about 1 micro meter. Ellipsometry is based on the samples interaction with polarized light and enables the characterization of ultra-thin films. The thickness of ALD-structures, printed at variable process parameters or with different materials was characterized by imaging ellipsometry. The standard characterization was done with a fixed angle of incidence system, equipped with a high power LED-HUB (SIMoN, EP4, Accurion GmbH) at an AOI of 60° and selected wavelength. Additionally, microscopic maps at different AOIs and wavelength of selected samples were recorded.

DS 4.18 Tue 10:00 P

Electrical transport properties of Vanadium-doped $Bi_2Te_{2.4}Se_{0.6}$ — Ch. Riha[1], B. Düzel[1], K. Graser[1], •O. Chiatti[1], E. Golias[2], J. Sánchez-Barriga[2], O. Rader[2], O. Tereshchenko[3], and S. F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Helmholtz-Zentrum-Berlin für Materialien und Energie, 12489 Berlin, Germany — [3]Physics Department, Novosibirsk State University, 630090 Novosibirsk, Russia

Transport in the topological surface states (TSSs) of topological insulators, such as Bi_2Se_3, can be masked by unintentional bulk doping. The alloy $Bi_2Te_{2.4}Se_{0.6}$ is a promising candidate to investigate TSSs, because in $Bi_2Te_{3-y}Se_y$ materials bulk *n*-type doping tends to be suppressed. In this work [1], single crystals of $V_xBi_{2-x}Te_{2.4}Se_{0.6}$, with $x = 0.015$ and 0.03, are grown by the Bridgman method. Angle-resolved photoemission spectroscopy shows gapless TSSs for both Vanadium concentrations. The resistivity, the Hall charge carrier density, and the mobility for temperatures from 0.3 to 300 K are strongly dependent on the Vanadium concentration, with carrier densities as low as 1.5×10^{16} cm^{-3} and mobilities as high as 570 cm^2/Vs. Below 10 K, resistivity, carrier density, and mobility are constant, as expected for gapless TSSs. Also, the magnetoresistance shows for both Vanadium concentrations weak antilocalization, which is analyzed with the Hikami-Larkin-Nagaoka model and yields phase-coherence lengths of up to 250 nm for $x = 0.015$.

[1] C. Riha *et al.*, Phys. Status Solidi B, 2000088 (2020)

DS 4.19 Tue 10:00 P

Magnetotransport and thermoelectric properties of vanadium disulfide (VS_2) flakes — •Yejin Lee[1,2], Gyu-Hyeon Park[1,2], Grigory Shipunov[1], Geishendorf Kevin[1], Bernd Buechner[1], Kornelius Nielsch[1,2], Saicharan Aswatham[1], and Andy Thomas[1,2] — [1]IFW Dresden — [2]Technische Universität Dresden

Two-dimensional transition metal dichalcogenides (TMDCs) have drawn extensive interest due to their intriguing electrical transport properties. Vanadium disulfide (VS_2) is a member of metallic TMDCs and interestingly, theoretical calculations have predicted magnetic characteristics. Here, we investigate magnetotransport and thermoelectric properties of exfoliated VS_2 flakes from a single crystal grown by chemical vapor transport technique. The magnetotransport characterizations were performed in an external magnetic field of up to 9 T. We found that the VS_2 flake exhibits a specific temperature dependence at around 21 K, which is consistent with the presence of a weak magnetic anomaly seen in the single crystal. In addition, a negative magnetoresistance is observed with a steep decrease at 2.5 T and below 20 K, where the slope of the magnetic field dependent Hall resistance changes. Furthermore, Seebeck coefficients are evaluated and it indicates a p-n type transition in the low temperature regime if a single band model is assumed. This findings provide further insight into the magnetotransport and thermoelectric properties of van Der Waals TMDCs.

DS 4.20 Tue 10:00 P

Influence of the module number on the folding process in thin spider silk films — •Mirjam Hofmaier[1,3], Birgit Urban[1], Sarah Lentz[4], Thomas Scheibel[4], Andreas Fery[1,3], and Martin Müller[1,2] — [1]Leibniz Institute of Polymer Research Dresden, Institute of Physical Chemistry and Polymer Physics, Hohe Str. 6, 01069 Dresden — [2]Technical University Dresden, Chair of Macromolecular Chemistry, 01062 Dresden — [3]Technical University Dresden, Chair of Physical Chemistry of Polymeric Materials, 01062 Dresden — [4]University of Bayreuth, Chair of Biomaterials, Prof.-Rüdiger-Bormann Str. 1, 95447 Bayreuth

Aiming at a better understanding of the folding process in recombinantly produced[1], multiblockcopolymer-like spider silks, herein we report experimental work on thin films of eADF4(Cx) proteins with x = 1-16 modules. Thin eADF4(Cx) films were characterized as-cast and during methanol post-treatment (pt) using dichroic attenuated total reflection (ATR-) FTIR spectroscopy, circular dichroism (CD), and scanning force microscopy (SFM).[2]

During post-treatment, FTIR reveals an increasing β-sheet content from < 10% to > 28 % and a decreasing random coil content from > 65% to < 50%, which could be confirmed by CD analysis.[2-3] An out-of-plane orientation of the antiparallel β-sheets of the crystalline blocks could be suggested by dichroic ATR-FTIR spectroscopy.[2]

[1] D. Huemmerich et al., Biochem., 2004, 43, 13604-13612. [2] M. Hofmaier et al., JPC B, 2021, 125, 1061-1071. [3] C. Borkner et al., ACS Appl. Polym. Mater., 2019, 1, 3366-3374.

DS 4.21 Tue 10:00 P

Enhancement of the Raman Emission in Hexagonal Boron Nitride — •Felix Schaumburg, Marcel Ney, Vasilis Dergianlis, Günther Prinz, Martin Paul Geller, and Axel Lorke — Faculty of Physics and CENIDE, University Duisburg-Essen, Germany

Optical spectroscopy, especially Raman- and photoluminescence (PL)-spectroscopy, is commonly used to study the optical properties of two-dimensional materials. In order to obtain the highest signal, it is important to reduce spurious effects, such as backscattered laser light.

We studied a number of exfoliated h-BN flakes with different thicknesses on a silicon (Si) substrate with a 300 nm silicon dioxide (SiO_2) top-layer. With changing the h-BN layer-thickness, we found a specific thickness, where all Raman signals showed maximum intensity, whereas the backscattered laser light was almost completely suppressed. To explain the increased signal, we calculated the reflectivity of the layer system (air, h-BN, SiO_2, Si) for different h-BN layer thickness, by using the transfer-matrix-algorithm. For our 532 nm excitation laser, the minimum surface reflectivity was found for a layer thickness of around 160 nm. With AFM measurements, we were able to confirm that the thickness of the samples, with the strongest Raman signal, corresponds almost exactly to the calculated thickness.

Our results suggest that the PL from defects will also be strongly enhanced for an h-BN thickness of 160 nm and an excitation laser wavelength of 532 nm. This optimal thickness for the defect state PL emission can easily be calculated for other excitation laser wavelengths, as well as for other materials.

DS 4.22 Tue 10:00 P

Vibrational spectroscopic characterization of local electrochemical modification of graphene — Tilmann Neubert[1,2,3,4], Jörg Rappich[1], Kannan Balasubramanian[3,4], and •Karsten Hinrichs[2,3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489, Berlin — [2]ISAS - e.V., In Situ Spectroscopy Group, Schwarzschildstr. 8, 12489 Berlin — [3]HU Berlin, School of Analytical Sciences Adlershof (SALSA), Unter den Linden 6, 10117 Berlin — [4]Department of Chemistry, HU Berlin, Unter den Linden 6, 10117 Berlin

Local properties of an electrochemical modification and the underlying graphene between the contacts of a field effect transistor (FET) were analyzed by Raman and infrared (IR) spectroscopies. IR spectroscopic ellipsometry (IRSE) enabled us to probe spots from about 0.1 to a few mm, IR microscopy of a few 10 μm, Raman of about 1 μm, photothermal AFM-IR at the nm-scale. For graphene surfaces modified electrochemically with maleimidophenyl (MP) or 4-Aminophenyl acetic acid (4-APhAA) the interpretation of Raman spectra allowed a detailed characterization of the graphene properties whereas IR is used for identification of characteristic molecular vibrations of the functional layers. The Raman spectra reveal if the electrochemically formed oligomers are covalently bound or physically adsorbed. AFM-profiles and IRSE interpretation reveal similar thicknesses of the deposited (a few nm thick) layers. Funding: EFRE 1.8/13 and SALSA.

DS 4.23 Tue 10:00 P

The Dielectric Tensor of Microtextured Squaraine Thin Films obtained by Imaging Mueller Matrix Ellipsometry — •Manuela Schiek[1], Sebastian Funke[2], Matthias Duwe[2], Peter H. Thiesen[2], Kurt Hingerl[1], and Frank Balzer[3] — [1]Johannes Kepler University of Linz, Austria. — [2]Accurion GmbH Göttingen, Germany. — [3]University of Southern Denmark, DK.

Imaging Mueller matrix ellipsometry combines the power of variable angle spectroscopic ellipsometry and optical microscopy mapping. Here we illustrate the determination of the full biaxial dielectric tensor of an organic material crystallizing in an orthorhombic phase. This is achieved by analyzing thin film samples with a single crystallographic orientation parallel to the substrate subdivided in micro-sized rotational domains. Oscillator dispersion relations reasonably model the diagonal tensor components and reproduce well the Davydov splitting of the material.

[1] Funke, Duwe, Balzer, Thiesen, Hingerl, Schiek. J. Phys. Chem. Lett. 19 (2021) 3053.

DS 4.24 Tue 10:00 P

Modelling of Two-Dimensional Electronic Spectroscopy Response of a Plasmon-Exciton System — •Marti Bosch[1], Antonietta De Sio[2], Christoph Lienau[2], and Erich Runge[1] — [1]TU Ilmenau — [2]Universität Oldenburg

Two-dimensional electronic spectroscopy (2DES) records the optical response of a system after the interaction with three timely delayed laser pulses. The dynamics and electronic couplings in complex optical systems can be analyzed with a high temporal resolution by correlating the excitation and emission intensities as a function of the time delay as well as the used frequencies. The interpretation of 2DES experimental results is challenging and it is often useful to support them with numerical calculations. In this work, we present the semi-classical calculations of the third order non-linear response signal of a plasmon-exciton system. We model the response signal of coupled two-level systems based on a perturbative density matrix approach [1] and implement the non-unitary time evolution of the system using the Lindblad formalism. We discuss the differences appearing for fermionic and bosonic systems and compare the results to preliminary experimental results. [1] Mukamel, S. (1995) Principles of nonlinear optical spectroscopy. O.U.P, New York

DS 4.25 Tue 10:00 P

Surface-localized phonon modes on the Si(553)-Au surface — •Julian Plaickner[1,2], Eugen Speiser[1], Sandhya Chandola[1,2], Christian Braun[3], Wolf Gero Schmidt[3], Norbert Esser[2,4], and Simone Sanna[5] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn Meitner Platz 1, 14109 Berlin — [2]Leibniz-Institut für Analytische Wissenschaften, ISAS e.V., Schwarzschildstraße 8, 12489 Berlin — [3]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, 33095 Paderborn — [4]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstraße 36, 10623 Berlin — [5]Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus Liebig Universität Gießen, Heinrich Buff Ring 16, 35392 Gießen

The Si(553)-Au surface is investigated with Raman spectroscopy and ab-initio calculations. A characterization of the phonon modes is provided below and above the phase transition temperature (Phys. Rev. B 103, 115441 (2021)). Some phonon modes shows a significant temperature dependence. The analysis of the calculated displacement patterns indicates that these modes are localized at the Si step edge or involve a change of the Au-Au bond length. The large temperature-induced frequency shift observed for transversal Au-related modes demonstrates that the dimerization is significantly affected by the phase transition due to charge transfer between Au- and Si-related states. The charge transfer leads to Raman scattering by charge density fluctuations, which is responsible for the detected Raman activity even for such modes that should be silent due to symmetry.

DS 4.26 Tue 10:00 P

Femtosecond Spectrostroscopic Ellipsometry — •Shirly Espinoza — ELI Beamlines, Institute of Physics, Czech Academy of Science, Prague, Czech Republic

The current status of a versatile experimental platform dedicated to ultrafast pump-probe ellipsometry with time resolution about 100 fs will be presented. The setup measures the ellipsometric spectra in the range 350-750 nm. The monochromatic pump beam can be chosen from 350 nm to 2 um. This setup give information of ultrafast changes on the optical properties of the materials forming a thin film. Recent results and ideas for expansion of the capabilities of the setup will be presented for discussion.

DS 4.27 Tue 10:00 P

Metal-insulator transition via ion irradiation in epitaxial La0.7Sr0.3MnO3-δ thin films — Lei Cao[1], Andreas Herklotz[2], Diana Rata[2], Chenyang Yin[3], Oleg Petracic[3], Ulrich Kentsch[1], Manfred Helm[1], and •Shengqiang Zhou[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, 01328, Germany — [2]Institute of Physics, Martin Luther University Halle-Wittenberg, Halle, 06120, Germany — [3]Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, Forschungszentrum Jülich GmbH Jülich, 52425, Germany

Complex oxides provide rich physics related to ionic defects. For the proper tuning of functionalities in oxide heterostructures, it is highly desired to develop fast, effective and low temperature routes for the dynamic modification of defect concentration and distribution. In this work, we report on the use of helium-irradiation to efficiently control the vacancy profiles in epitaxial La0.7Sr0.3MnO3-δ thin films. The viability of this approach is supported by the lattice expansion in the out-of-plane lattice direction and dramatic change in physical properties, i.e., a transition from ferromagnetic metallic to antiferromagnetic insulating. In particular, a significant increase of resistivity up to four orders of magnitude is evidenced at room temperature, upon irradiation by highly energetic He-ions. Our result offers an attractive means for tuning the emergent physical properties of oxide thin films, via strong coupling between strain, defects and valence.

The work at HZDR is supported by DFG (ZH 225/10-1).

DS 5: Focus Session: Highlights of Materials Science and Applied Physics I (joint session DS/HL)

Jointly organized on the occasion of the 60th anniversary of the *physica status solidi* journals (*pss*, http://www.pss-journals.com), this Focus Session features several invited presentations, talks and posters from key contributors on core condensed matter and applied physics topics. Highlights comprise the latest results on diamond, nitride semiconductors, organic materials, two-dimensional and quantum systems, oxides, magnetic materials, solar cells, thermoelectrics and more.

physica status solidi was launched by Akademie-Verlag Berlin in July 1961 and is published by Wiley-VCH Berlin and Weinheim today, supported by Wiley colleagues in China and the US. While in its first three decades it served as an East-West forum for solid state physics, since 1990 it has evolved into a family of journals with international author- and readership in a globalized scientific world. Its professional editorial services include topical curation, peer review organization, technical editing, special issue and hybrid open access publication.

The Focus session celebrates the numerous close collaborations and the steady support which the journals receive from their Advisory Board members, authors, reviewers and guest editors, including many members of the DPG and the condensed matter physics community in Germany.

(More information on '60 years of *pss*' is available at http://bit.ly/60_years_pss)

Organizers: Stefan Hildebrandt (Editor-in-Chief, pss), Norbert Esser (TU Berlin, ISAS) and Stephan Reitzenstein (TU Berlin)

Time: Tuesday 13:30–16:15 Location: H3

Topical Talk DS 5.1 Tue 13:30 H3

Single crystal diamond grown by CVD: state of the art, current challenges and applications — •Jean-Charles Arnault[1], Samuel Saada[2], and Victor Ralchenko[3,4] — [1]NIMBE, UMR CEA-CNRS 3685, Université Paris-Saclay, F-91191 Gif sur Yvette, France — [2]CEA, LIST, DM2I, F-91191 Gif-sur-Yvette, France — [3]Prokhorov General Physics Institute of Russian Academy of Sciences, Vavilov str. 38, Moscow 119991, Russia — [4]Harbin Institute of Technology, Harbin 150080, P.R. China

Single crystal diamond is the material of choice for future power electronics. Its electrical and thermal properties outperform those of other wide band gap semiconductors like 4H-SiC, GaN or Ga2O3. In addition, diamond can host a wide range of color centers (NV, SiV, GeV,...) that bring optical and spin properties suitable for quantum applications. This explains the ultrafast development of quantum applications based on diamond materials within the last years. For both application fields, diamond films of excellent crystalline quality are required and an accurate tuning of dopants is needed. This talk will draw the state of art of single crystal diamond grown by CVD either starting with diamond substrate (homoepitaxy) or controlling diamond epitaxial nucleation on a foreign substrate (heteroepitaxy). Progresses on substrates, growth mechanisms and reduction of structural defects, doping, upscaling and applications will be reviewed. In light of last progresses, future challenges and the respective roles of homoepitaxial and heteroepitaxial materials in the applications roadmap will be discussed.

Topical Talk DS 5.2 Tue 14:00 H3

Tuning Semiconductor Mode-Locked Laser Frequency Combs by Gain and Cavity Design — Stefan Meinecke and •Kathy Lüdge — Institute of Theoretical Physics, Technische Univ. Berlin

Passively mode-locked semiconductor lasers produce sequences of short optical pulses at high repetition rates without the need for an external driving frequency. They find applications in optical data communication and metrology and are promising candidates for comb generation in all-optical integration schemes [1].

The gain material as well as the cavity design play a crucial role for their performance and can be designed easily via epitaxial growth. We explore the pulse performance optimization of a three-section tapered quantum-dot laser by means of a numerical model that assumes both the microscopic charge-carrier scattering processes as well as the light-propagation along the device. Motivated by an experimentally characterized device [2], we utilize pulse peak power, pulse width and long-term timing jitter to characterize the performance. The results predict optimal configurations for both the angle of the tapered gain section and the position of the saturable absorber section. These findings can be interpreted and understood in terms of the gain and absorption recovery processes within the active regions of the laser and thus explain why the nano-structured quantum-dot gain medium is especially suited for optimizing the pulse performance.

[1] R. Guzmán et al., Opt. Lett. 42, 2318 (2017).
[2] S. Meinecke et al., Sci. Rep. 9, 1783 (2019).

Topical Talk DS 5.3 Tue 14:30 H3

Monolayer-thick GaN/AlN heterostructures for UVB & UVC ranges: technology, design and properties — Valentin Jmerik, Alexey Toropov, Valery Davydov, and •Sergey Ivanov — Ioffe Institute, Polytekhnicheskaya 26, Saint Petersburg, 194921, Russia

The development of monolayer (ML)-thick GaN/AlN multilayer heterostructures for deep ultraviolet (UV) optoelectronics is discussed. Analysis of plasma-assisted molecular beam epitaxy and metal-organic vapor phase epitaxy show that extreme interface sharpness and sub-ML accuracy in controlling the layer thickness are the main advantages of the former, while the lowest density of threading dislocations and wide possibilities for the implementation of various two-dimensional growth mechanisms are the attractive features of the latter. The structural properties of ML GaN/AlN heterostructures are evaluated comparatively by X-ray diffraction, scanning transmission electron microscopy and Raman spectroscopy. Studies of the optical properties of ML-thick GaN/AlN quantum wells (QWs) reveal that quenching of the Stark effect, suppression of polarization switching, as well as a true excitonic nature of the UV-emission in ultra-thin (1-2ML) QWs ensure a high internal quantum yield of 75% in such structures emitting at 235 nm. High optical quality of 100-nm-thick layers of ML-GaN/AlN digital alloys is confirmed by the optically pumped stimulated emissions in the range 262-290 nm with a minimum threshold of 700kW/cm2. The possibilities of using ML-GaN/AlN MQWs to fabricate powerful (Watt-range) electron-beam pumped UVC-emitters in the spectral range 240-260 nm are demonstrated.

15 minutes break

Topical Talk DS 5.4 Tue 15:15 H3

Optical and vibrational properties of layered 2D materials — •Janina Maultzsch — Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Atomically thin layered crystals have received great attention due to their fascinating physical properties. By deterministic stacking and twisting of these two-dimensional (2D) materials, an almost unlimited variety of material's combinations and resulting physical properties can be achieved. The properties can be further modified by chemical functionalization of the surface. In this talk I will present theoretical predictions on novel 2D antimony oxide structures which show tunable electronic properties depending on the oxygen content. Second, based on recent experiments on chemically functionalized MoS_2 layers, we present transitions from the 2H to the 1T' phase along with the characteristic phonon modes of the 1T' phase of MoS_2.

Topical Talk DS 5.5 Tue 15:45 H3

Organic/inorganic low dimensional material systems: Fundamental aspects and device applications — •Emil List-Kratochvil — Institut für Physik, Institut für Chemie & IRIS Adlershof, Humboldt-Universität zu Berlin, Zum Großen Windkanal 2, 12489 Berlin, Germany — Helmholtz-Zentrum für Materialien und Energie GmbH, HySPRINT Helmholtz Innovation Lab, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The ability to form heterostructures from different materials, yet from the same material class, has revolutionized electronic and optical technologies during the past decades. To explore novel electronic and optoelectronic functionalities based on heterostructures in a natural next step we have turned to systematically explore hybrid inorganic/organic materials systems (HIOS) in heterostructures combining materials from dissimilar material classes. Among different aspects in this HIOS research endeavour, it was found that an in-depth understanding and control over the energy level alignment in HIOS is the key to attain novel electronic and optoelectronic functionalities. In this contribution, we report on fundamental aspects of the self-assembled monolayer formation on different metal oxide and 2D semiconductors such as transition metal dichalcogenides, observations of switching processes and successful implementations in diode, light emitting diode, electrolyte gated field effect transistor and neuromorphic plasmonic device structures.

DS 6: Focus Session: Topological Phenomena in Synthetic Matter (joint session DS/HL)

Topological insulators are a striking example of materials in which topological invariants are manifested in robustness against perturbations. Topology has emerged as an abstract, yet surprisingly powerful, new paradigm for controlling the flow of an excitation, e.g. the flow of electrons or light. This interdisciplinary Focus Session aims at discussing the latest experimental and theoretical results in the fast developing field of topological phenomena in synthetic matter. The recent merging of topology and cold atoms, photonics, mechanics and many more fields promises a considerable impact on these disciplines. We bring together leading theoretical and experimental experts from the fields of topological phenomena in synthetic matter to discuss recent progress and interdisciplinary synergy emerging at the interface of these fields. Furthermore, we give an overview to young scientists of exciting possibilities of interdisciplinary research in these fields with the special focus on the practical applications of fundamental science.

Organizer: Sebastian Klembt (Julius-Maximilians-Universität Würzburg)

Time: Thursday 13:30–16:15 Location: H1

Topical Talk DS 6.1 Thu 13:30 H1

Exceptional Topology of Non-Hermitian Systems: from Theoretical Foundations to Novel Quantum Sensors — •Jan Carl Budich — Institute of Theoretical Physics, TU Dresden, Dresden, Germany

In a broad variety of physical settings ranging from classical meta-materials to open quantum systems, non-Hermitian (NH) Hamiltonians have proven to be a powerful and conceptually simple tool for effectively describing dissipation. Motivated by recent experimental discoveries, investigating the topological properties of such NH systems has become a major focus of current research. In this talk, I give a brief introduction to this rapidly growing field, and present our latest results. Specifically, we discuss the occurrence of novel topological phases unique to NH systems. There, the role of spectral degeneracies familiar from Hermitian systems such as Weyl semimetals is played by exceptional points at which the effective NH Hamiltonian becomes non-diagonalizable. Furthermore, we show how guiding principles of topological matter such as the bulk boundary correspondence are qualitatively changed in the NH realm. Finally, we demonstrate that the sensitivity of NH systems to small changes in the boundary conditions may be harnessed to devise novel high-precision sensors.

Topical Talk DS 6.2 Thu 14:00 H1

In situ fabrication of (Bi,Sb)-based topological insulator - superconductor hybrid devices — •Peter Schüffelgen — Forschungszentrum Jülich

With their experimental verification in 2007, topological insulators render a new and fascinating material class. A band inversion in the bulk of a 3D topological insulator creates a 2D metallic Dirac system at the physical surface of those 3D crystals. The surface Dirac states are topologically protected and have their spin locked to their momentum. This intrinsic quantum spin texture promises to enable fundamentally new, yet elusive quantum technologies, such as Majorana quantum bits. In this talk, I will introduce the material class of (Bi,Sb)-based topological insulators and discuss experimental challenges. I will present an in situ process that makes it possible to construct hybrid devices comprised of topological and superconductive nanostructures fully under ultra-high vacuum conditions via molecular beam epitaxy. A combination of stencil lithography and selective area growth allows for the realization of a variety of superconductor-topological insulator hybrid devices and solves the associated fabrication challenges.

Topical Talk DS 6.3 Thu 14:30 H1

Atomic monolayers as two-dimensional topological insulators — •Ralph Claessen — Physikalisches Institut und Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany

Two-dimensional topological insulators (2D-TIs) are characterized by hosting spin-polarized conducting band states at their one-dimensional (1D) edges, giving rise to the quantum spin Hall (QSH) effect. As pointed out in the seminal work of Kane and Mele, graphene would constitute the most simple realization of a QSH insulator if it were not for its almost negligible spin-orbit interaction. It has been suggested that going to heavier group IV monolayers (such as the Sn-derived "stanene") could remedy this problem, but a convincing demonstration of such 2D TIs is still lacking. Recently we discovered that the neighboring groups III and V in the Periodic Table provide a promising alternative. Here I will discuss rational design, epitaxial synthesis, as well as ARPES and STM studies of two such synthetic QSH insulators, namely Bi (bismuthene) and In (indenene) monolayers grown on SiC(0001) substrates.

15 minutes break

Topical Talk DS 6.4 Thu 15:15 H1

Topological Insulator Lasers — •Mordechai Segev — Technion - Israel Institute of Technology

Topological Insulator Lasers are semiconductor emitters fabricated on a potential landscape designed to harness the features of topological insulators to force injection-locking of the emitters, making them act as a single coherent laser. The concepts underlying topological insulator lasers will be reviewed along with the recent progress.

Topical Talk DS 6.5 Thu 15:45 H1

TBA — •Morais Smith —

DS 7: Thin Oxides and Organic Thin Films (joint session DS/CPP)

Time: Thursday 15:15–16:15 Location: H5

DS 7.1 Thu 15:15 H5

Hybrid electronic states in epitaxially layered perovskite oxide electrocatalysts for water electrolysis — •Lisa Heymann[1], Moritz Weber[1], Marcus Wohlgemuth[1], Felix Gunkel[1], and Christoph Baeumer[1,2] — [1]Peter Grunenberg Institute and JARA-FIT, Forschungszentrum Juelich GmbH, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, Netherlands

In electrochemical water splitting catalyzed by perovskite oxides (ABO_3), the B-O hybridization degree has a major impact on the electrocatalytic activity. Additionally, space charge layers at the interface to the electrolyte may hamper the electron transfer into the electrode, complicating the analysis of hybridization phenomena. The goal in this work was to explore whether A site doping in cobaltites ($ACoO_3$) has a major impact on the oxygen evolution reaction (OER) through a different degree of hybridization or the extend of a surface space charge layer. We investigated $La_{0.6}Sr_{0.4}CoO_3$ and $LaCoO_3$ bilayer structures in epitaxial thin films that enabled us to create a near surface depth profile of both, the hybridization degree and the doping concentration confirmed by x-ray photoelectron spectroscopy (XPS). In a Mott Schottky (MS) analysis, we showed that in the OER potential regime the catalytic activity is not limited by a space charge layer. Therefore, we can correlate the observed OER activity trend to the degree of hybridization in cobaltites. The combined XPS and MS analysis enables to differentiate between the influence of the hybridization degree and intrinsic space charge layers, which are indistinguishable in a sole physical or electrochemical characterization.

DS 7.2 Thu 15:30 H5

Tailored electrical characteristics in TiOx/HfOx-based memristive device for targeting neuromorphic computing — •Seongae Park[1,2], Stefan Klett[1], Tzvetan Ivanov[1,2], Andrea Knauer[2], Joachim Doell[2], and Martin Ziegler[1,2] — [1]Dep. of Electrical Engineering and Information Technology, TU Ilmenau — [2]Inst. of Micro and Nanotechnologies MacroNano, TU Ilmenau

Over the last few years, memristive devices have shown their high potential for neuromorphic computing. In particular, redox-based memristive devices have become the focus of research interest, since they enable precise emulation of synaptic functionality through local ionic processes. However, for targeted device functionality, a detailed understanding of ionic processes at the atomic level is required, which is often severely hampered by coupled electronic and ionic processes. In this talk, the bi-layer oxide system TiOx/HfOx is presented. In a combined approach using a 4-inch wafer process technology and a physical device model, we show the contribution of physical device parameters such as device area size, the thickness of HfOx, interface modification, as well as the stoichiometry of HfOx to the electrical characteristics. Furthermore, we present how those parameters can be tuned for customized device functionalities. In that respect, memristive devices with tailored I-V characteristics and analog resistive switching are obtained that own an intrinsic self-compliance and do not need electroforming-free cycles.

DS 7.3 Thu 15:45 H5

Arrangement and electronic properties of cobalt phthalocyanine molecules on Si(111) ($\sqrt{3} \times \sqrt{3}$) R30°-B — •Milan Kubicki, Martin Franz, Susi Lindner, Holger Eisele, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

The formation of self-assembled monolayers of organic molecular materials on solid surfaces is an important subject because of their possible application in advanced optical and electronic devices. Here, the molecular arrangement and the interfacial electronic properties of cobalt phthalocyanine (CoPc) on the deactivated Si(111) ($\sqrt{3} \times \sqrt{3}$) R30°-B surface are studied by scanning tunneling microscopy and spectroscopy [1,2]. It is found that for submonolayer coverages the CoPc molecules lie flat on the Si surface with the Co d_{z^2} orbital of the molecule forming a hybrid state with the p_z orbital of the Si adatom at the surface. For multilayer coverages in contrast, the CoPc molecules are tilted with respect to the Si surface forming highly ordered organic molecular films, and the electronic properties resemble those of pure CoPc.

[1] S. Lindner, M. Franz, M. Kubicki, S. Appelfeller, M. Dähne, and H. Eisele, Phys. Rev. B **100**, 245301 (2019).
[2] M. Kubicki, S. Lindner, M. Franz, H. Eisele, and M.Dähne, J. Vac. Sci. Technol. B **38**, 042803 (2020).

DS 7.4 Thu 16:00 H5

Experimental Quantification of Interaction Energies in Organic Monolayers — •Pierre-Martin Dombrowski, Stefan Renato Kachel, Leonard Neuhaus, Tobias Breuer, J. Michael Gottfried, and Gregor Witte — Philipps-Universität Marburg, Germany

The formation of molecular nanostructures is determined by the interplay of intermolecular and molecule-substrate interactions. However, these interactions are experimentally hardly accessible. Temperature-programmed desorption (TPD) is a fairly well-established experimental technique capable of quantifying both types of interaction, but its quantitative analysis is by no means trivial. In the present study, we analyse the desorption kinetics of the two organic semiconductors pentacene (PEN) and perfluoropentacene (PFP) from Au(111) and MoS_2 surfaces to show the potential of TPD, but also highlight challenges for large adsorbates. Combining TPD with scanning tunnelling microscopy, work function measurements and theoretical modelling, we show that intermolecular interactions are dominated by the intramolecular charge distribution, resulting in net intermolecular repulsion in unitary and attractive interactions in mixed PEN:PFP monolayers. We determine the coverage-dependent prefactor of desorption with unprecedented precision and correlate its evolution with the activation of specific degrees of freedom of motion of adsorbed molecules. Lastly, we compare differences in molecule-substrate interactions on Au(111) and MoS_2, revealing that (sub-)monolayers on MoS_2 are stabilized only by entropy.

DS 8: Annual General Meeting of the Thin Films Division

Time: Thursday 18:00–19:00 Location: MVDS

Annual General Meeting

DS 9: Focus Session: Highlights of Materials Science and Applied Physics II (joint session DS/HL)

Jointly organized on the occasion of the 60th anniversary of the *physica status solidi* journals (*pss*, http://www.pss-journals.com), this Focus Session features several invited presentations, talks and posters from key contributors on core condensed matter and applied physics topics. Highlights comprise the latest results on diamond, nitride semiconductors, organic materials, two-dimensional and quantum systems, oxides, magnetic materials, solar cells, thermoelectrics and more.

physica status solidi was launched by Akademie-Verlag Berlin in July 1961 and is published by Wiley-VCH Berlin and Weinheim today, supported by Wiley colleagues in China and the US. While in its first three decades it served as an East-West forum for solid state physics, since 1990 it has evolved into a family of journals with international author- and readership in a globalized scientific world. Its professional editorial services include topical curation, peer review organization, technical editing, special issue and hybrid open access publication.

The Focus session celebrates the numerous close collaborations and the steady support which the journals receive from their Advisory Board members, authors, reviewers and guest editors, including many members of the DPG and the condensed matter physics community in Germany.

(More information on '60 years of *pss*' is available at http://bit.ly/60_years_pss)

Organizers: Stefan Hildebrandt (Editor-in-Chief, pss), Norbert Esser (TU Berlin, ISAS) and Stephan Reitzenstein (TU Berlin)

Time: Friday 10:00–11:00 Location: H1

DS 9.1 Fri 10:00 H1

Additive manufacturing of permanent magnets based on $(CoCuFeZr)_{17}Sm_2$ — •Dagmar Goll, Felix Trauter, Philipp Braun, Judith Laukart, Ralf Löffler, Ute Golla-Schindler, and Gerhard Schneider — Aalen University, Materials Research Institute, Beethovenstr. 1, 73430 Aalen, Germany

Lab-scale additive manufacturing of $(CoCuFeZr)_{17}Sm_2$-based powder was performed to realize CoSm printed parts with hard magnetic properties. For manufacturing a special inert gas process chamber for laser powder bed fusion was used. A three-step annealing procedure analogous to sintered magnets was applied. This led to a coercivity of 2.77 T, remanence of 0.78 T and maximum energy density of 109.4 kJ/m^3 for the printed parts. Compared to an isotropic sintered magnet of comparable composition and annealing procedure, the coercivity is of the same order. Due to the texture of the printed parts the remanence is 24 % larger.

DS 9.2 Fri 10:15 H1

Structure solution of a large unit cell approximant derived from $SrTiO_3$ on Pt(111) — •Stefan Förster[1], Sebastian Schenk[1], Oliver Krahn[1], Holger L. Meyerheim[2], Marc DeBoissieu[3], and Wolf Widdra[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [3]Universite Grenoble Alps, CNRS, SIMaP, Saint-Martin d'Hères, France

The discovery of two-dimensional oxide quasicrystals (OQC) has caused a great amount of interest in aperiodic structure formation from perovskite materials on metal surfaces [1]. In recent years, a plethora of surface science techniques has been applied to OQCs to get an understanding of this peculiar materials system on the fundamental level [2]. In this contribution, we present low-temperature scanning tunneling microscopy (STM) and surface x-ray diffraction (SXRD) investigation of the largest unit cell approximant known so far in 2D systems. Its unit cell covers an area of approximately 44 Å × 44 Å and has p2gg symmetry. STM measurements show 48 atoms in the unit cell forming the vertices of 48 triangles, 18 squares and 6 rhombuses. The structure has been solved utilizing over 300 independent reflections measured by SXRD with an R-factor better than 0.20. From this analysis a profound understanding of the decoration of all tiles with Sr, Ti, and O ions is derived, which solves the structure of the parent OQC.

[1] S. Förster et. al., Nature 502, 215 (2013).
[2] S. Förster et al., Phys. Status Solidi B 257, 1900624 (2020).

DS 9.3 Fri 10:30 H1

Surface reconstructions: challenges and opportunities for the growth of perovskite oxides — Giada Franceschi, Michael Schmid, Ulrike Diebold, and •Michele Riva — Institute of Applied Physics, TU Wien, Austria

Achieving atomically flat and stoichiometric films of complex multicomponent oxides is crucial for integrating these materials in emerging technologies. While pulsed laser deposition (PLD) can in principle produce these high-quality films, experiments often show rough surfaces and nonstoichiometric compositions.

To understand the cause, we follow the growth at the atomic scale from its early stages, using STM. We focus on $SrTiO_3(110)$ and $La_{0.8}Sr_{0.2}MnO_3(110)$ films. For both, the non-stoichiometries introduced during growth accumulate at the surface. As a result, their surface structure evolves along phase diagrams of surface structure vs. composition [1,2,3]. This can drastically degrade the surface morphology: pits develop on reconstructed areas with different sticking [4]; ill-defined oxide clusters nucleate when the non-stoichiometry introduced is too large to be accommodated in the surface by changing its structure. On the flip side, one can take advantage of the high sensitivity of surface structures to composition deviations to grow films with thickness of several tens of nanometers retaining atomically flat surfaces, and with stoichiometry control better than 0.1% [1].

[1] Phys. Rev. Mater. **3**, 043802 (2019). [2] J. Mater. Chem. A **8**, 22947 (2020). [3] arXiv:2010.05205 (2020). [4] Phys. Rev. Res. **1**, 033059 (2019).

DS 9.4 Fri 10:45 H1

Investigation of Spin Pumping through α-Sn Interlayer — •Leszek Gladczuk[1], Lukasz Gladczuik[2], Piotr Dluzewski[1], Gerrit van der Laan[3], and Thorsten Hesjedal[2] — [1]Institute of Physics, Polish Academy of Science — [2]Department of Physics, Clarendon Laboratory, University of Oxford — [3]Diamond Light Source, Harwell Science and Innovation Campus

Elemental tin in the α-phase is an intriguing member of the family of topological quantum materials. In thin films, with decreasing thickness, α-Sn transforms from a 3D topological Dirac semimetal (TDS) to a 2D topological insulator (TI). Getting access to and making use of its topological surface states is challenging and requires interfacing to a magnetically ordered material. Recently we have successfully performed an epitaxial growth of α-Sn thin films on Co, forming the core of a spin-valve structure, is reported. Time- and element-selective ferromagnetic resonance experiments were conducted to investigate the presence of spin pumping through the spin-valve structure. A rigorous statistical analysis of the experimental data using a model based on the Landau-Lifshitz-Gilbert-Slonczewski equation was applied. A strong exchange coupling contribution was found, however no unambiguous proof for spin pumping. Nevertheless, the incorporation of α-Sn into a spin valve remains a promising approach given its simplicity as an elemental TI and its room-temperature application potential.

DS 10: Focus Session: Highlights of Materials Science and Applied Physics III (joint session DS/HL)

Time: Friday 11:15–13:00 Location: H1

DS 10.1 Fri 11:15 H1

Free-Standing ZnSe-Based Microdisk Resonators - Influence of Edge Roughness on the Optical Quality and Degradation Reduction with Supported Geometry — •Wilken Seemann[1], Alexander Kothe[1], Christian Tessarek[1], Gesa Schmidt[2], Siqi Qiao[2], Nils von den Driesch[2], Jan Wiersig[3], Alexander Pawlis[2], Gordon Callsen[1], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany — [3]Institut für Physik, Universität Magdeburg, Germany

Free-standing microdisks with ZnCdSe quantum wells in ZnMgSe barriers are analyzed using micro-photoluminescence (μPL). Stimulated emission into whispering gallery modes (WGMs) is demonstrated. Deformation functions of the resonators are determined via scanning electron microscopy (SEM). A correlation between edge roughness and optical quality is found. These results are confirmed by calculations based on the boundary element method using the measured deformation functions.

To reduce degradation in the ZnSe structures a fabrication technique new to this material system is introduced. It yields "supported" disks with no underetching which enhances the mechanical stability of the resonator and its thermal contact to the substrate. SEM measurements reveal an excellent structural quality of these resonators. The formation of WGMs in supported ZnSe:Cl resonators is demonstrated in μPL and confirmed by theoretical calculations.

DS 10.2 Fri 11:30 H1

Pyramid formation by etching of InGaN/GaN quantum well structures grown on N-face GaN for nano optical light emitters — •Uwe Rossow, Savutjan Sidikejiang, Samar Hagag, Philipp Henning, Rodrigo de Vasconcellos Lourenco, Heiko Bremers, and Andreas Hangleiter — TU Braunschweig, Inst. f. Angewandte Physik

While growth processes of $In_xGa_{1-x}N$/GaN quantum well structures on the Ga-face of GaN buffer layers are already optimized to obtain high quantum efficiency, the growth on N-face has gained momentum only in the last years. Compared to Ga-face $In_xGa_{1-x}N$ layers are more stable on N-face and the surface can easily be structured by wet chemical etching, which usually leads to the formation of pyramids on the surface. This allows a new way to realize nano optical light emitters which offers the possibility to produce structures with similar emission properties. First we grow $In_xGa_{1-x}N$/GaN (single or multi) quantum well structures on N-face GaN. In a second step pyramids are formed by KOH etching. We demonstrate that pyramids with smooth side facets of the type $(1\bar{1}0\bar{1})$ and sharp tips in the nanometer range can be achieved without any sign of damage. TEM reveals that InGaN quantum dot-like structures are present in the pyramids and in photoluminescence narrow emission lines are observed. The etching process depends on electrolyte composition and temperature, defects at the surface and surface morphology. A better control of this process is required to achieve reproducible nano structures.

DS 10.3 Fri 11:45 H1

Bulk and interfacial effects in the Co/Ni_xMn_{100-x} exchange-bias system due to creation of defects by Ar^+ sputtering — •Tauqir Shinwari[1], Ismet Gelen[1], Yasser A. Shokr[1,2], Ivar Kumberg[1], Ikram Ullah[3], Muhammad Sajjad[3], M. Yaqoob Khan[3], and Wolfgang Kuch[1] — [1]Freie Universität Berlin, Arnimallee 14, Berlin 14195, Germany — [2]Faculty of Science, Department of Physics, Helwan University, 17119 Cairo, Egypt — [3]Department of Physics, Kohat University of Science and Technology, Kohat, Khyber Pakhtunkhwa 26000, Pakistan

A series of experiments is carried out to identify the contribution of interface and bulk antiferromagnetic (AFM) spins to exchange bias (EB) in ultrathin epitaxial ferromagnetic (FM)/AFM bilayer samples. These are single-crystalline AFM Ni_xMn_{100-x} and FM Co layers on $Cu_3Au(001)$, in which structural or chemical defects are introduced by controlled Ar^+ sputtering at the surface of the AFM layer or at a certain depth inside the AFM layer. Comparison of the magnetic properties measured by magneto-optical Kerr effect for sputtered and non-sputtered parts of the same sample then allows a precise determination of the influence of sputtering on the AFM layer during the sample preparation. The results show that the creation of defects in the bulk of the AFM layer enhances the magnitude of EB and its blocking temperature, but not the ones at the interface. We also observed that the deeper the insertion of defects in the AFM layer, the higher the EB field and the larger the coercivity. These findings are discussed as the effect of additional pinning centers in the bulk of the AFM layer.

DS 10.4 Fri 12:00 H1

Study of annealing effect on RF-sputtered Bi2Te3 thin films with full figure of merit characterization. — •Gyuhyeon Park, Maksim Naumochkin, Kornelius Nielsch, and Heiko Reith — Leibniz Institute for Solid State and Materials Research Dresden (IFW Dresden), Institute for Metallic Materials, Helmholtzstrasse 20, 01069 Dresden, Germany

Thermoelectric (TE) devices enable the direct conversion of heat into electricity and vice versa. The demand of micro TE harvesting or Peltier cooling devices for application in autonomous sensor systems required for the internet of things (IoT) will prospectively drastically increase in the coming years. Such microdevices are typically fabricated using electrodeposition or physical vapor deposition, where the successful optimization of the thermoelectric figure of merit, zT, which is the key enabler for the introduction of these devices to application. Accordingly, thin film fabrication methods and material investigation are of high interest. In this study, we report on the thermoelectric characterization of RF sputtered n-Bi2Te3 thin films with various thicknesses. For the in-plane Seebeck coefficient, Hall coefficient, electrical, and thermal conductivity measurement a thin film analyzer (TFA) has been used. We will discuss the influence of temperature effects on the transport properties, including in-situ annealing experiments and the relation to the structure, grain size, and chemical composition which was analyzed with XRD, SEM and EDX.

DS 10.5 Fri 12:15 H1

Passivating polysilicon recombination junctions for crystalline silicon solar cells — •Franz-Josef Haug[1], Audrey Morisset[1], Philippe Wyss[1], Mario Lehmann[1], Aicha Hessler-Wyser[1], Andrea Ingenito[1], Quentin Jeangros[1], Christophe Ballif[1], Shyam Kumar[2], Santhana Eswara[2], and Nathalie Valle[2] — [1]Ecole Poiytechnique Fédérale de Lausanne (EPFL), School of Engineering, PV-Lab, Switzerland — [2]Luxembourg Institute of Science and Technology (LIST), Materials Research and Technology Department, Luxembourg

We investigate polysilicon recombination junctions, whose n-type bottom layer also acts as passivating contact to the silicon surface. They are a key element in tandem devices with a silicon bottom cell, and they could be used to simplify the processing sequence of single-junction cells with interdigitated back contacts. Processing requires high temperatures to crystallize the layers, however, this step can also deteriorate the tunnelling junction by diffusion of dopants. We analyse depth profiles of the doping concentrations in the layers and diffusion across the interface between them by secondary ion mass spectrometry (SIMS) in dynamic mode. We show that undesired diffusion is suppressed by modifying the interface with C, O, or a combination of these. Moreover, we demonstrate that this modification does not interfere with the diffusion of H which is an essential element to passivate defects at the wafer surface. Thus, we find implied open-circuit voltages up to 740 mV for contact resistivities less than 40 mΩcm2, and we demonstrate tandem cells with efficiency above 20%.

DS 10.6 Fri 12:30 H1

Homoepitaxial diamond lateral growth: a new methodology for the next generation of power devices — •Fernando Lloret[1], Daniel Araujo[2], David Eon[3], and Etienne Bustarret[3] — [1]Department of Applied Physics, University of Cádiz, 11510, Puerto Real (Cádiz) Spain — [2]Department of Material Science, University of Cádiz, 11510, Puerto Real (Cádiz) Spain — [3]Univ. Grenoble-Alpes, CNRS, Institut Néel, 38000 Grenoble, France

Diamond is expected to be the base material for future power electronic devices. However, the technological steps and the particularities inherent to the material remain impassable issues for its industrial implementation. Shortcomings such as the high density of substrate defects and small substrate sizes (less than 1 cm2), the large number of required non-fully-controlled technology steps (etch and deposition or growth) or electrical problems related to the classical geometries (high electric fields, leakages*) can be overcome by using lateral growth. The progress of this promising diamond deposition methodology, capable of drastically reducing defects density, promoting selective doping and providing a wealth of alternative geometries for the device, is here reviewed.

DS 10.7 Fri 12:45 H1

Impact of electrical current on single GaAs nanowire structure — •Ullrich Pietsch[1], Danial Bahrami[1], Ali AlHassan[1], Arman Davtyan[1], Taseer Anjum[1], Ren Zhe[2], Rainer Timm[2], Lutz Geelhaar[3], Jesus Herranz[3], and Dmiri Novikov[4] — [1]University of Siegen, Siegen, Germany — [2]University of Lund, Lund , Sweden — [3]Paul Drude Institute, Berlin, Germany — [4]DESY, Hamburg, Germany

The impact of electrical current on the structure of single free-standing Be-doped GaAs nanowires grown on a Si 111 substrate has been investigated by X-ray nano-diffraction before and after the application of an electrical current. The conductivity measurements of same nanowires in their as-grown geometry have been realized via W-probes installed inside a dual beam focused ion beam/scanning electron microscopy chamber. Comparing reciprocal space maps of the 111 Bragg reflection before and after the conductivity measurement, we find a deformation of the hexagonal nanowire cross-section, tilting and bending with respect to the substrate normal. For electrical current densities above 347 A/mm^2, the diffraction pattern was completely distorted. Confirmed by SEM the reconstructed cross-section of the illuminated nanowire shows elongation of two pairs of opposing side facets accompanied by shrinkage of the third pair of facets. To explain our findings, we suggest material melting due to Joule heating during voltage/current application accompanied by anisotropic deformations induced by the W-probe.

DS 11: 2D semiconductors and van der Waals heterostructures II (joint session HL/DS)

Time: Friday 13:30–14:45 Location: H4

See HL 25 for details of this session.

Dynamics and Statistical Physics Division
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Overview of Invited Talks and Sessions

(Lecture halls H2 and H6; Poster P)

Invited Talks

DY 2.1	Tue	10:00–10:30	H6	**Local Versus Global Two-Photon Interference in Quantum Networks** — •Sonja Barkhofen, Thomas Nitsche, Syamsundar De, Evan Meyer-Scott, Johannes Tiedau, Jan Sperling, Aurél Gábris, Igor Jex, Christine Silberhorn
DY 9.1	Wed	13:30–14:00	H6	**Nanofriction in Ion Coulomb Systems** — •Tanja Mehlstäubler
DY 10.1	Wed	15:00–15:30	H6	**Effect of fibrosis on propagation on non-linear waves and onset of arrhythmias in cardiac tissue** — •Alexander Panfilov, Timur Nezlobinsky, Farhad Pashakhanloo
DY 10.4	Wed	16:00–16:30	H6	**Chaos and nonlinear dynamics in the heart: Experiments and simulations of arrhythmias and defibrillation** — •Flavio fenton
DY 13.1	Thu	13:30–14:00	H2	**Multi-scale modeling of dyadic structure-function relation in ventricular cardiac myocytes** — •Martin Falcke, Filippo G. Cosi, Wolfgang Giese, Wilhelm Neubert, Stefan Luther, Nagaiah Chmakuri, Ulrich Parlitz
DY 13.4	Thu	14:45–15:15	H2	**Cardiac repolarization dynamics and arrhythmias in healthy and diseased hearts** — •Esther Pueyo
DY 13.7	Thu	15:45–16:15	H2	**Dynamics of paroxysmal tachycardias** — •Gil Bub
DY 18.1	Fri	13:30–14:00	ESS	**Network-Induced Multistability Through Lossy Coupling** — •Jürgen Kurths
DY 18.2	Fri	14:00–14:30	ESS	**Control of synchronization in two-layer power grids** — •Simona Olmi, Carl Totz, Eckehard Schöll
DY 18.3	Fri	15:00–15:30	ESS	**Relay and complete synchronization of chimeras and solitary states in heterogeneous networks of chaotic maps** — Elena Rybalova, Eckehard Schöll, •Galina Strelkova
DY 18.4	Fri	15:30–16:00	ESS	**A bridge between the fractal geometry of the Mandelbrot set and partially synchronized dynamics of chimera states.** — •Ralph G Andrejzak

Invited talks of the joint symposium Topological constraints in biological and synthetic soft matter (SYSM)

See SYSM for the full program of the symposium.

SYSM 1.1	Mon	10:00–10:30	Audimax 1	**Interphase Chromatin Undergoes a Local Sol-Gel Transition Upon Cell Differentiation** — •Alexandra Zidovska
SYSM 1.2	Mon	10:30–11:00	Audimax 1	**Topological Tuning of DNA Mobility in Entangled Solutions of Supercoiled Plasmids** — •Jan Smrek, Jonathan Garamella, Rae Robertson-Anderson, Davide Michieletto
SYSM 1.3	Mon	11:15–11:45	Audimax 1	**Dynamics of macromolecular networks under topological and environmental constraints: some outstanding challenges** — •Dimitris Vlassopoulos
SYSM 1.4	Mon	11:45–12:15	Audimax 1	**Supercoiling in a Protein Increases its Stability** — •Joanna Sulkowska, Szymon Niewieczerzał
SYSM 1.5	Mon	12:15–12:45	Audimax 1	**Topology for soft matter photonics** — •Igor Musevic

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium The Physics of CoViD Infections (SYCO)

See SYCO for the full program of the symposium.

SYCO 1.1	Mon	13:30–14:00	Audimax 1	**A Tethered Ligand Assay to Probe SARS-CoV-2:ACE2 Interactions** — Magnus Bauer, Sophia Gruber, Adina Hausch, Lukas Milles, Thomas Nicolaus, Leonard Schendel, Pilar Lopez Navajas, Erik Procko, Daniel Lietha, Rafael Bernadi, Hermann Gaub, •Jan Lipfert
SYCO 1.2	Mon	14:00–14:30	Audimax 1	**From molecular simulations towards antiviral therapeutics against COVID-19** — •Rebecca Wade
SYCO 1.3	Mon	14:45–15:15	Audimax 1	**The physical phenotype of blood cells is altered in COVID-19** — Markéta Kubánková, Martin Kräter, Bettina Hohberger, •Jochen Guck
SYCO 1.4	Mon	15:15–15:45	Audimax 1	**Extended lifetime of respiratory droplets in a turbulent vapor puff and its implications on airborne disease transmission** — •Detlef Lohse, Kai Leong Chong, Chong Shen Ng, Naoki Hori, Morgan Li, Rui Yang, Roberto Verzicco
SYCO 1.5	Mon	15:45–16:15	Audimax 1	**Beyond the demographic vaccine distribution: Where, when and to whom should vaccines be provided first?** — •Benno Liebchen, Jens Grauer, Fabian Schwarzendahl, Hartmut Löwen

Invited talks of the joint symposium Amorphous materials: structure, dynamics, properties (SYAM)

See SYAM for the full program of the symposium.

SYAM 1.1	Tue	13:30–14:00	Audimax 1	**Glassy dynamics of vitrimers** — •Liesbeth Janssen
SYAM 1.2	Tue	14:00–14:30	Audimax 1	**Liquid-Liquid Phase Transition in Thin Vapor-Deposited Glass Films** — •Zahra Fakhraai
SYAM 1.3	Tue	14:30–15:00	Audimax 1	**Connection between structural properties and atomic motion in ultraviscous metallic liquids close to the dynamical arrest** — •Beatrice Ruta, Nico Neuber, Isabella Gallino, Ralf Busch
SYAM 1.4	Tue	15:15–15:45	Audimax 1	**Signatures of the spatial extent of plastic events in the yielding transition in amorphous solids** — •Celine Ruscher, Daniel Korchinski, Joerg Rottler
SYAM 1.5	Tue	15:45–16:15	Audimax 1	**Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment** — •Olfa D'Angelo, W. Till Kranz

Invited talks of the joint symposium Facets of many-body quantum chaos (SYQC)

See SYQC for the full program of the symposium.

SYQC 1.1	Tue	13:30–14:00	Audimax 2	**Holographic interpretation of SYK quantum chaos** — •Alexander Altland
SYQC 1.2	Tue	14:00–14:30	Audimax 2	**Non-Fermi liquids and the lattice** — •Sean Hartnoll
SYQC 1.3	Tue	14:30–15:00	Audimax 2	**Dual-unitary circuits: non-equilibrium dynamics and spectral statistics** — •Bruno Bertini
SYQC 1.4	Tue	15:15–15:45	Audimax 2	**Post-Ehrenfest many-body quantum interferences in ultracold atoms** — •Steven Tomsovic
SYQC 1.5	Tue	15:45–16:15	Audimax 2	**Dynamics in unitary and non-unitary quantum circuits** — •Vedika Khemani

Invited talks of the joint symposium Advanced neuromorphic computing hardware: Towards efficient machine learning (SYNC)

See SYNC for the full program of the symposium.

SYNC 1.1	Wed	10:00–10:30	Audimax 1	**Equilibrium Propagation: a Road for Physics-Based Learning** — •Damien Querlioz
SYNC 1.2	Wed	10:30–11:00	Audimax 1	**Machine Learning and Neuromorphic Computing: Why Physics and Complex Systems are Indispensable** — •Ingo Fischer
SYNC 1.3	Wed	11:00–11:30	Audimax 1	**Photonic Tensor Core Processor and Photonic Memristor for Machine Intelligence** — •Volker Sorger
SYNC 1.4	Wed	11:45–12:15	Audimax 1	**Material learning with disordered dopant networks** — •Wilfred van der Wiel
SYNC 1.5	Wed	12:15–12:45	Audimax 1	**In-memory computing with non-volatile analog devices for machine learning applications** — •John Paul Strachan

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Diversity on the Device Scale (SYHN)

See SYHN for the full program of the symposium.

SYHN 1.1	Thu	10:00–10:30	Audimax 1	**Scaling behavior of stiffness and strength of hierarchical network nanomaterials** — •Shan Shi
SYHN 1.2	Thu	10:30–11:00	Audimax 1	**Functional and programmable DNA nanotechnology** — •Laura Na Liu
SYHN 1.3	Thu	11:15–11:45	Audimax 1	**Multivalent nanoparticles for targeted binding** — •Stefano Angioletti-Uberti
SYHN 1.4	Thu	11:45–12:15	Audimax 1	**Programming Nanoscale Self-Assembly** — •Oleg Gang
SYHN 1.5	Thu	12:15–12:45	Audimax 1	**Achieving Global Tunability via Local Programming of a Structure's Composition** — •Jochen Mueller

Invited talks of the joint symposium Climate and energy: Challenges and options from a physics perspectiv (SYCE)

See SYCE for the full program of the symposium.

SYCE 1.1	Thu	13:30–14:00	Audimax 1	**The challenge of anthropogenic climate change - Earth system analysis can guide climate mitigation policy** — •Matthias Hofmann

SYCE 1.2	Thu	14:00–14:30	Audimax 1	**Towards a carbon-free energy system: Expectations from R&D in renewable energy technologies** — •Bernd Rech, Rutger Schlatmann
SYCE 1.3	Thu	14:30–15:00	Audimax 1	**Decarbonizing the Heating Sector - Challenges and Solutions** — •Florian Weiser
SYCE 1.4	Thu	15:15–15:45	Audimax 1	**A carbon-free Energy System in 2050: Modelling the Energy Transition** — •Christoph Kost, Philip Sterchele, Hans-Martin Henning
SYCE 1.5	Thu	15:45–16:15	Audimax 1	**The transition of the electricity system to 100% renewable energy: agent-based modeling of investment decisions under climate policies** — •Kristian Lindgren

Invited talks of the joint symposium Active nematics: From 2D to 3D (SYAN)

See SYAN for the full program of the symposium.

SYAN 1.1	Fri	10:00–10:30	Audimax 1	**Corrugated patterns made from an active nematic sheet** — •Anis Senoussi, Shunichi Kashida, Raphaël Voituriez, Jean-Christophe Galas, Ananyo Maitra, Estevez-Torres André
SYAN 1.2	Fri	10:30–11:00	Audimax 1	**Wrinkling instability in 3D active nematics** — •Isabella Guido
SYAN 1.3	Fri	11:15–11:45	Audimax 1	**Three-dimensional active nematic defects and their energetics** — •Miha Ravnik
SYAN 1.4	Fri	11:45–12:15	Audimax 1	**Liquid-crystal organization of liver tissue** — •Benjamin M Friedrich, Hernan Morales-Navarrete, Andre Scholich, Hidenori Nonaka, Fabian Segovia Miranda, Steffen Lange, Jens Karschau, Yannis Kalaidzidis, Frank Jülicher, Marino Zerial
SYAN 1.5	Fri	12:15–12:45	Audimax 1	**Machine learning active nematic hydrodynamics** — •Vincenzo Vitelli

Sessions

DY 1.1–1.4	Mon	10:00–11:15	H1	**Statistical physics of biological systems (joint session BP/DY)**
DY 2.1–2.7	Tue	10:00–12:15	H6	**Quantum Chaos**
DY 3.1–3.11	Tue	17:30–19:30	P	**Poster Sesssion I: Quantum Chaos and Many-Body Quantum Dynamics**
DY 4.1–4.10	Tue	17:30–19:30	P	**Poster Session II: Nonlinear Dynamics, Simulations and Machine Learning**
DY 5.1–5.15	Tue	17:30–19:30	P	**Poster Session III: Statistical Physics, Complex Fluids and Soft Matter**
DY 6.1–6.8	Wed	10:00–12:45	H3	**Soft Matter (joint session CPP/DY)**
DY 7.1–7.11	Wed	10:00–13:00	H6	**Focus Session: Facets of Many-Body Quantum Chaos (organised by Markus Heyl and Klaus Richter) (joint session DY/TT)**
DY 8.1–8.7	Wed	11:15–13:00	H7	**Quantum Computing (joint session TT/DY)**
DY 9.1–9.4	Wed	13:30–14:45	H6	**Many-Body Quantum Dynamics I (joint session DY/TT)**
DY 10.1–10.4	Wed	15:00–16:30	H6	**Focus session: Nonlinear Dynamics of the Heart I (organized by Markus Bär, Stefan Luther and Ulrich Parlitz)**
DY 11.1–11.6	Thu	10:00–11:30	H2	**Many-Body Quantum Dynamics II (joint session DY/TT)**
DY 12.1–12.5	Thu	11:45–13:00	H2	**Active Matter (joint session DY/BP/CPP)**
DY 13.1–13.7	Thu	13:30–16:15	H2	**Focus session: Nonlinear Dynamics of the Heart II (organized by Markus Bär, Stefan Luther and Ulrich Parlitz)**
DY 14	Thu	18:00–19:00	MVDY	**Mitgliederversammlung Fachverband DY**
DY 15.1–15.4	Fri	10:00–11:00	H2	**Condensed-Matter Simulations augmented by Advanced Statistical Methodologies (joint session DY/CPP)**
DY 16.1–16.5	Fri	11:15–12:30	H2	**Machine Learning in Dynamical Systems and Statistical Physics (joint session DY/BP)**
DY 17.1–17.5	Fri	13:30–15:00	H3	**Theory and Simulation (joint session CPP/DY)**
DY 18.1–18.4	Fri	13:30–16:00	ESS	**Symposium: Synchronization Patterns in Complex Dynamical Networks (organized by Jakub Sawicki, Sabine Klapp, Markus Bär and Jens Christian Claussen) (joint session DY/SOE)**
DY 19.1–19.6	Fri	13:30–15:00	H6	**Transport (joint session TT/DY)**

Annual General Meeting of the Dynamics and Statistical Physics Division

Donnerstag, 30. September 2021 18:00–19:00 MVDY

- Bericht DY Aktivitäten und Entwicklung 2020 - 21
- Planung Frühjahrstagung Regensburg 2022
- Verschiedenes

Sessions

– Invited Talks, Contributed Talks, and Posters –

DY 1: Statistical physics of biological systems (joint session BP/DY)

Time: Monday 10:00–11:15 Location: H1

See BP 1 for details of this session.

DY 2: Quantum Chaos

Time: Tuesday 10:00–12:15 Location: H6

Invited Talk DY 2.1 Tue 10:00 H6

Local Versus Global Two-Photon Interference in Quantum Networks — •Sonja Barkhofen[1], Thomas Nitsche[1], Syamsundar De[1], Evan Meyer-Scott[1], Johannes Tiedau[1], Jan Sperling[1], Aurél Gábris[2,3], Igor Jex[2], and Christine Silberhorn[1] — [1]Applied Physics, University of Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany — [2]Department of Physics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Brehová 7, 115 19 Praha 1-Stare Mesto, Czech Republic — [3]Wigner Research Centre for Physics, Konkoly-Thege M. út 29-33, H-1121 Budapest, Hungary

We devise an approach to characterizing the intricate interplay between classical and quantum interference of two-photon states in a network, which comprises multiple time-bin modes. By controlling the phases of delocalized single photons, we manipulate the global mode structure, resulting in distinct two- photon interference phenomena for time-bin resolved (local) and time-bucket (global) coincidence detection. This coherent control over the photons' mode structure allows for synthesizing two-photon interference patterns, where local measurements yield standard Hong-Ou-Mandel dips while the global two-photon visibility is governed by the overlap of the delocalized single-photon states. Thus, our experiment introduces a method for engineering distributed quantum interferences in networks.

DY 2.2 Tue 10:30 H6

Interplay between coherent and incoherent decay processes in chaotic systems: the role of quantum interference — •Camilo Alfonso Moreno Jaimes and Juan-Diego Urbina — Regensburg University, Regensburg, Germany

The population decay due to a small opening in an otherwise closed cavity supporting chaotic classical dynamics displays a quantum correction on top of the classical exponential form, a pure manifestation of quantum coherence that acquires a universal form and can be explained by path interference. Being coherent, such enhancement is prone to decoherence effects due to the coupling of the system to an external environment. We study this interplay between incoherent and coherent quantum corrections to decay by evaluating, within a Caldeira-Leggett scenario, off-diagonal contributions to the decoherence functional coming from pairs of correlated classical paths in the time regime where dissipative effects are neglected and decoherence does not affect the classical dynamics, but quantum interference must be accounted for. We find that the competing effects of interference and decoherence lead to a universal nonmonotonic form for the survival probability depending only on the coupling strength and macroscopic parameters of the cavity.

DY 2.3 Tue 10:45 H6

Geometry of complex instability in four-dimensional symplectic maps — •Jonas Stöber and Arnd Bäcker — TU Dresden, Institut für Theoretische Physik

In four-dimensional symplectic maps complex instability of periodic orbits is possible, which cannot occur for the two-dimensional case. We investigate the transition from stable to complex unstable dynamics of a fixed point under parameter variation. The change in the geometry of regular structures is visualized using three-dimensional phase-space slices and in frequency space using the example of two coupled standard maps. The chaotic dynamics is studied using escape time plots and two-dimensional invariant manifolds associated with the complex unstable fixed point. Based on a normal-form description, we investigate the underlying transport mechanism by visualizing the escape paths and the long-time confinement in the surrounding of the complex unstable fixed point.

15 min. break.

DY 2.4 Tue 11:15 H6

Chaos induced by interface produces universal Hong-Ou-Mandel correlations in topological insulators — •Andreas Bereczuk, Juan Diego Urbina, Cosimo Gorini, and Klaus Richter — Institut of Theoretical Physics, University Regensburg, Germany

The celebrated Hong-Ou-Mandel (HOM) effect [1] is a known coherent manifestation of the indistinguishable-distinguishable transition that is experimentally accessible through measurements of the transmission probability for two-body fermionic states propagating through a quantum point contact in electron quantum optics [2]. As shown in
[3, 4], universal HOM correlations are visible by substituting the quantum point contact by a chaotic cavity in a mesoscopic regime [3] where universal correlations of the scattering matrix entries at different energies enter. We present here a numerical analysis of this correlators for a HOM setup with normal cavities playing the role of complex beam splitters and edge states of a topologiocal insulator instead of waveguides. Our main observation is the emergence of universal HOM correlations in this setup where chaotic dynamics is driven by the high reflectivity due to mode mismatch at the interfaces.

[1] C. K. Hong, Z. Y. Ou and L. Mandel, Phys. Rev. Lett. 59, 2044 (1987)
[2] E. Bocquillon et al., Annalen der Physik 526, 1 (2014)
[3] J. D. Urbina et al., Phys. Rev. Lett. 116, 100401 (2016)
[4] A. Bereczuk et al., Phys. Rev. E 103, 052209 (2021)

DY 2.5 Tue 11:30 H6

Dirac fermion optics and directed emission from single- and bilayer graphene cavities — •Jule Katharina Schrepfer[1], Szu-Chao Chen[2], Ming-Hao Liu[2], Klaus Richter[3], and Martina Hentschel[4] — [1]Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]National Cheng Kung University, Tainan 70101, Taiwan — [3]Universität Regensburg, 93040 Regensburg, Germany — [4]Technische Universität Chemnitz, 09107 Chemnitz, Germany

High-mobility graphene hosting massless charge carriers with linear dispersion provides a promising platform for electron optics phenomena. Inspired by the physics of dielectric optical micro-cavities where the photon emission characteristics can be efficiently tuned via the cavity shape, we study corresponding mechanisms for trapped Dirac fermionic resonant states in deformed microdisk graphene billiards and directed emission from those. In such graphene devices a back-gatevoltage provides an additional tunable parameter to mimic different effective refractive indices and thereby the corresponding Fresnel laws at the boundaries. Moreover, cavities based on single-layer and double-layer graphene exhibit Klein- and anti-Klein tunneling. Moreover,we find a variety of different emission characteristics depending on the position of the source where charge carriers are fed into the cavites. Combining quantum mechanical simulations with optical ray tracing and a corresponding phase-space analysis, we demonstrate strong confinement of the emitted charge carriers in the mid field of single-layer graphene systems and can relate this to a lensing effect. For bilayer graphene, trapping of the resonant states is more efficient.

DY 2.6 Tue 11:45 H6

Optical microcavities in a ray picture with phase information — •Lukas Seemann — TU Chemnitz

Ray-wave correspondence has proven a useful tool to describe various aspects of optical microcavities, for example the far-field emission of deformed microdisk resonators. However, for more complicated settings such as coupled microcavities, interference effects will become important [1]. To this end we expand the ray description by the phase information and include the phase collected by the light ray along its trajectory [2] into the model. We explore the chances as well as possible limitations of this approach in various examples and investigate to what extent a ray model with phase information can deepen ray-wave correspondence.

[1] J. Kreismann, J. Kim, M. Bosch, M. Hein, S. Sinzinger, and M. Hentschel, Super-directional light emission and emission reversal from micro cavity arrays, Phys. Rev. Res. 1, 033171(1-5) (2019).
[2] M. Hentschel and M. Vojta, Multiple beam interference in a quadrupolar glass fiber, Opt. Lett. 26, 1764-1766 (2001).

DY 2.7 Tue 12:00 H6

Emergent fractal phase in energy stratified random models — •Anton Kutlin and Ivan Khaymovich — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187-Dresden, Germany

We study the effects of partial correlations in kinetic hopping terms of long-range disordered random matrix models on their localization properties. We consider a set of models interpolating between fully-localized Richardson's model and the celebrated Rosenzweig-Porter model (with implemented translation-invariant symmetry). In order to do this, we propose the energy-stratified spectral structure of the hopping term, allowing one to gradually decrease the range of correlations. We show both analytically and numerically that any deviation from the completely correlated case leads to the emergent non-ergodic delocalization in the system unlike the predictions of localization of cooperative shielding. In order to describe the models with correlated kinetic terms, we develop the generalization of the Dyson Brownian motion and cavity approaches basing on stochastic matrix process with independent rank-one matrix increments and examine its applicability to the above set of models

DY 3: Poster Sesssion I: Quantum Chaos and Many-Body Quantum Dynamics

Time: Tuesday 17:30–19:30 Location: P

DY 3.1 Tue 17:30 P

Drift-induced Delocalization Transition in Resonance Channels — •Jan Robert Schmidt, Arnd Bäcker, and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik, Dresden

In higher-dimensional Hamiltonian systems resonance channels play a prominent role. Transport is typically slow due to Arnold diffusion, leading quantum mechanically to dynamical localization. Resonance channels widen as they approach the chaotic sea. We show that this induces (i) classically a drift and (ii) quantum mechanically leads to delocalization if the drift is strong enough. We propose a scaling of the delocalization transition by a single transition parameter. These phenomena are confirmed in a 4D symplectic map with a large resonance channel.

DY 3.2 Tue 17:30 P

Dynamics of NV centers interacting with background spins — •Lukas Voss and Jürgen Stockburger — Institute for Complex Quantum Systems, Ulm University

The nitrogen vacancy (NV) center in diamond is considered to be one of the most promising physical systems for application in emerging quantum technologies such as quantum sensing and quantum computing [1]. The corresponding protocols are highly sensitive to the interactions of NV centers with either ^{13}C background spins or other NV centers.

The number of spins typically involved is too large for direct methods of propagation (curse of dimensionality). As a remedy, we modify a stochastic jump method for coherent quantum dynamics introduced by Breuer [2], which greatly reduces the dimension of the state space of the propagation (sum vs. product spaces).

We demonstrate this technique for an NV center and several nuclear background spins and find attractive performance characteristics. Further investigations are aimed at clustering a large number of background spins. Treating intra-cluster interactions by unitary propagation while applying the jump approach to inter-cluster interactions will further improve simulation performance.

[1] MW Doherty et al., *Physics Reports* **528**, 1 (2013)
[2] H-P Breuer *Physical Review A* **69**, 122 (2004)

DY 3.3 Tue 17:30 P

Quantum signatures of partial barriers in 4D symplectic maps — •Jonas Stöber, Arnd Bäcker, and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik

Partial transport barriers in the chaotic sea of Hamiltonian systems restrict classical chaotic transport, as they only allow for a small flux between phase-space regions. Quantum mechanically for 2D symplectic maps one has a universal quantum localizing transition. The scaling parameter is the ratio of flux to the Planck cell of size h, such that quantum transport is suppressed if h is much greater than the flux, while mimicking classical transport if h is much smaller.

In a higher-dimensional 4D map one naively expects that the relevant scaling parameter is the same, but now with a Planck cell of size h squared. We show that due to dynamical localization along resonance channels the localization length modifies the scaling parameter. This is demonstrated for coupled kicked rotors for a partial barrier that generalizes a cantorus to higher dimensions.

DY 3.4 Tue 17:30 P

Enhanced state transfer by complex instability in coupled kicked tops — •Maximilian Kieler and Arnd Bäcker — Technische Universität Dresden, Institut für Theoretische Physik and Center for Dynamics, Dresden, Germany

By considering coupled kicked tops we provide a mechanism for a fast transfer between two specific states representing bits. This crucially relies on that fact that the semiclassical limit corresponds to a higher-dimensional system which allows for more types of stability of fixed points than the two-dimensional case. Tuning the parameters, the coupled kicked tops have fixed points with complex instability. Quantum mechanically this allows for a rapid transfer between coherent states located at these points, which is much faster than the coexisting dynamical tunneling.

DY 3.5 Tue 17:30 P

Fermionic duality beyond weak coupling: General simplifications of open-system dynamics — •Valentin Bruch[1], Konstantin Nestmann[1], Jens Schulenborg[2], and Maarten Wegewijs[1,3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany and JARA-FIT, 52056 Aachen — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen — [3]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

A large class of fermionic open systems obeys a powerful dissipative analogue of the "symmetry" of hermitian conjugation in closed quantum systems. This *fermionic duality relation* applies to quantum-impurity transport models with strong interactions and hybridization exhibiting many-body and memory effects. Here we extend this relation from the time-nonlocal memory-kernel approach (Nakajima-Zwanzig) to prominent quantum-information inspired approaches in their exact formulation [arXiv:2104.11202]. These include the Kraus-operator decomposition of the dynamical map as well as the time-convolutionless quantum master equation with a time-local generator and generalized Lindblad jump-operators. Whereas in some of these formulations this yields a strong restriction on the involved quantities, in others it can be exploited to partially by-pass nontrivial time-evolution calculations. Fermionic duality also offers new insights into the divisibility and causal structure of the dynamics and applied to nonperturbative semigroup approximations [Phys. Rev. X 11, 021041 (2021)] it provides a new way to construct initial-slip corrections.

DY 3.6 Tue 17:30 P

Quantum dynamics and thermodynamics in nanosystems with strong electronic-vibrational coupling under external driving — •Jakob Bätge[1], Wenjie Dou[2], Amikam Levy[3], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg, Freiburg, Germany — [2]School of Science, Westlake University, Hangzhou, China — [3]Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel

The development and optimization of quantum devices increase the interest in dynamics and thermodynamics of systems on the scale of single atoms and molecules. In this contribution, we investigate the nonequilibrium quantum dynamics of a time-dependent driven nanosystem with interacting electronic and vibrational degrees of freedom utilizing the numerically exact hierarchical equations of motion approach for multiple fermionic and bosonic environments [1]. We analyze the role of vibrations in the electronic friction induced by electronic-vibrational coupling and identify the adiabatic and nonadiabatic contributions to thermodynamic quantities[2].

[1] J. Bätge *et al.*, Phys. Rev. B **103**, 235413 (2021)
[2] W. Dou *et al.*, Phys. Rev. B **101**, 184304 (2020)

DY 3.7 Tue 17:30 P

Floquet prethermalization and Rabi oscillations in optically excited Hubbard clusters — •Junichi Okamoto[1,2] and Francesco Peronaci[3] — [1]Institute of Physics, University of Freiburg, Germany — [2]EUCOR Centre for Quantum Science and Quantum Computing, University of Freiburg, Germany — [3]Max Planck Institute for the Physics of Complex Systems, Germany

Floquet engineering is a growing field of study to realize exotic many-body quantum states beyond the conventional material science in equilibrium. The Floquet picture in terms of effective Hamiltonians is valid in the limit of high-frequency drive, where the heating rate is suppressed. In contrast, when the drive frequency is comparable to the energies of the system, the effect of heating is non-negligible, and the analysis becomes intricate. However, even in this case, the existence of quasi-steady states, so-called Floquet prethermal states (FPSs), has been demonstrated, which expands the boundary of Floquet engineering to a realistic drive range. In this work, we have investigated the optically excited Hubbard clusters by exact diagonalization. We show that FPSs emerge not only off resonance but also for resonant excitation, provided a small field amplitude. Notably, FPSs at resonance occur with Rabi oscillations. At stronger fields, thermalization to infinite temperature is observed. We elucidate the origin of the FPSs using time-dependent perturbation theory and the two-site Hubbard model. A finite-size analysis substantiates the main findings.

DY 3.8 Tue 17:30 P

Transmission through three-terminal microwave graphs with orthogonal, unitary and symplectic symmetry — Felipe de Jesús Castañeda-Ramírez[1], Angel M. Martínez-Argüello[2], •Tobias Hofmann[3], Aimaiti Rehemanjiang[3], Moisés Martínez-Mares[1], José A. Méndez-Bermúdez[4], Ulrich Kuhl[5], and Hans-Jürgen Stöckmann[3] — [1]Departamento de Física, Universidad Autónoma Metropolitana-Iztapalapa, Apartado Postal 55-534, 09340 Ciudad de México, Mexico — [2]Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Apartado Postal 48-3, 62210 Cuernavaca, Mor., Mexico — [3]Fachbereich Physik der Philipps-Universität Marburg, D-35032 Marburg, Germany — [4]Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apartado Postal J-48, 72570 Puebla, Pue., Mexico — [5]Université Côte d'Azur, CNRS, Institut de Physique de Nice (INPHYNI), 06108 Nice, France

Transmission measurements through three-port microwave graphs are performed, in analogy to three-terminal voltage drop devices, with orthogonal, unitary, and symplectic symmetry. The terminal used as a probe is symmetrically located between two different chaotic subgraphs of the same mean density of states. Each subgraph is connected to one port, the input and the output, respectively. We find a good agreement with theoretical predictions, provided the effects of dissipation and imperfect coupling to the ports is considered. This extends previous studies using an asymmetric probe position [1].

[1] A. M. Martínez-Argüello et.al, Phys. Rev. B **98** (7) (2018) 075311.

DY 3.9 Tue 17:30 P

Heat transport through a superconducting artificial atom — •Meng Xu, Juergen Stockburge, and Joachim Ankerhold — ICQ and IQST, Ulm University, Germany

Theoretical studies of photonic heat transport and rectification in superconducting platforms play an important role not only in understanding current experimental findings but also in designing and potentially improving future architectures to control heat, for example in circuit Quantum Electrodynamics (cQED). Moreover, fundamental questions regarding signatures of quantum mechanics in thermodynamic properties of devices at nanoscales have not been answered yet and require advanced simulation techniques beyond conventional perturbative treatments

Quantum heat transfer through a generic superconducting set-up consisting of a tunable transmon qubit placed between resonators that are terminated by thermal reservoirs is explored. Applying the numerical exact hierarchical equation of motion (HEOM) approach, steady-state properties are revealed, and experimentally relevant parameter sets are identified. Benchmark results are compared with predictions based on approximate treatments to demonstrate their failure in broad ranges of parameter space. These findings may allow improving future designs for heat control in superconducting devices.

DY 3.10 Tue 17:30 P

Interaction-driven dynamical quantum phase transitions in a strongly correlated bosonic system — •Sebastian Stumper[1], Michael Thoss[1,2], and Junichi Okamoto[1,2] — [1]Institute of Physics, University of Freiburg — [2]EUCOR Centre for Quantum Science and Quantum Computing, University of Freiburg

We investigate the dynamical quantum phase transitions (DQPTs) in the one-dimensional extended Bose-Hubbard model after a sudden quench of the nearest-neighbor interaction strength. We show that interaction-driven DQPTs can appear after quenches between two topologically trivial insulating phases based on extensive matrix-product-states simulations. The threshold value of the quench parameter for the DQPTs does not coincide with the equilibrium phase boundaries, which is contrary to the DQPTs between topologically distinct phases. Furthermore, we define a new set of string and parity order parameters to characterize the dynamics and find a close connection between DQPTs and these order parameters for both types of quenches. Finally, the timescales of DQPTs are also studied, revealing different kinds of power laws for the topological and interaction-driven cases.

DY 3.11 Tue 17:30 P

A particle conserving framework to transport in AC-driven quantum dots contacted to superconducting leads — •Julian Siegl[1], Jordi Pico-Cortes[1,2], and Milena Grifoni[1] — [1]Universität Regensburg — [2]Universidad Autónoma de Madrid

Transport through an interacting quantum dot coupled to superconducting leads and subject to DC and AC-bias is studied within a particle conserving framework. In this formulation, charge conservation during tunneling of an electron out of the dot includes processes where a quasiparticle is destroyed in the superconductor and simultaneously a Cooper pair is created. This possibility gives rise to non vanishing coherences of the density matrix involving Cooper pairs and states with zero or double occupancy in the quantum dot. In the sequential tunneling regime (second order in the tunneling), the *anomalous* contribution to the current due to the coherences is negligible and quasiparticle transport dominates. Here, the combination of AC and DC bias gives rise to stability diagrams whose features cannot be explained within the simple Tien-Gordon theory. At higher orders the coherences are responsible for the supercurrent in the junction.

DY 4: Poster Session II: Nonlinear Dynamics, Simulations and Machine Learning

Time: Tuesday 17:30–19:30 Location: P

DY 4.1 Tue 17:30 P

Memory effects and stochastic forces on a passive particle in an active bath — •Jeanine Shea[1], Friederike Schmid[1], and Gerhard Jung[2] — [1]Johannes Gutenberg University — [2]University of Innsbruck

Implicit models of passive, equilibrium systems have been used for many years to study and understand the physical behavior of these systems. Given the success of understanding equilibrium systems through models, recent studies have focused on mapping non-equilibrium systems onto modified equilibrium models to better understand non-equilibrium behavior. In particular, active systems are non-equilibrium systems which are highly pertinent to biological studies and which exhibit vastly different behavior than strictly passive systems. These distinctive dynamics are not limited to purely active systems, but can also be transferred to passive particles in active systems. As such, the behavior of passive particles immersed in active systems can significantly differ from that in a passive system. We investigate the dissipative and stochastic forces which act on one fundamental example of such a system, that of a colloid in a bath of active particles.

DY 4.2 Tue 17:30 P

Epidemic modeling with delay-differential equations including saturation effects by isolation and contact restriction — •Susanne Kiefer and Edeltraud Gehrig — RheinMain University of Applied Science, Germany

Delay differential equation enable a realistic modeling of epidemics since they allow the inclusion of incubation periods, recovery times or the influence of a quarantine. A systematic modelling of the influence of parameters and their mutual dependence is of high importance when analyzing the behavior of the numbers of infected, susceptible and recovered persons. In this work we present and compare epidemic models with variable delays and saturation parameters. Thereby we consider both, a delay term describing the influence of incubation time as well as a delay for an inclusion of recovery. Our stability analysis and modeling of the temporal behavior allow for a determination of critical regimes where, depending on model approach, a delay may turn the system into instable behavior. A rise in amplitude of the characteristic oscillations shows a strong dependence on delay. This behavior may be controlled by parameters describing quarantine rules. Results of our simulations reveal an influence of parameters describing isolation of infected persons and contact restrictions on the dynamics and particularly on the transition to unstable behavior. A thorough adjustment of contact restriction and isolation may allow to shift the onset of instability and to adjust restriction rules. Thereby the range of control options of each of these parameters critically depends on initial values, infection and recovery rates as well on the delays.

DY 4.3 Tue 17:30 P

Interplay of viscosity and surface tension for ripple formation by external laser melting — •Klaus Morawetz[1,2], Sarah Trinschek[1], and Evgeny Gurevich[1] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

A model for ripple formation on liquid surfaces exposed to an external laser or particle beam and a variable ground is developed. Starting from the Navier Stokes equation the coupled equations for the velocity potential and the surface height are derived with special attention to viscosity. Linear stability analysis provides the formation of a damped gravitation wave modified by an interplay between the external beam, the viscosity, and the surface tension. The resulting wavelengths are in the order of the ripples occurring in laser welding experiments hinting to their hydrodynamical origin. The stability due to the periodic time-dependence of the external beam is discussed with the help of Floquet multipliers showing that the ripple formation could be triggered by an external excitation with frequencies in the order of the repetition rate of the laser. The weak nonlinear stability analysis provides ranges where hexagonal or stripe structures can appear. The orientation of stripe structures and ripples are shown to be dependent on the incident angle and a minimal angle is reported. Two models are presented to couple the external current to the gradient of the surface. Numerical simulations confirm the findings. arXiv:2107.02651

DY 4.4 Tue 17:30 P

Observation of phase synchronization and alignment during free induction decay of quantum spins with Heisenberg interactions — •Patrick Vorndamme[1], Heinz-Jürgen Schmidt[2], Christian Schröder[1,3], and Jürgen Schnack[1] — [1]Bielefeld University, 33615 Bielefeld, Germany — [2]Osnabrück University, Barbarastraße 7, 49076 Osnabrück, Germany — [3]Bielefeld Institute for Applied Materials Research, 33619 Bielefeld, Germany

Equilibration of observables in closed quantum systems that are described by a unitary time evolution is a meanwhile well-established phenomenon. Here we report the surprising theoretical observation that spin rings with nearest-neighbor or long-range isotropic Heisenberg interaction not only equilibrate but moreover also synchronize the directions of the expectation values of the individual spins. Here, we observe mutual synchronization of local spin directions in closed systems under unitary time evolution. This synchronization is independent of whether the interaction is ferro- or antiferromagnetic. In our numerical simulations, we investigate the free induction decay of an ensemble of quantum spins by solving the time-dependent Schrödinger equation numerically exactly. The synchronization is very robust against for instance random fluctuations of the Heisenberg couplings and inhomogeneous magnetic fields. Synchronization is not observed with strong enough symmetry-breaking interactions such as the dipolar interaction. We also compare our results to closed-system classical spin dynamics which does not exhibit phase synchronization due to the lack of entanglement. (arxiv:2104.05748)

DY 4.5 Tue 17:30 P

Neural Network-Based Approaches for Multiscale Modelling of Topological Defects — •Kyra Klos[1], Karin Everschor-Sitte[2], and Friederike Schmid[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]University of Duisburg-Essen, Duisburg, Germany

Topological defects and their dynamics are a heavily researched topic in a wide range of physics fields.[1]

Due to the multiscale character of those defect structures, numerically simulating a large number of them in full microscopic detail gets highly complicated, as the large size of associated deformation fields around each core leads to a complex interaction pattern.

To give a possible insight into the connection between the macroscopic (particle) description of a model with topological defects and the underlying microscopic true structure, the use of neural networks is proposed. Starting with a spin-dynamic simulated microscopic model as input [2,3], a fully convolutional network (FCN)[4] is used to simplify the complex defect structure of the microscopic theory without loss of valuable information. This allows the extraction of the configuration and location of the topological defects.

[1] Mermin, N. D., Rev. Mod. Phys. 51, 591, (1979)
[2] Leoncini, X. et. al., Phys. Rev. E 57(6), 6377, (1998)
[3] Cerruti-Sola, M. et. al., Phys. Rev. E 61(5A), 5171, (2000)
[4] Long, J. et. al., IEEE, 39(4), 640, (2017)

DY 4.6 Tue 17:30 P

Nonlinear dynamics in intra-cavity pumped thin-disk lasers — •Sarah Trinschek, Christian Vorholt, and Ulrich Wittrock — Münster University of Applied Sciences, Germany

For an intra-cavity pumped Yb:YAG thin-disk laser, complex dynamics of the laser output power can be observed. The gain medium of this laser is residing in the resonator of a conventional, diode-pumped Yb:YAG thin-disk laser. We present illustrative experimental results and a detailed analysis of the nonlinear dynamics of the laser in the framework of a rate-equation model. Despite stable continuous-wave pumping, periodic pulse trains and chaotic fluctuations of the optical power of both lasers occur. The dynamics is not driven by external perturbations but arises naturally in this laser system due to cross-saturation effects of the two gain media. The qualitative type of dynamics can be controlled by the resonator length of the diode-pumped laser but the detailed behaviour of the laser is complex and also shows hysteresis and multistability.

DY 4.7 Tue 17:30 P

Quantitative Waveform Sampling on Atomic Scales — Dominik Peller[1], Carmen Roelcke[1], •Lukas Kastner[1], Thomas Buchner[1], Alexander Neef[1], Johannes Hayes[1], Franco Bonafé[2], Dominik Sidler[2], Michael Ruggenthaler[2], Angel Rubio[2,3,4], Rupert Huber[1], and Jascha Repp[1] — [1]University of Regensburg, Germany — [2]MPSD, MPG, Hamburg, Germany — [3]CCQ, Flatiron Institute, New York, USA — [4]UPV/EHU, San Sebastían, Spain

Using a single molecule as a local field sensor, we precisely sample the absolute field strength and temporal evolution of tip-confined near-field transients in a lightwave-driven scanning tunnelling microscope. To develop a comprehensive understanding of the extracted atomic-scale nearfield, we simulated the far-to-near-field transfer with classical electrodynamics and include time-dependent density functional theory to validate our calibration and conclusions.

DY 4.8 Tue 17:30 P

Calculating Raman Spectra using Kernel-Based Machine Learning — •Manuel Grumet[1], Karin S. Thalmann[1], Tomáš Bučko[2,3], and David A. Egger[1] — [1]Technical University of Munich, Germany — [2]Comenius University in Bratislava, Slovakia — [3]Slovak Academy of Sciences, Slovakia

First-principles theoretical predictions of Raman spectra are possible using either a phonon-based approach or molecular dynamics (MD) simulations. In both cases, the polarizability tensor of the system, α, is the central quantity. Specifically, the Raman spectrum is obtained from Fourier-transformed velocity autocorrelation functions (VACs) of tensor invariants of α in the MD method [1]. This requires a large number of evaluations of α and thus leads to high computational cost.

We use kernel-based machine learning (ML) to reduce the number of polarizability calculations needed. In this approach, a subset of all configurations serves as a training data set, and polarizabilities for all other configurations are predicted using ML methods. In particular, we obtain the polarizabilites using kernel ridge regression with descriptors based on the atomic neighbourhood density around each atom [2,3].

We apply these methods to a number of test systems, consisting of small molecules and simple solids. We compare different descriptors with regard to the size of the training data set required to obtain accurate predictions for polarizabilties and Raman spectra.

[1] M. Thomas et al., Phys. Chem. Chem. Phys. **15**, 6608 (2013)
[2] N. Raimbault et al., New J. Phys. **21**, 105001 (2019)
[3] A. P. Bartók et al., Phys. Rev. B **87**, 184115 (2013)

DY 4.9 Tue 17:30 P

Machine learning generators of open system Lindblad dynamics — •Francesco Carnazza[1], Dominik Zietlow[2], Federico Carollo[1], Sabine Andergassen[1], Georg Martius[2], and Igor Lesonovsky[1,3] — [1]Institut für Theoretische Physik and Center for Quantum Science, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [2]Max Planck Institute for Intelligent Systems, Max-Planck-Ring 4, 72076 Tübingen, Germany — [3]School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, UK

In recent years artificial neural network methods have established themselves as a versatile tool to encode the state of both closed and open quantum systems. We are interested in the question whether they can learn the generator of an effective open quantum dynamics which governs a small system of interest that is embedded within a larger one (Paolo Mazza et al. 2020 https://doi.org/10.1103/PhysRevResearch.3.023084). The model we consider is a spin chain where the system of interest is formed by two spins which are coupled to a "bath" consisting of the rest of the chain. The whole chain is evolved according to an transverse field Ising Hamiltonian. From the reduced density matrix, obtained by tracing out the bath degrees of freedom, the two-body correlations are determined, which are subsequently used to train the network. A simple architecture is adopted in order to have the possibility to "look inside" the network and to see whether the learned dynamics is indeed governed by a time-local Lindblad generator.

DY 4.10 Tue 17:30 P

Modelling a highly adaptive, nonlinear acoustic sensor — •Philipp Hövel[1], Thomas Meurer[2], Martin Ziegler[3], and Claudia Lenk[3] — [1]University College Cork, Ireland — [2]Kiel University, Germany — [3]Technische Universität Ilmenau, Germany

Hearing is a remarkable sense both in terms of physiology and signal processing. In biology, hearing exhibits amazing sensing properties, in particular for low-volume sounds and noisy environments, which is known as the "cocktail party effect". For many state-of-the-art technological implementations, speech recognition remains a challenging task in these hard-to-hear situations and varying surroundings.

In this contribution, we present a mathematical model of a novel, adaptive, bio-inspired acoustic sensor with integrated signal processing functionality, whose sensing and processing properties can be widely tuned using real-time feedback. We show that dynamical switching between linear and nonlinear characteristics improves detection of signals in noisy conditions, increases the dynamic range of the sensor, and enables adaptation to changing acoustic environments. We demonstrate that the dynamical switching can be attributed to a Hopf bifurcation, and its dependence of sensor and feedback parameters is validated in experiments, and highlight the applicability and conceptual advantages of the acoustic sensor.

DY 5: Poster Session III: Statistical Physics, Complex Fluids and Soft Matter

Time: Tuesday 17:30–19:30 Location: P

DY 5.1 Tue 17:30 P

Correlational entropy by nonlocal quantum kinetic theory — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

The nonlocal kinetic equation unifies the achievements of the transport in dense quantum gases with the Landau theory of quasiclassical transport in Fermi systems. Large cancellations in the off-shell motion appear which are hidden usually in non-Markovian behaviors [1]. The remaining corrections are expressed in terms of shifts in space and time that characterize the non-locality of the scattering process [2]. In this way quantum transport is possible to recast into a quasi-classical picture [3]. The balance equations for the density, momentum, energy and entropy include besides quasiparticle also the correlated two-particle contributions beyond the Landau theory [4]. The medium effects on binary collisions are shown to mediate the latent heat, i.e., an energy conversion between correlation and thermal energy. For Maxwellian particles a sign change of the latent heat is reported at a universal ratio of scattering length to the thermal De Broglie wavelength. This is interpreted as a change from correlational heating to cooling [5]. [1] Ann. Phys. 294 (2001) 135, [2] Phys. Rev. C 59 (1999) 3052, [3] "'Interacting Systems far from Equilibrium -Quantum Kinetic Theory"' Oxford University Press, (2017) ISBN 9780198797241, [4] Phys. Rev. E 96 (2017) 032106, [5] Phys. Rev. B 97 (2018) 195142

DY 5.2 Tue 17:30 P

Toolbox for quantifying memory in dynamics along reaction coordinates — Alessio Lapolla and •Aljaz Godec — Mathematical bioPhysics Group, Max Planck Institute for Biophysical Chemistry

Memory effects in time series of experimental observables are ubiquitous and may have important consequences for the interpretation of kinetic data. They may even affect the function of biomolecular nanomachines such as enzymes. We propose a set of complementary methods for quantifying conclusively the magnitude and duration of memory in a time series of a reaction coordinate [1]. The toolbox is general, easy to use, and does not rely on any underlying microscopic model. As a proof of concept we apply it to the analysis of memory in the dynamics of the end-to-end distance of the analytically solvable Rouse-polymer model, an experimental time series of extensions of a single DNA hairpin measured by optical tweezers, and the fraction of native contacts in a small protein probed by atomistic molecular dynamics simulations.

[1] A. Lapolla and A. Godec, Phys. Rev. Research 3, L022018 (2021)

DY 5.3 Tue 17:30 P

Depinning of confined colloidal dispersions under oscillatory shear — •Marcel Hülsberg and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Strongly confined colloidal dispersions under shear exhibit a variety of dynamical phenomena, including a depinning transition similar to single particles that are driven over a periodic substrate potential [1].

Here, we investigate the depinning behavior of these systems under pure oscillatory shearing with shear rate $\dot{\gamma}(t) = \dot{\gamma}_0 \cos(\omega t)$, as it is a common scenario in rheological experiments [2].

The colloids' depinning behavior is assessed from a microscopic level based on particle trajectories, which are obtained from overdamped Brownian Dynamics simulations. The numerical approach is complemented by an analytic one based on a single-particle model in the limit of weak driving.

Investigating a broad spectrum of shear rate amplitudes $\dot{\gamma}_0$ and frequencies ω, we observe complete pinning as well as temporary depinning behaviour. We discover that temporary depinning occurs for shear rate amplitudes above a frequency-dependent critical amplitude $\dot{\gamma}_0^{\mathrm{crit}}(\omega)$, for which we attain a functional expression. This allows us to identify the dominant system-intrinsic time scale that dictates the scaling behavior of $\dot{\gamma}_0^{\mathrm{crit}}$ with driving frequency ω.

Finally, we discuss the connection between depinning and structural changes in the system.

[1] S. Gerloff and S.H.L. Klapp, Phys. Rev. E **94**(6), 062605 (2016)
[2] J.M. Brader, et al., Phys. Rev. E **82**(6), 061401 (2010)

DY 5.4 Tue 17:30 P

Emergence of collective motion in two-dimensional colloidal systems with delayed feedback — •Robin A. Kopp and Sabine H. L. Klapp — ITP, TU Berlin, Berlin, Germany

In recent years, delayed feedback (dFB) in colloidal systems has become an active and promising field of study [1,2,3], key topics being history dependence and the manipulation of transport properties. Here we study the dynamics of a two-dimensional colloidal suspension, subject to time-delayed feedback. To this end we perform overdamped Brownian dynamics simulations, where the particles interact through a Weeks-Chandler-Andersen (WCA) potential. Furthermore, each particle is subject to a Gaussian, repulsive feedback potential (cf. [1]), that depends on the difference of the particle position at the current time, $\mathbf{r}_i(t)$ and the particle position at an earlier time, $\mathbf{r}_i(t-\tau_{\mathrm{delay}})$. We observe the emergence of collective motion characterized by a nonzero mean velocity. After quantitatively studying this phenomenon, we also provide a possible explanation combining single-particle and mean-field-like effects.

[1] S. Tarama, S. U. Egelhaaf, and H. Löwen, Physical Review E **100**, 022609 (2019)
[2] R. Gernert and S. H. L. Klapp, Physical Review E **92**, 022132 (2015)
[3] S. A. M. Loos, and S. H. L. Klapp, Scientific Reports **9**, 2491 (2019)

DY 5.5 Tue 17:30 P

Brownian magneto-gyrator as a tunable microengine — •Iman Abdoli[1], René Wittmann[2], Joseph Michael Brader[3], Jens-Uwe Sommer[1,4], Hartmut Löwen[2], and Abhinav Sharma[1,4] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Dresden, 01069, Germany — [2]Institut für Theoretische Physik II, Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Düsseldorf, 40225, Germany — [3]Department de Physique, Université de Fribourg, CH-1700 Fribourg, Switzerland — [4]Technische Universität Dresden, Institut für Theoretische Physik, Dresden, 01069, Germany

A Brownian particle performs gyrating motion around a potential energy minimum when subjected to thermal noises from two different heat baths. Here, we propose a magneto-gyrator made of a single charged Brownian particle that is steered by an external magnetic field. Key properties, such as the direction of gyration, the torque exerted by the engine on the confining potential and the maximum power delivered by the microengine can be tuned by varying the strength and direction of the applied magnetic field. Further tunability is obtained with a potential that couples the spatial degrees of freedom. We show that in this generic scenario, the microengine can be stalled and even reversed by the magnetic field. Finally, we highlight a property of the magneto-gyrator that has no counterpart in the overdamped approximation–the heat loss from the hot to cold bath requires explicit knowledge of the mass of the particle. Consequently, the efficiency of the microengine is mass-dependent even in the overdamped limit.

DY 5.6 Tue 17:30 P

Broadband frequency filters with quantum dot chains — •Tilmann Ehrlich[1] and Gernot Schaller[1,2] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

Two-terminal electronic transport systems with a rectangular transmission can violate standard thermodynamic uncertainty relations. This is possible beyond the linear response regime and for parameters that are not accessible with rate equations obeying detailed-balance. Looser bounds originating from fluctuation theorem symmetries alone remain respected. We demonstrate that optimal finite-sized quantum dot chains can implement rectangular transmission functions with high accuracy and discuss the resulting violations of standard thermodynamic uncertainty relations as well as heat engine performance.

[1] arXiv:2103.04322, to appear in PRB

DY 5.7 Tue 17:30 P

Cosmological and Elementary Particles Explained by Phase Transitions Derived by Quantum Gravity — •Hans-Otto Carmesin — Gymnasium Athenaeum, Harsefelder Straße 40, 21680 Stade — Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — Universität Bremen, Fachbereich 1, Postfach 330440, 28334 Bremen

In the early universe, the density was very high. As a consequence, there occurred gravitational instabilities and corresponding dimensional phase transitions, see Carmesin, Hans-Otto (March 2021): Quanta of Spacetime Explain Observations, Dark Energy, Graviton and Nonlocality. Berlin, Dr. Köster Verlag. These transitions are very robust, as they occur in three very different physical systems.

Based on the quantum states corresponding to these dimensional transitions, we derive many excitation modes that include the formation of neutrinos, of the Higgs boson, of the quanta of dark energy, and of many novel elementary particles, see Carmesin, Hans-Otto (August 2021): Cosmological and Elementary Particles Explained by Quantum Gravity. Berlin, Dr. Köster Verlag. These particles range form the Planck scale to the lightest particles, and so they solve the hierarchy problem of particle physics.

All results are derived by quantum gravity and are in precise accordance with observation. I emphasize that the only numerical input used in my theory is the present day time after Big Bang combined with the universal constants G, c, k_B and h.

DY 5.8 Tue 17:30 P

Dimensional Phase Transitions of a Bose Gas in the Early Universe — •Paul Sawitzki[1] and Hans-Otto Carmesin[1,2,3] — [1]Gymnasium Athenaeum, Harsefelder Straße 40, 21680 Stade — [2]Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — [3]Universität Bremen, Fachbereich 1, Postfach 330440, 28334 Bremen

In the early universe, the density was very high. As a consequence, there occurred gravitational instabilities and corresponding dimensional phase transitions, see Carmesin, Hans-Otto (March 2021): Quanta of Spacetime Explain Observations, Dark Energy, Graviton and Nonlocality. Berlin, Dr. Köster Verlag. These transitions are very robust, as they occur in three very different physical systems. Here we derive these transitions for the case of a Bose gas.

These transitions are essential for various fields of cosmology, including the so-called era of 'cosmic inflation' and the solution of the horizon problem.

All results are derived by quantum gravity and are in precise accordance with observation. We emphasize that the only numerical input used in the theory is the present day time after Big Bang combined with the universal constants G, c, k_B and h.

DY 5.9 Tue 17:30 P

Diagrammatic expansion of the two-point effective action around non-Gaussian theories — •Tobias Kühn and Frédéric van Wijland — Laboratoire Matière et Systèmes Complexes, Université de Paris

Consider a many-body problem, such as one involving interacting spins, particles or the time series of a random signal, of which we know the corresponding one- and two-point correlation functions. We suppose that the distribution of the spin values (or particle positions,...) is written in a Boltzmann form with a Hamiltonian possessing one- and two-body interactions only. How does one choose the corresponding couplings so that the distribution generates the prescribed statistics? This so-called inverse problem is conveniently described by the second Legendre transform of the cumulant-generating function, the two-point effective action, whose arguments are means and correlations. The couplings we seek for are then explicitly given by its derivatives. Weak correlation approximations have been proven useful to compute the two-point effective action (Sessak & Monasson 2009). As long as the one-body problem is described by independent Gaussian distributions, they can be routinely derived using diagrammatic methods dating back to Feynman, Luttinger and Ward. Here we explain how similar diagrammatics can be extended to the case in which the one-body problem is not of a Gaussian nature. We discuss how this can prove useful in inference problems pertaining to neuroscience and other complex systems. Another possible application is the derivation of mean-field theories self-consistently taking into account pairwise correlations.

DY 5.10 Tue 17:30 P

Charged Liquid Bridges — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

A new solution of a charged catenary is presented which allows to determine the static and dynamical stability conditions where charged liquid bridges are possible. The creeping height, the bridge radius and length as well as the shape of the bridge is calculated showing an asymmetric profile in agreement with observations. The flow profile is calculated from the Navier Stokes equation leading to a mean velocity which combines charge transport with neutral mass flow and which describes recent experiments on water bridges. The velocity profile in a water bridge is reanalyzed. Assuming hypothetically that the bulk charge has a radial distribution, a surface potential is formed that is analogous to the Zeta potential. The Navier*Stokes equation is solved, neglecting the convective term; then, analytically and for special field and potential ranges, a sign change of the total mass flow is reported caused by the radial charge distribution. [Water 9 (2017) 353, Phys. Rev. E 86 (2012) 026302, errata Phys. Rev. 86 (2013) 069904, AIP Advances 2 (2012) 022146-1-6]

DY 5.11 Tue 17:30 P

Ornstein-Zernike relation in hypergraphs — •Christian Faber[1,2,3], Till Kranz[2,3], and Matthias Sperl[3,2] — [1]Jülich Supercomputing Centre, FZ Jülich — [2]Institut für Theoretische Physik, Uni Köln — [3]Institut für Materialphysik im Weltraum, DLR Köln

The pair correlation function is an important input to describe equilibrium phase transitions and the glass transitions [1]. An Ornstein-Zernike relation can be used to represent the pair correlation function in a form that is easy to approximate and that allows an intuitive representation in terms of graphs [2]. However, this graphical representation is limited to pairwise interactions between particles and recent analyses show that some systems, such as foams, cannot be adequately represented with pair interactions [3]. To be able to specify a meaningful Ornstein-Zernike relation for such systems, we have started from scratch and have introduced hypergraphs for multi-body interactions. With these we are able to represent the Ornstein-Zernike relation for multi-body interactions and to give a graphical meaning to the individual terms. We will discuss the similarities and differences between the relation for pair- and for multi-body interactions.

[1] W. Götze, *Zeitschrift f. Physik B Condensed Matter* **60**, 2 (1985).
[2] M. Wortis, "Linked Cluster Expansion" in *Phase Transitions and Critical Phenomena*, C. Domb, M.S. Green, Eds. (Academic Press, London, 1974), vol. 3.
[3] G. Ginot, R. Höhler, S. Mariot, A. Kraynik, W. Drenckhan, *Soft Matter* **15.22**, 4570-4582 (2019).

DY 5.12 Tue 17:30 P

Phase behaviour of a generalized chiral Lebwohl-Lasher model — •Anja Kuhnhold and Philipp Elsässer — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

The Lebwohl-Lasher (LL) model is a simple model to study the isotropic-nematic (IN) transition of liquid-crystalline systems. Particles are described by unit vectors that sit on a simple cubic lattice and only interact with nearest neighbours; the interaction potential has a minimum for parallel orientation of the particles' axes, which drives the IN transition.

Fish and Vink generalized the LL model so that the sharpness of the potential can be tuned and with that the type of phase transition in the 2D limit [1]. Memmer et al. added a chiral interaction to the LL model. They studied the resulting cholesteric phase (where the orientation of particles is parallel within a layer but is rotated between layers) and its behaviour when confined between aligning surfaces [2]. We combine both extensions to the generalized chiral Lebwohl-Lasher model and study the isotropic-cholesteric transition depending on the sharpness parameter, the chirality, and the dimensionality of the system. We use a Wang-Landau Monte-Carlo method to simulate the system and apply finite-size scaling to identify the type of phase transitions.

[1] J.M. Fish, R.L.C. Vink, PRE **81**, 021705 (2010).
[2] R. Memmer, O. Fliegans, PCCP **5**, 558 (2003).

DY 5.13 Tue 17:30 P

Microsecond XPCS on soft matter probed at the European XFEL — •Francesco Dallari and Felix Lehmkühler — Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

Many soft-matter systems are composed of nanoparticles or macromolecules dispersed in water. The characteristic time at the relevant length-scales of few nanometers falls therefore in the (sub)microsecond time-scales, making the measurement of the dynamical properties for these system an extremely challenging (often impossible) task at third generation synchrotron light sources. With the recent development of hard X-ray free electron lasers (XFELs) and fourth generation light sources, time-resolved experiments in this time- and length-scale regimes have become accessible. Here we present the first results on prototypical charge-stabilized silica nanoparticles dispersed in water both in diluted [1] and concentrated [2] systems. Tuning the pulse fluence we are able to probe and describe with thermodynamical models the diffusion properties in stationary systems and in systems driven by the XFEL pulses.

[1] F. Lehmkühler, F. Dallari, A. Jain, et al. (2020). PNAS, 117, 24110-24116. https://doi.org/10.1073/pnas.2003337117
[2] F. Dallari, ,A. Jain, F. Lehmkühler, et al. (2021). IUCrJ 8, https://doi.org/10.1107/S2052252521006333.

DY 5.14 Tue 17:30 P

Efficient Event-Driven Simulation of the Bubbling Instability in a Fluidised Bed — Raphael Biertz[1], •Till Kranz[1,2], and Matthias Sperl[2,1] — [1]Institut für Theoretische Physik, Uni Köln — [2]Institut für Materialphysik im Weltraum, DLR Köln

Two-phase flows, comprised of granular particles and an interstitial molecular fluid occur in many places in nature and industry. The prototypical setup for this kind of complex fluid is a fluidised bed. At sufficient fluidisation flow rates, the particulate phase displays a bubbling instability with close packed and very dilute regions [1].

While pure granular fluids are efficiently simulated by event-driven molecular dynamics algorithms, the two-phase flow problem is still a numerical challenge. Here, we discuss that an implicit model of the fluidising fluid in combination with a event-driven approach for the particles [2] can faithfully capture the bubbling instability [3].

[1] Jackson, R., *The Dynamics of Fluidized Particles*, Cambridge University Press, 2000
[2] Fiege, A., Zippelius, A., J. Phys.: Conf. Ser. **759**, 012001 (2016)
[3] Biertz, R., Sperl, M., Kranz, W. T., in preparation

DY 5.15 Tue 17:30 P

Topological optimization of microfluidic Tesla valves for applications with low Reynold numbers — •Sebastian Bohm[1], Hai Binh Phi[2], Ayaka Moriyama[3], and Erich Runge[1] — [1]TU Ilmenau, FG Theoretische Physik I, DE — [2]TU Ilmenau, FG Mikrosystemtechnik, DE — [3]Carleton College, Physics Department, USA

Passive Tesla valves represent a promising method for rectifying flows in microfluidic systems because no moving parts are needed. The efficiency of the valves is characterised by the diodicity which can be defined as the pressure drop ratio of the forward and the reverse flow direction. To obtain efficient valve designs, topological optimization has proven to be a particularly suitable method [1]. The challenge is the dependency of the diodicity on the Reynolds number. Normally, the valves are only efficient at Reynolds numbers much greater than 100. In microfluidics, Reynolds numbers are usually very low, which hitherto limits the applicability of Tesla valves. Therefore a novel approach for the topological optimization of valves that work at very small Reynolds numbers is presented: To ensure that the optimization yields meaningful designs, a customized objective function is introduced and a multi-stage optimization procedure is used. In addition, a method is presented to optimize the diodicity over a given range of Reynolds numbers simultaneously. The resulting valves achieve a diodicity of up to 2 already at Reynolds numbers smaller than 20. The simulated predictions are in close agreement to experimental results.

[1] S. Lin et al., *Topology Optimization of Fixed-Geometry Fluid Diodes*, J. Mech. Des., 137 **(8)**, (2015)

DY 6: Soft Matter (joint session CPP/DY)

Time: Wednesday 10:00–12:45 Location: H3

See CPP 7 for details of this session.

DY 7: Focus Session: Facets of Many-Body Quantum Chaos (organised by Markus Heyl and Klaus Richter) (joint session DY/TT)

This session covers the same topics as the TT-DY-MA symposium with the same name and five invited speakers on Tuesday, September 28th.

Time: Wednesday 10:00–13:00 Location: H6

DY 7.1 Wed 10:00 H6

Probing many-body quantum chaos with quantum simulators using randomized measurements — Lata K Joshi[1,2], •Andreas Elben[1,2,3], Amit Vikram[4,5], Benoit Vermersch[1,2,6], Victor Galitski[4], and Peter Zoller[1,2] — [1]Center for Quantum Physics, University of Innsbruck, Innsbruck A-6020, Austria — [2]Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, Innsbruck A-6020, Austria — [3]Institute for Quantum Information and Matter and Walter Burke Institute for Theoretical Physics, California Institute of Technology, Pasadena, CA 91125, USA — [4]Joint Quantum Institute, University of Maryland, College Park, MD 20742, USA — [5]Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD 20742, USA — [6]Univ. Grenoble Alpes, CNRS, LPMMC, 38000 Grenoble, France

Randomized measurements provide a novel toolbox to probe many-body quantum chaos in quantum simulators, utilizing observables such as out-of-time ordered correlators and spectral form factors (SFFs). Here, I will focus on a protocol to access the SFF, characterizing the energy eigenvalue statistics, in quantum spin models. In addition, I will introduce partial spectral form factors (pSFFs) which refer to subsystems of the many-body system and reveal unique insights into energy eigenstate statistics. I will show that our randomized measurement protocol allows to access both, SFF and pSFFs. It provides thus a unified testbed to probe many-body quantum chaotic behavior, thermalization and many-body localization in closed quantum systems.

DY 7.2 Wed 10:15 H6

Exploring the bound on chaos due to quantum criticality — •Mathias Steinhuber, Juan-Diego Urbina, and Klaus Richter — University of Regensburg, Regensburg, Germany

The 'bound on chaos' proposed by Maldacena, Shenker and Stanford [1] predicts a temperature-dependent upper bound on the initial exponential growth rate $\lambda_{\text{OTOC}} \leq 2\pi T$ for out-of-time-order correlators (OTOCs) in quantum systems with chaotic classical limit. We explore the temperature dependence of the quantum Lyapunov exponent λ_{OTOC} in Bose-Hubbard systems near criticality of the ground state [2]. We find the conditions for a non-trivial temperature dependence satisfying the bound, indicating the requirement that the system shows signatures of classical instability at the ground state while reaching the semiclassical regime at the same time. This is guaranteed by many-body systems with a well defined mean-field limit close to a bifurcation [3].

[1] Maldacena J., Shenker S. H. & Stanford D. A bound on chaos. Journal of High Energy Physics 2016, 106 (2016).
[2] Hummel, Q., Geiger, B., Urbina, J. D. & Richter, K. Reversible Quantum Information Spreading in Many-Body Systems near Criticality. Phys. Rev. Let. 123, 160401 (2019).
[3] Eilbeck, J., Lomdahl, P. & Scott, A. The discrete self-trapping equation. Physica D: Nonlinear Phenomena 16, 318-338 (1985).

DY 7.3 Wed 10:30 H6

Critically slow operator dynamics in constrained many-body systems — •Johannes Feldmeier[1,2] and Michael Knap[1,2] — [1]Technical University of Munich — [2]Munich Center for Quantum Science and Technology (MCQST)

The far-from-equilibrium dynamics of generic interacting quantum systems is characterized by a handful of universal guiding principles, among them the ballistic spreading of initially local operators. Here, we show that in certain constrained many-body systems the structure of conservation laws can cause a drastic modification of this universal behavior. As an example, we study operator growth characterized by out-of-time-order correlations (OTOCs) in a dipole-conserving fracton chain. We identify a critical point with sub-ballistically moving OTOC front, that separates a ballistic from a dynamically frozen phase. This critical point is tied to an underlying localization transition and we use its associated scaling properties to derive an effective description of the moving operator front via a biased random walk with long waiting times. We support our arguments numerically using classically simulable automaton circuits.

DY 7.4 Wed 10:45 H6

Universal equilibration dynamics of the Sachdev-Ye-Kitaev model — •Soumik Bandyopadhyay, Philipp Uhrich, Alessio Paviglianiti, and Philipp Hauke — INO-CNR BEC Center and Department of Physics, University of Trento, Via Sommarive 14, I-38123 Trento, Italy

The Sachdev-Ye-Kitaev (SYK) model was introduced in the context of explaining the properties of "strange metals," and has been found to manifest the characteristics of a quantum theory which is holographically dual to extremal charged black holes with two-dimensional anti-de Sitter horizons. Being maximally chaotic, black holes are the best known scramblers of quantum information in nature. Same features are shared by the SYK model, which has triggered a massive interest in its chaotic dynamics. Yet, many questions about the dynamics of the SYK model remain open. In this presentation, we shall be discussing the equilibration process of a fermionic system under the SYK Hamiltonian evolution. Our study, based on a state-of-the-art exact diagonalization method, reveals that the system exhibits an universal equilibration process. By devising a master equation for disordered systems, we successfully explain some of the key features of this dynamics. We infer the universality from the spectral analysis of the corresponding Liouvillian. We expect our findings shed light on challenging questions for systems far from equilibrium, such as, thermalization of closed and disordered quantum many-body systems.

DY 7.5 Wed 11:00 H6

Periodic orbit sums and their relation to JT gravity correlators — •Fabian Haneder, Torsten Weber, Camilo Moreno, Juan Diego Urbina, and Klaus Richter — University of Regensburg, Germany

Jackiw-Teitelboim (JT) gravity is a two-dimensional dilaton gravity theory originally used to describe the near-horizon physics of charged, static black holes, but has recently garnered much attention due to its exact duality to a particular double-scaled Hermitian matrix model [1]. Applications are believed to be as a toy model for the black hole information paradox, the AdS/CFT correspondence, and holography and quantum gravity more generally.

The duality with a matrix model suggests the existence of a classical chaotic system which, after semiclassical (periodic orbit) quantisation [2], leads to the same spectral correlations. Finding such a system would solve the long-standing problem of identifying a single dual, rather than an ensemble of theories, as expected from orthodox AdS/CFT.

In this contribution, we will give a very brief overview of the JT/matrix model duality and show the structural similarity of JT correlators and stochastically projected periodic orbit sums, at the level of the one-point function, as well as propose a candidate dual system.

[1] P. Saad, S. Shenker, D. Stanford, arXiv:1903.11115
[2] See e.g. M. Gutzwiller, *Chaos in classical and quantum mechanics*, Springer 2019

DY 7.6 Wed 11:15 H6

Entanglement entropy of fractal states — Giuseppe De Tomasi[1] and •Ivan Khaymovich[2] — [1]T.C.M. Group, Cavendish Laboratory, JJ Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [2]Max Planck Institute for the Physics of Complex Systems

In this talk we will discuss the relations between entanglement (and Renyi) entropies and fractal dimensions D_q of many-body wavefunctions.

As a simple example we introduce a new class of *sparse* random pure states being fractal in the corresponding computational basis and show that their entropies reach the upper bound of Page value for fractal dimension larger than the subsystem size ($D_q > 0.5$ for equipartitioning) and grow linearly with D_q otherwise.

Moreover this dependence poses the upper bound for entanglement and Renyi entropies for any multifractal states and uncovers the relation between multifractality and entanglement properties of many-body wavefunctions.

15 min. break.

DY 7.7 Wed 11:45 H6

Chaos for Interacting Bosons and Random Two-Body Hamiltonians — Lukas Pausch[1], Edoardo Carnio[1,2], Andreas Buchleitner[1,2], and •Alberto Rodríguez[3] — [1]Physikalisches Institut, Albert-Ludwigs-Universität-Freiburg, Hermann-Herder-Straße 3, D-79104, Freiburg, Germany — [2]EUCOR Centre for Quantum Science and Quantum Computing, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, D-79104, Freiburg, Germany — [3]Departamento de Física Fundamental, Universidad de Salamanca, E-37008 Salamanca, Spain

We investigate the chaotic phase of the Bose-Hubbard model [1] in relation to the bosonic embedded random-matrix ensemble, which mirrors the dominant few-body nature of many-particle interactions, and hence the Fock space sparsity of quantum many-body systems. Within the chaotic regime, mean and fluctuations of the fractal dimensions of Bose-Hubbard eigenstates show clear fingerprints of ergodicity and are well described by the embedded ensemble, which is furthermore able to capture the energy dependence of the chaotic phase. Despite such agreement, the distributions of the fractal dimensions for these two models depart from each other and from the Gaussian orthogonal ensemble as Hilbert space grows.

[1] L. Pausch et al, Phys. Rev. Lett. **126**, 150601 (2021).

DY 7.8 Wed 12:00 H6

Orthogonal quantum many-body scars — •Hongzheng Zhao[1], Adam Smith Smith[2], Florian Mintert[1], and Johannes Knolle[1,3,4] — [1]Blackett Laboratory, Imperial College London, London, United Kingdom — [2]School of Physics and Astronomy, University of Nottingham, University Park, Nottingham, United Kingdom — [3]Department of Physics TQM, Technical University of Munich, Munich, Germany — [4]Munich Center for Quantum Science and Technology, Munich, Germany

Quantum many-body scars have been put forward as counterexamples to the Eigenstate Thermalization Hypothesis. These atypical states are observed in a range of correlated models as long-lived oscillations of local observables in quench experiments starting from selected initial states. The long-time memory is a manifestation of quantum non-ergodicity generally linked to a sub-extensive generation of entanglement entropy, the latter of which is widely used as a diagnostic for identifying quantum many-body scars numerically as low entanglement outliers. Here we show that, by adding kinetic constraints to a fractionalized orthogonal metal, we can construct a minimal model with orthogonal quantum many-body scars leading to persistent oscillations with infinite lifetime coexisting with rapid volume-law entanglement generation. Our example provides new insights into the link between quantum ergodicity and many-body entanglement while opening new avenues for exotic non-equilibrium dynamics in strongly correlated multi-component quantum systems. Reference: https://arxiv.org/abs/2102.07672

DY 7.9 Wed 12:15 H6

Genuine many-body quantum scarring in a periodic Bose-Hubbard ring — •Quirin Hummel and Peter Schlagheck — Université de Liège (Belgium)

Quantum scars have been known for decades to exist in quantum systems of low dimensionality (e.g. “quantum billiards”): While most eigenstates of a classically chaotic system are typically spread across the accessible phase space, individual states exist that are concentrated along unstable classical periodic orbits. On the other hand, recent studies in many-body quantum systems that admit no known meaningful classical limits have revealed eigenstates - now termed “quantum many-body scars” - that feature quantum mechanical properties reminiscent of scenarios of quantum scarring. An unambiguous classification as scars in the original sense, however, remains controversial, if not fundamentally impossible due to the lack of a classical limit. In order to bridge this gap, we investigate the phenomenon of quantum scarring in the prototypical Bose-Hubbard model, a many-body quantum system that combines both, a well-defined formally classical description and the typical high-dimensionality of many-body systems identified with the number of sites that constitute the one-body state space.

DY 7.10 Wed 12:30 H6

Quantum scars of bosons with correlated hopping — •Ana Hudomal[1,2], Ivana Vasić[2], Nicolas Regnault[3,4], and Zlatko Papić[1] — [1]School of Physics and Astronomy, University of Leeds, United Kingdom — [2]Institute of Physics Belgrade, University of Belgrade, Serbia — [3]Joseph Henry Laboratories and Department of Physics, Princeton University, USA — [4]Laboratoire de Physique de l'École Normale Supérieure, ENS, CNRS, Paris, France

Recent experiments have shown that preparing an array of Rydberg atoms in a certain initial state can lead to unusually slow thermalization and persistent density oscillations [1]. This type of non-ergodic behavior has been attributed to the existence of “quantum many-body scars”, i.e., atypical eigenstates that have high overlaps with a small subset of vectors in the Hilbert space. Periodic dynamics and many-body scars are believed to originate from a “hard” kinetic constraint: due to strong interactions, no two neighbouring Rydberg atoms are both allowed to be excited. Here we propose a realization of quantum many-body scars in a 1D bosonic lattice model with a “soft” constraint: there are no restrictions on the allowed boson states, but the amplitude of a hop depends on the occupancy of the hopping site. We find that this model exhibits similar phenomenology to the Rydberg atom chain, including weakly entangled eigenstates at high energy densities and the presence of a large number of exact zero energy states [2].

[1] H. Bernien et al., Nature **551**, 579 (2017).
[2] A. Hudomal et al., Commun. Phys. **3**, 99 (2020).

DY 7.11 Wed 12:45 H6

Quantum local random networks and the statistical robustness of quantum scars — •Federica Maria Surace[1,2], Marcello Dalmonte[1,2], and Alessandro Silva[1] — [1]International School for Advanced Studies (SISSA), via Bonomea 265, 34136 Trieste, Italy — [2]The Abdus Salam International Centre for Theoretical Physics (ICTP), Strada Costiera 11, 34151 Trieste, Italy

We investigate the emergence of quantum scars in a general ensemble of random Hamiltonians (of which the PXP is a particular realization), that we refer to as quantum local random networks. We find two types of scars, that we call stochastic and statistical. We identify specific signatures of the localized nature of these eigenstates by analyzing a combination of indicators of quantum ergodicity and properties related to the network structure of the model. Within this parallelism, we associate the emergence of statistical scars to the presence of motifs in the network, that reflects how these are associated to links with anomalously small connectivity (as measured, e.g., by their betweenness). Most remarkably, statistical scars appear at well-defined values of energy, predicted solely on the basis of network theory. We study the scaling of the number of statistical scars with system size: below a threshold connectivity, we find that the number of statistical scars increases with system size. This allows to define the concept of statistical stability of quantum scars.

DY 8: Quantum Computing (joint session TT/DY)

Time: Wednesday 11:15–13:00 Location: H7

See TT 13 for details of this session.

DY 9: Many-Body Quantum Dynamics I (joint session DY/TT)

Time: Wednesday 13:30–14:45 Location: H6

Invited Talk DY 9.1 Wed 13:30 H6

Nanofriction in Ion Coulomb Systems — •Tanja Mehlstäubler — PTB, Bundesallee 100, 38116 Braunschweig

Single trapped and laser-cooled ions in Paul traps allow for a high degree of control of atomic quantum systems. They are the basis for modern atomic clocks, quantum computers and quantum simulators. Our research aims to use ion Coulomb crystals, i.e. many-body systems with complex dynamics, for precision spectroscopy. This paves the way to novel optical frequency standards for applications such as relativistic geodesy and quantum simulators in which complex dynamics becomes accessible with atomic resolution. The high-level of control of self-organized Coulomb crystals opens up a fascinating insight into the non-equilibrium dynamics of coupled many-body systems, displaying atomic friction and symmetry-breaking phase transitions. We discuss the creation of topological defects and Kibble-Zurek tests in 2D crystals and present recent results on the study of tribology and transport mediated by the topological defect.

DY 9.2 Wed 14:00 H6

Quantum many-body scars in tilted Fermi-Hubbard chains — •Jean-Yves Desaules[1], Ana Hudomal[1,2], Christopher Turner[1], and Zlatko Papić[1] — [1]School of Physics and Astronomy, University of Leeds, Leeds, United Kingdom — [2]Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia

Motivated by recent observations of ergodicity breaking due to Hilbert space fragmentation in 1D Fermi-Hubbard chains with a tilted potential [Scherg et al., arXiv:2010.12965], we show that the same system also hosts quantum many-body scars in a regime U=Δ>J at electronic filling factor ν=1. We numerically demonstrate that the scarring phenomenology in this model is similar to other known realisations such as Rydberg atom chains, including persistent dynamical revivals and ergodicity-breaking many-body eigenstates. At the same time, we show that the mechanism of scarring in the Fermi-Hubbard model is different from other examples in the literature: the scars originate from a subgraph, representing a free spin-1 paramagnet, which is weakly connected to the rest of the Hamiltonian's adjacency graph. Our work demonstrates that correlated fermions in tilted optical lattices provide a platform for understanding the interplay of many-body scarring and other forms of ergodicity breaking, such as localisation and Hilbert space fragmentation.

DY 9.3 Wed 14:15 H6

(Classical) Prethermal phases of matter — •Andrea Pizzi[1], Andreas Nunnenkamp[2], and Johannes Knolle[3] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [2]School of Physics and Astronomy and Centre for the Mathematics and Theoretical Physics of Quantum Non-Equilibrium Systems, University of Nottingham, Nottingham, NG7 2RD, United Kingdom — [3]Department of Physics, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany

Systems subject to a high-frequency drive can spend an exponentially long time in a prethermal regime, in which novel phases of matter with no equilibrium counterpart can be realized. Due to the notorious computational challenges of quantum many-body systems, numerical investigations in this direction have remained limited to one spatial dimension, in which long-range interactions have been proven a necessity. Here, we show that prethermal non-equilibrium phases of matter are not restricted to the quantum domain. Studying the Hamiltonian dynamics of a large three-dimensional lattice of classical spins, we provide the first numerical proof of prethermal phases of matter in a system with short-range interactions. Concretely, we find higher-order as well as fractional discrete time crystals breaking the time-translational symmetry of the drive with unexpectedly large integer as well as fractional periods. Our work paves the way towards the exploration of novel prethermal phenomena by means of classical Hamiltonian dynamics with virtually no limitations on the system's geometry or size, and thus with direct implications for experiments.

DY 9.4 Wed 14:30 H6

Master equations for Wigner functions with spontaneous collapse and their relation to thermodynamic irreversibility* — •Michael te Vrugt[1,2], Gyula I. Tóth[3], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — [2]Philosophisches Seminar, Westfälische Wilhelms-Universität Münster, D-48143 Münster, Germany — [3]Interdisciplinary Centre for Mathematical Modelling and Department of Mathematical Sciences, Loughborough University, Loughborough, LE11 3TU, United Kingdom

Wigner functions allow for a reformulation of quantum mechanics in phase space. They are, as shown in our recent work [1], very useful for understanding effects of spontaneous collapses of the wavefunction as predicted by the Ghirardi-Rimini-Weber (GRW) theory. We derive the dynamic equations for the Wigner function in the GRW theory and its most important variants. The results are used to test, via computer simulations, David Albert's suggestion that the stochasticity induced by spontaneous collapses is responsible for the emergence of thermodynamic irreversibility. We do not observe the equilibration mechanism proposed by Albert, suggesting that GRW theory cannot explain the approach to thermal equilibrium.

[1] M. te Vrugt, G. I. Tóth, R. Wittkowski, arXiv:2106.00137 (2021)

Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1

DY 10: Focus session: Nonlinear Dynamics of the Heart I (organized by Markus Bär, Stefan Luther and Ulrich Parlitz)

Time: Wednesday 15:00–16:30 Location: H6

Invited Talk DY 10.1 Wed 15:00 H6

Effect of fibrosis on propagation on non-linear waves and onset of arrhythmias in cardiac tissue — •Alexander Panfilov[1,2], Timur Nezlobinsky[1,2], and Farhad Pashakhanloo[3] — [1]Department of Physics and Astronomy, Ghent Unibversity, Belgium — [2]Ural Federal University, Ekaterinburg, Russia — [3]Cardiovascular Division, Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, Massachusetts, 02115, USA

Cardiac fibrosis is a well-known arrhythmogenic condition which can lead to sudden cardiac death. Physically, fibrosis can be viewed as a large number of small obstacles in an excitable medium, which may create nonlinear wave turbulence or reentry. The relation between the specific texture of fibrosis and the onset of reentry is of great theoretical and practical importance. In my talk I present results of several recent studies which show how basic properties of wave propagation are affected by fibrosis. We also characterize properties of fibrotic texture which led to cardiac arrhythmias and propose a concept of minimal functional cluster which allows quantitatively predict the arrhythmia probability for different fibrosis densities and tissue excitabilities.

DY 10.2 Wed 15:30 H6

The mechanism of defibrillation of cardiac tissue by time-periodic low-energy shocks I: Refractory boundary length is key for prediction of success probabilities — •Markus Bär, Pavel Buran, and Thomas Niedermayer — Physikalisch-Technische Bundesanstalt, Abbestr. 2 - 12, 10587 Berlin

Rotating excitation waves and electrical turbulence in cardiac tissue are associated with arrhythmias such as life-threatening ventricular fibrillation. Experimental studies have shown that a periodic sequence of four or more electrical far-field pulses is able to terminate fibrillation with less energy than a single shock protocol. During this so-called periodic low-energy anti-fibrillatory pacing (LEAP), only tissue near sufficiently large conduction heterogeneities, such as large coronary arteries, is activated. By means of simulation of the impact of periodic pacing on fibrillation in a two-dimensional electrophysiological model exhibiting multiple stable spirals (vortices) with a representative array of heterogeneities, we show that the success probability for defibrillation depends exponentially on the length of the refractory boundary, i. e. the total length of the borders between refractory and excitable parts of the tissue. This exponential dependency is also derived analytically from simple arguments assuming that successful defibrillation by a low energy shock requires not only to annihilate all vortices, but also needs to prevent initiation of new vortices in the vulnerable excitable region near the refractory boundary.

DY 10.3 Wed 15:45 H6

The mechanism of defibrillation of cardiac tissue by time-periodic low-energy shocks II: Subsequent shortening of refractory boundary length enables low energy antifibrillatory pacing (LEAP) — •Pavel Buran, Thomas Niedermayer, and Markus Bär — Physikalisch-Technische Bundesanstalt, Abbestr. 2 - 12, 10587 Berlin

We present a generic mechanism for the success of LEAP protocols, which covers termination of multiple stable rotors as well as of states of spatiotemporal chaos. Previously, we found that knowledge of the refractory boundary length is sufficient to estimate the success probability of an individual LEAP pulse which is found to decay exponentially with this length in a medium with stable spirals. This result is also found in simulations of cardiac models exhibiting spatiotemporal chaos. Whereas single shock defibrillation requires instantaneous annihilation of all existing vortices, during LEAP the defibrillation process is more gradual and is based on a subsequent shortening of the total refractory boundary length. The average shortening factor, i. e. the ratio between the refractory boundary lengths just before subsequent pulses during periodic pacing can be determined numerically both for media with spatiotemporal chaos and multiple stable spirals and provides a good indicator for the efficiency of a given LEAP protocol.

Invited Talk DY 10.4 Wed 16:00 H6

Chaos and nonlinear dynamics in the heart: Experiments and simulations of arrhythmias and defibrillation — •Flavio fenton — School of Physics, Georgia Institute of Technology, Atlanta, GA

In this talk we present experimental examples of chaotic dynamics including unstable periodic orbits (period 3 and higher orders) in the heart. As a nonlinear system we further demonstrate a universal mechanism for terminating spiral waves in generic excitable media using an established topological framework. Under this mechanism it is possible to explain when defibrillation shocks, by high- or low-energy methods, succeed or fail. Furthermore, it is also possible to design a single minimal stimulus capable to defibrillate, at any time, any turbulent state driven by multiple spiral waves. We demonstrate this in a variety of cardiac tissue models. The theory described here shows how this mechanism underlies all successful defibrillation and can be used to further develop existing and future low-energy defibrillation strategies.

DY 11: Many-Body Quantum Dynamics II (joint session DY/TT)

Time: Thursday 10:00–11:30 Location: H2

DY 11.1 Thu 10:00 H2

Anderson localization of composite particles — •Fumika Suzuki[1], Mikhail Lemeshko[2], Wojciech Zurek[3], and Roman Krems[4] — [1]IST Austria (Institute of Science and Technology Austria) — [2]IST Austria (Institute of Science and Technology Austria) — [3]Los Alamos National Laboratory — [4]University of British Columbia

We investigate the effect of coupling between translational and internal degrees of freedom of composite quantum particles on their localization in a random potential. We show that entanglement between the two degrees of freedom weakens localization due to the upper bound imposed on the inverse participation ratio by purity of a quantum state. We perform numerical calculations for a two-particle system bound by a harmonic force in a 1D disordered lattice and a rigid rotor in a 2D disordered lattice. We illustrate that the coupling has a dramatic effect on localization properties, even with a small number of internal states participating in quantum dynamics.

arXiv:2011.06279

DY 11.2 Thu 10:15 H2

An SYK-inspired model with density-density interactions — •Johannes Dieplinger[1], Soumya Bera[2], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, D-93040, Germany — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

Strong electron-electron interactions are challenging to capture theoretically. A rare example of an analytically tractable model is the Sachdev-Ye-Kitaev (SYK) model, which owes its tractability to the structureless and therefore artificial design: interactions are restricted to two body terms, whose matrix elements are randomly chosen and therefore do not commute with the local density, a fundamental symmetry of realistic electron-electron interactions. We here investigate a derivative of the SYK model, restoring this fundamental symmetry [1]. It features density-density-type interactions as well as a randomized single body term. We present numerical evidence that this model has a rich phase structure, featuring two integrable phases separated by several intermediate phases, including a chaotic one. The latter exhibits several key characterstics of the SYK model including the spectral and wave function statistics and therefore should be adiabatically connected to the non-Fermi liquid phase of the original SYK model. Thus, the presented model provides a further element for bridging the SYK-model and microscopic realism.

[1] J. Dieplinger, S. Bera, F. Evers, Annals of Physics, 168503 (2021)

DY 11.3 Thu 10:30 H2

Disorder-Free Localization in an Interacting 2D Lattice Gauge Theory — •Peter Karpov[1,2], Roberto Verdel[1], Yi-Ping Huang[3], Markus Schmitt[4], and Markus Heyl[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]National Univesity of Science and Technology "MISiS", Moscow, Russia — [3]National Tsing Hua University, Hsinchu, Taiwan — [4]University of Cologne, Cologne, Germany

Disorder-free localization has been recently introduced as a mechanism for ergodicity breaking in low-dimensional homogeneous lattice gauge theories caused by local constraints. We show that also genuinely interacting systems in two spatial dimensions can become nonergodic due to this mechanism. This is all the more surprising since the conventional many-body localization is conjectured to be unstable in two dimensions; hence the gauge constraints represent an alternative robust localization mechanism for interacting models in higher dimensions.

Specifically, we demonstrate nonergodic behavior in the quantum link model by obtaining a bound on the localization-delocalization transition through a unconventional percolation problem implying a fragmentation of Hilbert space. We study the quantum dynamics in this system by introducing the method of "variational classical networks", an efficient representation of the wave function in terms of a network of classical spins. We show that propagation of line defects has different light cone structures in the localized and ergodic phases.

[1] P. Karpov et al, Phys. Rev. Lett. **126**, 130401 (2021).
[2] R. Verdel et al, Phys. Rev. B **103**, 165103 (2021).

DY 11.4 Thu 10:45 H2

Superradiant many-qubit absorption refrigerator — Michal Kloc[1], Kurt Meier[1], Kimon Hadjikyriakos[2], and •Gernot Schaller[3] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328, Dresden, Germany

We show that the lower levels of a large-spin network with a collective antiferromagnetic interaction and collective couplings to three reservoirs may function as a quantum absorption refrigerator. In appropriate regimes, the steady-state cooling current of this refrigerator scales quadratically with the size of the working medium, i.e., the number of spins. The same scaling is observed for the noise and the entropy production rate.

[1] arXiv:2106.04164

DY 11.5 Thu 11:00 H2

Bose condensation of squeezed light — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

Light with an effective chemical potential and no mass is shown to possess a general phase-transition curve to Bose-Einstein condensation. This limiting density and temperature range is found by the diverging in-medium potential range of effective interaction. While usually the absorption and emission with Dye molecules is considered, here it is proposed that squeezing can create also such an effective chemical potential. The equivalence of squeezed light with a complex Bogoliubov transformation of interacting Bose system with finite lifetime is established with the help of which an effective gap is deduced. This gap phase creates a finite condensate in agreement with the general limiting density and temperature range. The phase diagram for condensation is presented due to squeezing and the appearance of two gaps is discussed. Phys. Rev. B 99 (2019) 205124

DY 11.6 Thu 11:15 H2

Interplay of thermal and plasmonic THz nonlinearities on graphene — Jeongwoo Han[1], Mattew L. Chin[2], •Stephan Winnerl[3], Thomas E. Murphy[2], and Martin Mittendorff[1] — [1]Department of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]University of Maryland, College Park, MD 20740, United States of America — [3]Helmholtz-Zentrum Dresden- Rossendorf, 01328 Dresden, Germany

Due to the linear dispersion, graphene has attracted much attention as a material platform of nonlinear optics, in particular in the infrared regime. While for higher photon energies the nonlinearities are mostly related to interband transitions and Pauli blocking, in the infrared regime intraband and thermal effects dominate. Here we present the experimental evidence of nonlinear THz absorption beyond thermal effects, i.e., plasmonic nonlinearity, by employing polarization-resolved terahertz pump-probe measurements on graphene disks. By varying the polarization between pump and probe beam, i.e., co- and cross-polarized configurations, we observe a significant polarization dependence of the pump-induced change in transmission. To quantitatively analyze this observation, we develop numerical simulation, allowing us to understand the interplay between thermal and plasmonic nonlinearities. While both contribute to the co-polarized configuration, thermal effects dominate the nonlinearity in the cross-polarized configuration.

DY 12: Active Matter (joint session DY/BP/CPP)

Time: Thursday 11:45–13:00 Location: H2

DY 12.1 Thu 11:45 H2

Orientation-dependent propulsion of active Brownian spheres: from advection to polygonal clusters* — •Jens Bickmann[1], Stephan Bröker[1], Michael E. Cates[2], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — [2]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom

Controllability of the collective dynamics of active Brownian particles is much desired for numerous potential future applications. In addition to the regular way of achieving control via external interventions, e.g., by traps, internal interventions in the dynamics of active Brownian particles become increasingly popular. Most often, internal intervention is achieved by a propulsion of the particles that depends on space, time, or orientation. Using field-theoretical modeling and particle-based simulations, we investigate systems of interacting active Brownian spheres in two spatial dimensions with an orientation-dependent propulsion. We show that different forms of orientation-dependent propulsion can give rise to advection, anomalous diffusion, and even the emergence of polygon-shaped clusters. **Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

DY 12.2 Thu 12:00 H2

The Anomalous Transport of Tracers in Active Baths — •Omer Granek[1], Yariv Kafri[1], and Julien Tailleur[2] — [1]Department of Physics, Technion-Israel Institute of Technology, Haifa, 3200003, Israel — [2]Université de Paris, Laboratoire Matière et Systèmes Complexes (MSC), UMR 7057 CNRS, F-75205 Paris, France

We derive the exact long-time dynamics of a tracer immersed in a one-dimensional active bath. In contrast to previous studies, we find that the damping and noise correlations possess long-time tails with exponents that depend on the tracer symmetry. For an asymmetric tracer, the tails lead to superdiffusion and friction that grows with time when the tracer is dragged at a constant speed. For a symmetric tracer, we recover normal diffusion and finite friction. However, when the symmetric tracer is small compared to the active-particle persistence length, the noise becomes anticorrelated at late times and the active contribution to the friction becomes negative: active particles then enhance motion rather than opposing it.

DY 12.3 Thu 12:15 H2

Forces on objects immersed in active fluids — Thomas Speck and •Ashreya Jayaram — Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7-9, 55128 Mainz, Germany

Depending on their shape, objects immersed in active fluids may be subjected to a net force or net torque. We show that in a finite, periodic system, the force/torque on such an object is determined by the vorticity of the polarization of the surrounding active fluid which in turn is localized to regions close to the object where its curvature changes. We find that the system size L has a colossal influence on the magnitude of the force which grows as L^2 before saturating to a constant. We relate this force to the current away from the body and substantiate our theoretical results with numerical simulations of active Brownian particles.

DY 12.4 Thu 12:30 H2

Active Cooling in Inertial Active Matter — •Lukas Hecht[1], Suvendu Mandal[2], Hartmut Löwen[2], and Benno Liebchen[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany — [2]Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

To cool down a target domain of an equilibrium system, the system must be coupled to an external bath to which heat can be transferred. However, active matter is intrinsically out of equilibrium and the active particles themselves do not obey the second law of thermodynamics. Therefore, we ask the question if we can actively cool down active particles in a target domain without transferring a significant amount of heat to particles in the environment.

In this work, we use the active Brownian particle (ABP) model with inertia to develop a route to cool down ABPs in a target domain without the need of an external bath. Such an active cooling requires two ingredients: First, we need the feature of inertial ABPs to undergo motility-induced phase separation into coexisting phases with different effective temperatures [1]. Second, a mechanism that localizes the phase-separated region in the target domain is required. We show several realizations of active cooling demonstrating how inertial effects in active matter can be utilized to actively cool down a target domain.

[1] S. Mandal, B. Liebchen, and H. Löwen, Phys. Rev. Lett. 123, 228001 (2019).

DY 12.5 Thu 12:45 H2

Arrested phase separation in nonreciprocally interacting colloids — •Sebastian Fehlinger and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Non-reciprocal interactions are wide spread in nature and can lead to a huge variety of phenomenons in many physical systems. For the specific case of a binary mixture of passive particles, the breaking of the action reaction principle can lead to formation of self-propelled dimers and other active molecules. For a small system size, these active molecules have already been realized in experiments based on phoretically interacting binary colloidal mixtures [1].

This work focuses on the numerical simulation of the Langevin equations describing many noninteracting colloids which we complement with a continuum theory. We find that the nonreciprocal attractions destabilize the uniform disordered phase and lead to clusters which grow in the course of the time. Surprisingly, for a wide parameter range, the clusters only grow up to a certain size such that coarsening is arrested. We attribute this to the spatiotemporal organization of the composition of the binary mixture within the cluster which essentially screens the phoretic attractions.

[1] F. Schmidt, B. Liebchen, H. Löwen, G. Volpe, J. Chem. Phys. 150, 094905 (2019).

DY 13: Focus session: Nonlinear Dynamics of the Heart II (organized by Markus Bär, Stefan Luther and Ulrich Parlitz)

Time: Thursday 13:30–16:15 Location: H2

Invited Talk DY 13.1 Thu 13:30 H2

Multi-scale modeling of dyadic structure-function relation in ventricular cardiac myocytes — •Martin Falcke[1], Filippo G. Cosi[2], Wolfgang Giese[1], Wilhelm Neubert[1], Stefan Luther[2], Nagaiah Chmakuri[3], and Ulrich Parlitz[2] — [1]Max Delbrück Center for Molecular Medicine in the Helmholtz Association, Berlin, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [3]IISER Thiruvananthapuram, India

Cardiovascular disease is often related to defects of sub-cellular components in cardiac myocytes, specifically in the dyadic cleft, which include changes in cleft geometry and channel placement. Modeling of these pathological changes requires both spatially resolved cleft as well as whole cell level descriptions. We use a multi-scale model to create dyadic structure-function relationships to explore the impact of molecular changes on whole cell electrophysiology and calcium cycling. This multi-scale model incorporates stochastic simulation of individual L-type calcium channels (LCC) and ryanodine receptor channels (RyRs), spatially detailed concentration dynamics in dyadic clefts, rabbit membrane potential dynamics, and a system of partial differential equations for myoplasmic and lumenal free calcium and calcium-binding molecules in the cell bulk. We found action potential duration, systolic and diastolic calcium to respond most sensitive to changes in LCC current. The RyR cluster structure inside dyadic clefts was found to affect all biomarkers investigated. The shape of clusters observed in experiments by Jayasinghe et al. and channel density within the cluster showed the strongest correlation to the effects on biomarkers.

DY 13.2 Thu 14:00 H2

Optogenetics control of spiral waves dynamics in cardiac tissue — Sayedeh Hussaini[1], Aidai Mamyraiym kyzy[1], Laura N. Diaz-Maue[1], Johannes Schroeder-Schetelig[1], Vishallini Venkatesan[1], Raul A. Quiñonez Uribe[1], Claudia Richter[1], Vadim Biktashev[2], Rupamanjari Majumder[1], Valentin Krinski[1], and •Stefan Luther[1] — [1]Research Group Biomedical Physics, Max Planck Institute for Dynamics and Self-Organization, G\"ottingen, Germany — [2]Exeter University, Exeter, England, United Kingdom

The heart is an excitable medium. The formation of spiral waves in the heart is the main cause of life-threatening cardiac arrhythmias. Defibrillation is a method to control these abnormal waves. Due to the significant side effects of this method, the development of alternative methods is needed. To do this, we need to deepen our knowledge of the dynamics of spiral waves. For this, Optogenetics has shown its great potential. In this work, using optogenetics we control the dynamics of a spiral wave in a two-dimensional domain of the mouse heart. We apply global and structured illumination patterns at different light intensities. In the sub-threshold regime illumination, we observed the tendency of the spiral wave to drift along the LI gradient. This observation provides us with a new mechanistic insight into optogenetic defibrillation. Global epicardial illumination of the cardiac surface leads to an intramural exponential decay of illumination which may cause the drift of a spiral wave towards the epicardium, where the wave may be terminated with supra-threshold illumination.

DY 13.3 Thu 14:15 H2

Spatiotemporal correlation of cardiac tissue and its variation in response to temperature — •Alessandro Loppini[1], Alessio Gizzi[1], Christian Cherubini[1], Flavio Fenton[2], and Simonetta Filippi[1] — [1]Unit of Nonlinear Physics and Mathematical Modeling, Campus Bio-Medico University of Rome, 00128 Rome, Italy — [2]School of Physics, Georgia Institute of Technology, Atlanta, Georgia, USA

Complex emergent dynamics are at the basis of life-threatening cardiac arrhythmias, including tachycardia and fibrillation. In the past years, a large number of studies have shown that such irregular rhythms in myocardium electrical oscillations are anticipated by cardiac alternans, are supported by nonlinearities, tissue heterogeneity, and anisotropy, and are further shaped by the mechanical and thermal state of the tissue. In this context, a comprehensive understanding of the appearance and development of impaired rhythms, starting from the underlying spatiotemporal dynamics, is required to prevent cardiac failure. In this contribution, we discuss a novel correlation analysis of cardiac activation maps accounting for thermal feedback, showing its application on canine ventricular tissues monitored via optical mapping. Specifically, we define a characteristic length able to describe the emergent synchronization of the tissue and analyze its variations at alternans onset and during their development at different temperatures. Computed results show that the characteristic length is significantly lower in the alternans regime compared to physiological rhythms. Also, we further show that thermal-induced changes in the underlying dynamic result in corresponding variations of the characteristic length.

15 min. break.

Invited Talk DY 13.4 Thu 14:45 H2

Cardiac repolarization dynamics and arrhythmias in healthy and diseased hearts — •Esther Pueyo — University of Zaragoza, Zaragoza, Spain

The electrical activity of the heart is the result of a set of complex nonlinear biophysical and biochemical processes occurring at different scales within the cardiac tissue. The variability arising from these processes translates into variability at the cell, tissue, organ and whole-body levels. The importance of investigating variability in cardiac electrical activity, in general, and in cardiac repolarization (i.e. the return of cells to their resting state after electrical activation), in particular, has been well documented, having shown value for diagnosis, monitoring and treatment of cardiac diseases.

In this talk, I will present studies combining computational, experimental and clinical methods to investigate temporal and spatial variability in cardiac repolarization. I will show the role of stochasticity in contributing to this variability in health and diseased hearts. The link between enhanced repolarization variability and pro-arrhythmia will be described, with emphasis on the role of the autonomic nervous system as a modulator of this link.

DY 13.5 Thu 15:15 H2

Using small perturbations and machine learning for the control of spiral wave chaos — •Thomas Lilienkamp — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The dynamics during life threatening cardiac arrhythmias like ventricular fibrillation is governed by chaotic spiral/scroll wave dynamics. In ex-vivo experiments and numerical simulations, a phenomenon called self-termination can be observed frequently, where the chaotic dynamics terminates by itself without any interaction. We demonstrate what implications this observation has on the structure of the state space, and how this structure can be exploited for an efficient control of the dynamics via small but finite perturbations (localized in space and time). We also discuss, how machine learning algorithms can be used for the control of such systems.

DY 13.6 Thu 15:30 H2

A simulation study of the effects of optogenetics on the human cardiac pacemaker: Prospects of Opto-ATP control. — Afnan Nabizath Mohamed Nazer[1], Sayedeh Hussaini[2,3], Raul A. Quinonez Uribe[2], Stefan Luther[2,3], and •Rupamanjari Majumder[1,2] — [1]University Medical Center Göttingen, 37075 Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — [3]Institute for the Dynamics of Complex Systems, Goettingen University, Goettingen, Germany

High-frequency electric spiral and scroll waves often occur in the heart during lethal cardiac arrhythmias. Treatment of such arrhythmias necessitates removal of these waves. Currently, the most effective approach to eliminating these waves is defibrillation, which involves delivering high-voltage shocks to the heart. However, the technique is accompanied by numerous negative side effects that make it suboptimal.

Optimizing defibrillation primarily requires reducing defibrillation energy. To this end, the approach that works best for tachycardic arrhythmias is anti-tachycardia pacing (ATP). ATP relies on the external application of a series of low-energy, high-frequency electrical pulses that stimulate the heart faster than the arrhythmia. A biological evolution of this approach would be to replace the external energy source with the heart's own pacemaker. But such a step would require deeper understanding of pacemaker function. Recently, optogenetics has emerged as a powerful tool in cardiac research. Using optogenetic simulations, I explore the possibility to realise ATP in human hearts.

Invited Talk DY 13.7 Thu 15:45 H2

Dynamics of paroxysmal tachycardias — •Gil Bub — McGill University, Montreal, Canada

Reentrant cardiac arrhythmias can start and stop spontaneously, giving rise to paroxysmal bursting rhythms. Experiments and simulations suggest that the dynamics of these paroxysmal reentrant waves may be natural consequences of structural heterogeneity, action potential restitution, and tissue fatigue. Recent experimental studies show that reentrant wave termination is linked to alternans, the beat-to-beat variation in action potential duration and velocity. The impact of alternans on termination was also confirmed using simulations that include restitution curve dynamics. Initiation of these waves, however, is less well understood. Current challenges include the development of imaging technologies that can observe rare spontaneous initiation events in multiple samples to gain mechanistic insights.

DY 14: Mitgliederversammlung Fachverband DY

Tagesordnung:

Bericht DY-Aktivitäten und Entwicklung 2020 - 21

Planung Regensburg 2022

Verschiedenes

Time: Thursday 18:00–19:00 Location: MVDY

60 Minuten

DY 15: Condensed-Matter Simulations augmented by Advanced Statistical Methodologies (joint session DY/CPP)

Time: Friday 10:00–11:00 Location: H2

DY 15.1 Fri 10:00 H2

Simple model to describe stability of thin domains — •Ruben Khachaturyan[1], Arne J. Klomp[2], Karsten Albe[2], and Anna Anna Grünebohm[1] — [1]Interdisciplinary Center for Advanced Materials Simulation, Ruhr-University Bochum — [2]Department of Materials Science, Technical University of Darmstadt, Darmstadt, Germany

Ferro domains are important for contemporary electronics, particularly decreasing domain size allowing for denser information storage per unit area. Thermal fluctuations limit domain stability, which is the key property for ferroic data storage. Therefore the ability to estimate the expected lifetime of a domain is of crucial importance. In this work, we simulate 180° domains in BaTiO3 with different widths at various temperatures using ab initio based molecular dynamics simulation employing LAMMPS and feram codes. We then derived a model to analyze the lifetime of the domains depending on their width and temperature. The model treats domain walls as fluctuating strings. String stiffness reflects the information about energy for domain wall roughening and thermal fluctuations are considered as a field of random forces. Our findings allowed us to interpret the stochastic nature of thin domain collapses and identify associated energies. With further development of the model, we are planning to consider the behavior of ferroelastic and ferromagnetic domain walls.

DY 15.2 Fri 10:15 H2

Population Annealing Monte Carlo Using the Rejection-Free n-Fold Way Update Applied to a Frustrated Ising Model on the Honeycomb Lattice — •Denis Gessert[1,2] and Martin Weigel[1,3] — [1]Centre for Fluid and Complex Systems, Coventry University, Coventry, CV1 5FB, United Kingdom — [2]Institut für Theoretische Physik, Leipzig University, Postfach 100920, D-04009 Leipzig, Germany — [3]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Population annealing (PA) is a MC method well suited for the study of systems with a rough free energy landscape, e.g. glassy systems. PA is similar to an equilibrium version of parallel simulated annealing runs with the addition of a resampling step at each temperature. While a large population may improve imperfect equilibration, it is evident PA will fail when almost no spins are flipped in the equilibration routine.

This is the case in systems with a low temperature phase transition where high Metropolis rejection rates make sampling phase space near infeasible. To overcome this slowdown we propose a combination of the PA framework with the rejection-free "n-fold way" update and achieve an exponential speed-up at low temperatures compared to Metropolis.

To test our method we study the Ising model with competing ferromagnetic nearest and antiferromagnetic next-to-nearest neighbor interactions of strengths $J_1 > 0$ and $J_2 < 0$, resp., on the honeycomb lattice. As T_c becomes arbitrarily small, when approaching the special point $J_2 = -J_1/4$ with $T_c = 0$, we consider this a good choice to test the efficacy of our method.

DY 15.3 Fri 10:30 H2

Noncontact friction: The role of viscous friction and its non-universality — •Miru Lee[1], Niklas Weber[2], Richard Vink[2], Cynthia Volkert[2], and Matthias Krüger[1] — [1]Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Obtaining theoretical predictions for friction during sliding motion is challenging due to the complex nature of the problem. In the so-called noncontact regime, the friction tensor is given by the leading order of the pairwise interactions between the probe and the surface atoms [1]. In such a regime, one can thus find an analytic expression of the friction tensor [2]. Starting from a stochastic viscoelastic solid model, we identify the two paradigmatic dissipation mechanisms [3]: phonon radiation, prevailing even in a purely elastic solid, and phonon damping, e.g., caused by viscous motion of crystal atoms. At small probe-surface separations, phonon damping dominates over phonon radiation, and vice versa at large separations. Phonon radiation is furthermore universal; there exists a general one-to-one mapping between the mean probe-surface force and the resulting friction. In contrast, phonon damping is non-universal, and no such general relation exists; it is subject to the details of the underlying pairwise interaction, e.g., the interaction range. For certain cases, the friction can even *decrease* with increasing surface area the probe interacts with.

[1] M. Lee, R. Vink, M. Krüger, Phys. Rev. B **101**, 235426 (2020)
[2] A. I. Volokitin, et. al., Phys. Rev. B **73**, 165423 (2006)
[3] M. Lee, R. Vink, C. Volkert, M. Krüger, In preparation.

DY 15.4 Fri 10:45 H2

Investigation of transferability in LDOS based DFT surrogate models for multiscale simulations — •Lenz Fiedler[1,2] and Attila Cangi[1,2] — [1]Center for Advanced Systems Understanding (CASUS) — [2]Helmholtz-Zentrum Dresden-Rossendorf

Density Functional Theory (DFT) is one of the most important computational tools for materials science, as it combines high accuracy with general computational feasibility. However, applications important to scientific progress can pose problems to even the most advanced and efficient DFT codes due to size and/or complexity of the underlying simulations. Namely the modeling of materials across multiple length and time scales at ambient or extreme conditions, necessary for the understanding of important physical phenomena such as radiation damages in fusion reactor walls, evade traditional ab-initio treatment. DFT surrogate models are a useful tool in achieving this goal by reproducing DFT results at drastically reduced computational cost by using machine learning methods. Yet, a lack of transferability of many approaches lead to repeated and costly training data generation procedures. Here, we present results of an investigation to transfer such machine learning DFT surrogate models between different simulation cell sizes, with the goal of reducing the overall amount of computational time for training data generation. The models are based upon the Materials Learning Algorithms (MALA) package [1] and the therein implemented LDOS based machine learning workflow [2].

[1]: https://github.com/mala-project
[2]: J. A. Ellis et al., Phys. Rev. B 104, 035120, 2021

DY 16: Machine Learning in Dynamical Systems and Statistical Physics (joint session DY/BP)

Time: Friday 11:15–12:30 Location: H2

DY 16.1 Fri 11:15 H2

Tayloring Reservoir Computing Performance via Delay Time Tuning — •Tobias Hülser, Felix Köster, and Kathy Lüdge — Institut für Theoretische Physik, TU Berlin

Reservoir Computing is a versatile, fast-trainable machine learning scheme that utilises the intrinsic information-processing capacities of dynamical systems. In recent years delay-based reservoir computing emerged as a promising, easy to implement alternative to classical reservoir computing. Previous work showed that a mismatch between input time and delay time enhances computational performance significantly[1]. For delays much higher than the input time, it was shown that certain inputs cannot be recalled by the network which lead to gaps in the memory capacity[2]. Via manipulating the delays in a system of ring-coupled Stuart-Landau oscillators, we show that some of the gaps can be closed. Moreover, we can tune the range of previous inputs the reservoir can memorise. Consequently, we find a significant increase in performance for nonlinear memory tasks and the NARMA10 task.

[1] S. Stelzer et al., Neural Networks 124, 158-169 (2020)
[2] F. Köster et al., Cogn. Comput. (2020)

DY 16.2 Fri 11:30 H2

Employing artificial neural networks to find reaction coordinates and pathways for self-assembly — •Jörn Appeldorn, Arash Nikoubashman, and Thomas Speck — Inst. für Physik, Universität Mainz, Germany

We study the spontaneous self-assembly of single-stranded DNA fragments using the coarse-grained oxDNA2 implementation [1]. A successful assembly is a rare event that requires crossing a free energy barrier. Advanced sampling methods like Markov state modeling allow to bridge these long time scales, but they require one or more collective variables (order parameters) that faithfully describe the transition towards the assembled state. Formulating an order parameter typically relies on physical insight, which is then verified, e.g., through a committor analysis. Here we explore the use of autoencoder neural networks to automatize this process and to find suitable collective variables based on structural information. For this step, one still needs to map configurations onto structural descriptors, which is a non-trivial task. Specifically, we investigate the latent space of EncoderMap [2] and how it changes with the amount of information contained in the descriptor. With this approach, we were able to determine the free energy landscape, the locations of the (meta)stable states, and the corresponding transition probabilities.

[1] - Snodin et al., J. Chem. Phys.(2015), 142, 234901 [2] - T. Lemke and and C. Peter,J.Chem.TheoryComput.(2019), 15, 1209-1215

DY 16.3 Fri 11:45 H2

Efficient Bayesian estimation of the generalized Langevin equation from data — •Clemens Willers and Kamps Oliver — Center for Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Correnssstr. 2, 48149 Münster, Germany

A recent topic of research attracting broad interest is the modeling of stochastic time series whose dynamics includes memory effects. To cover this non-Markovian case, the Langevin equation, which is frequently used in many fields of science, is extended by a memory kernel, yielding the generalized Langevin equation (GLE). Since a direct derivation of the GLE from basic mechanisms through the well known Mori-Zwanzig formalism is not accessible in many cases, it is a relevant question how to estimate the model solely based on measured data.

In our work we develop a realization of Bayesian estimation of the GLE. The Bayesian approach allows for the determination of both estimates and their credibility in a straightforward manner. To facilitate this method, we consider the GLE with white noise. Although this is an approximation, we still deal with a very general model class representing systems with memory.

Importantly for applications, we realize the method in a numerically efficient manner through a piecewise constant parameterization of the drift and diffusion functions of the model, a reformulation of the likelihood, and an effective initial guess for the estimate.

We illustrate our method by an example from turbulence. Here we are able to reproduce the autocorrelation function of the original data set, which is an essential characteristic of a turbulent flow.

DY 16.4 Fri 12:00 H2

Master memory function for delay-based reservoir computers — •Felix Köster[1], Serhiy Yanchuk[2], and Kathy Lüdge[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, 10623 Berlin — [2]Institut für Mathematik, TU Berlin, Str. des 17. Juni 136, 10587 Berlin

The reservoir computing scheme is a versatile machine learning mechanism, which shows promising results in time-dependent task predictions in comparable fast-training times. Delay-based reservoir computing is a modification in which a single dynamical node under the influence of feedback is used as a reservoir instead of a spatially extended system.

We show that many delay-based reservoir computers considered in the literature can be characterized by a universal master memory function (MMF). Once computed for two independent parameters, this function provides linear memory capacity for any delay-based single-variable reservoir with small inputs. Moreover, we propose an analytical description of the MMF that enables its efficient and fast computation. Our approach can be applied not only to the reservoirs governed by known dynamical rules such as Mackey-Glass or Ikeda-like systems but also to reservoirs whose dynamical model is not available.

DY 16.5 Fri 12:15 H2

Investigating the role of Chaos and characteristic time scales in Reservoir Computing — Marvin Schmidt[1,2], Yuriy Mokrousov[1,3], Stefan Blügel[1,3], Abigail Morrison[2,3,4], and •Daniele Pinna[1,3] — [1]Peter Grünberg Institute (PGI-1), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [2]Institute for Theoretical Neuroscience Institute of Neuroscience and Medicine (INM-6), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [3]Institute for Advanced Simulation (IAS-6), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [4]Computational and Systems Neuroscience & JARA-Institut Brain structure-function relationships (INM-10), Wilhelm-Johnen-Straße, 52428 Jülich, Germany

Reservoir Computing (RC) dynamical systems must retain information for long times and exhibit a rich representation of their driving. This talk highlights the importance of matching between input and dynamical timescales in RC systems close to chaos. We compare a chain of Fermi-Pasta-Ulam-Tsingou anharmonic oscillators and a sparsely connected network of spiking excitatory/inhibitory neurons. The first is toy model for magnetic spin-wave reservoirs while the latter that of a biological neural net. Both systems are shown to rely on a close matching of their relaxation timescales with the driving input signal's frequency in order to memorize and make precise use of the information injected. We argue that this is a general property of RC systems. We acknowledge the HGF-RSF project TOPOMANN for funding.

DY 17: Theory and Simulation (joint session CPP/DY)

Time: Friday 13:30–15:00 Location: H3

See CPP 15 for details of this session.

DY 18: Symposium: Synchronization Patterns in Complex Dynamical Networks (organized by Jakub Sawicki, Sabine Klapp, Markus Bär and Jens Christian Claussen) (joint session DY/SOE)

The program of this session is embedded in a symposium supported by DPG section DY and SOE as well as TU Berlin, SFB 910 and the BCSCCS e.V in Honor of Professor Eckehard Schöll's 70th Birthday. Eckehard Schöll has been the local organizer of the DPG-SKM conferences in Berlin for many years and was awarded the DPG badge of honour (Ehrennadel) for his service to the community.

Time: Friday 13:30–16:00 Location: ESS

Invited Talk DY 18.1 Fri 13:30 ESS

Network-Induced Multistability Through Lossy Coupling — •Jürgen Kurths — PIK, Potsdam, Germany — HU Berlin, Germany

The stability of synchronized networked systems is a multi-faceted challenge for many natural and technological fields, from cardiac and neuronal tissue pacemakers to power grids. For these, the ongoing transition to distributed renewable energy sources leads to a proliferation of dynamical actors. The desynchronization of a few or even one of those would likely result in a substantial blackout. Thus, the dynamical stability of the synchronous state has become a leading topic in power grid research. Here we uncover that, when taking into account physical losses in the network, the back-reaction of the network induces new exotic solitary states in the individual actors and the stability characteristics of the synchronous state are dramatically altered. These effects will have to be explicitly taken into account in the design of future power grids. We expect the results presented here to transfer to other systems of coupled heterogeneous Newtonian oscillators.

Invited Talk DY 18.2 Fri 14:00 ESS

Control of synchronization in two-layer power grids — •Simona Olmi[1], Carl Totz[2], and Eckehard Schöll[2] — [1]Istituto dei Sistemi Complessi - CNR - Firenze, Italy — [2]Technische Universität Berlin - Germany

In this talk we suggest to model the dynamics of power grids in terms of a two-layer network, and use the Italian high voltage power grid as a proof-of-principle example. The first layer in our model represents the power grid consisting of generators and consumers, while the second layer represents a dynamic communication network that serves as a controller of the first layer. In particular, the dynamics of the power grid is modelled by the Kuramoto model with inertia, while the communication layer provides a control signal P_i^c for each generator to improve frequency synchronization within the power grid. We propose different realizations of the communication layer topology and different ways to calculate the control signal. Then we conduct a systematic survey of the two-layer system against a multitude of different realistic perturbation scenarios, such as disconnecting generators, increasing demand of consumers, or generators with stochastic power output. When using a control topology that allows all generators to exchange information, we find that a control scheme aimed to minimize the frequency difference between adjacent nodes operates very efficiently even against the worst scenarios with the strongest perturbations.

30 min. break.

Invited Talk DY 18.3 Fri 15:00 ESS

Relay and complete synchronization of chimeras and solitary states in heterogeneous networks of chaotic maps — Elena Rybalova[1], Eckehard Schöll[2], and •Galina Strelkova[1] — [1]Institute of Physics, Saratov State University, Astrakhanskaya str. 83, Saratov 410012, Russia — [2]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

In this talk we discuss the phenomena of relay and complete synchronization in a heterogeneous three-layer network of chaotic maps. In the considered network two remote layers are not directly coupled but interact via a relay layer with which they are pairwise and symmetrically coupled. All the three layers represent rings of nonlocally coupled discrete-time oscillators but the relay layer is completely different in its spatiotemporal dynamics from that of the outer layers. We consider the cases when the individual elements of the relay layer and of the outer layers are described by Lozi maps and Henon maps, respectively, and vice versa. We establish and explore relay and complete synchronization of chimera structures and solitary state modes in a heterogeneous multiplex network and analyze the role of the relay layer structure in the resulted synchronous patterns. The results are illustrated by diagrams of desynchronized and synchronous regimes in the "inter-layer coupling - intra-layer coupling of the relay layer" parameter planes.

Invited Talk DY 18.4 Fri 15:30 ESS

A bridge between the fractal geometry of the Mandelbrot set and partially synchronized dynamics of chimera states. — •Ralph G Andrejzak — Universitat Pompeu Fabra, Barcelona, Catalonia, Spain

A simple quadratic map with a complex-valued parameter c allows one to generate enormously rich dynamics and patterns. Fractal Julia sets and the Mandelbrot set divide the complex plane into stable and divergent regions of the map's initial conditions and parameters c. What happens if one couples several quadratic maps? We address this question using a minimal two-population network of two pairs of two quadratic maps. In dependence on c, the network enters into qualitatively different dynamical states. The network iterates can diverge to infinity or remain bounded. Bounded solutions can get fully synchronized, fully desynchronized, or enter into different partially synchronized states, including a symmetry-broken chimera state. We will at first inspect examples for these different dynamical states in the domain of the complex-valued iterates of the network. We then illustrate that the boundaries between different dynamical states form intriguing fractal patterns in the domain of the complex-valued c.

DY 19: Transport (joint session TT/DY)

Time: Friday 13:30–15:00 Location: H6

See TT 28 for details of this session.

Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

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Overview of Invited Talks and Sessions

(Lecture halls H1, H3, H4, H5, and H7; Poster P)

Invited Talks

HL 1.1	Mon	10:00–10:30	H4	**Phonon Screening of Excitons in Halide Perovskites and Beyond** — •Marina Filip
HL 1.2	Mon	10:30–11:00	H4	**Anharmonic semiconductors - Lessons Learned from Halide perovskites** — •Omer Yaffe
HL 1.3	Mon	11:00–11:30	H4	**Exciton structure symmetry analysis for quantum-well layered halide perovskites and charge-energy transfer in presence of π-conjugated organic chromophores** — •Claudio Quarti
HL 1.4	Mon	11:45–12:15	H4	**Solid state ionics of hybrid halide perovskites: equilibrium situation and light effects** — •Alessandro Senocrate, Gee Yeong Kim, Tae-Youl Yang, Giuliano Gregori, Michael Grätzel, Joachim Maier
HL 1.5	Mon	12:15–12:45	H4	**Unifying Ultrafast Polarization Responses of Lead Halide Perovskites via Two-Dimensional Optical Kerr Effect** — •Sebastian F. Maehrlein
HL 5.1	Mon	13:30–14:00	H4	**The role of chalcogen vacancies for atomic defect emission in MoS_2** — Elmar Mitterreiter, Bruno Schuler, Daniel Hernangómez-Pérez, Julian Klein, Jonathan Finley, Sivan Refaely-Abramson, Alexander Holleitner, Alexander Weber-Bargioni, •Christoph Kastl
HL 7.1	Tue	10:00–10:30	H4	**Ultrafast Spin-Lasers** — Natalie Jung, Markus Lindemann, Tobias Pusch, Rainer Michalzik, Martin R. Hofmann, •Nils C. Gerhardt
HL 11.1	Tue	13:30–14:00	H4	**Modulation Doping in High-Mobility Alkaline-Earth Stannates** — •Bharat Jalan
HL 11.2	Tue	14:00–14:30	H4	**Ultrathin oxides on InGaN nanowires: Hybrid nanostructure photoelectrodes and optical analysis of chemical processes** — P. Neuderth, J. Schörmann, M. Coll, M. de la Mata, J. Arbiol, R. Marschall, •M. Eickhoff
HL 11.3	Tue	14:30–15:00	H4	**Doping and charge compensation mechanisms in semiconducting oxides** — •Andreas Klein
HL 11.4	Tue	15:00–15:30	H4	**Oxide Memristors for edge computing and secure electronics** — •Heidemarie Schmidt
HL 11.5	Tue	15:30–16:00	H4	**Integration of 33°Y-$LiNbO_3$ films with high-frequency BAW resonators** — Sondes Boujnah, Mihaela Ivan, Vincent Astié, Samuel Margueron, Mario Constanza, Jean-Manuel Decams, •Ausrine Bartasyte
HL 14.1	Wed	10:00–10:30	H4	**Quantum Interference of Identical Photons from Remote Quantum Dots** — •Giang N. Nguyen, Liang Zhai, Clemens Spinnler, Julian Ritzmann, Matthias C. Löbl, Andreas D. Wieck, Arne Ludwig, Alisa Javadi, Richard J. Warburton
HL 15.1	Thu	10:00–10:30	H4	**Quasi-instantaneous switch-off of deep-strong light-matter coupling** — •Christoph Lange, Joshua Mornhinweg, Maike Halbhuber, Viola Zeller, Cristiano Ciuti, Dominique Bougeard, Rupert Huber
HL 15.2	Thu	10:30–11:00	H4	**Lithium niobate nonlinear nanophotonics** — •Frank Setzpfandt
HL 15.3	Thu	11:00–11:30	H4	**Quadratic nanomaterials for integrated photonic devices** — •Rachel Grange
HL 15.4	Thu	11:45–12:15	H4	**Topological plasmonics: Ultrafast vector movies of plasmonic skyrmions on the nanoscale** — •Harald Giessen, Pascal Dreher, David Janoschka, Frank Meyer zu Heringdorf, Tim Davis, Bettina Frank
HL 15.5	Thu	12:15–12:45	H4	**Supercontinuum second-harmonic generation spectroscopy of 2D semiconductors** — •Steffen Michaelis de Vasconcellos
HL 18.1	Thu	13:30–14:00	H4	**Telecom wavelength quantum dot-based single-photon sources for quantum technologies** — •Anna Musial
HL 22.1	Fri	10:00–10:30	H4	**Two-dimensional gain materials for new nanolaser concepts** — •Christopher Gies
HL 22.2	Fri	10:30–11:00	H4	**Room-temperature polariton lattices for quantum simulation** — •Stephane Kena-Cohen
HL 22.3	Fri	11:00–11:30	H4	**Topological nanocavity lasers and topological high-power lasers** — •Yasutomo Ota, Yasuhiko Arakawa, Satoshi Iwamoto

HL 22.4	Fri	11:45–12:15	H4	**Topological Insulator Lasers** — •Miguel A. Bandres, Steffen Wittek, Gal Harari, Mordechai Segev, Demetrios N. Christodoulides, Mercedeh Khajavikhan
HL 22.5	Fri	12:15–12:45	H4	**When polariton condensates have dissipations or have no excitons** — •Hui Deng

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium Potentials for NVs sensing magnetic phases, textures and excitations (SYNV)

See SYNV for the full program of the symposium.

SYNV 1.1	Mon	13:30–14:00	Audimax 2	**Harnessing Nitrogen Vacancy Centers in Diamond for Next-Generation Quantum Science and Technology** — •Chunhui Du
SYNV 1.2	Mon	14:00–14:30	Audimax 2	**Nanoscale imaging of spin textures with single spins in diamond** — •Patrick Maletinsky
SYNV 1.3	Mon	14:30–15:00	Audimax 2	**Spin-based microscopy of 2D magnetic systems** — •Jörg Wrachtrup
SYNV 1.4	Mon	15:15–15:45	Audimax 2	**Exploring antiferromagnetic order at the nanoscale with a single spin microscope** — •Vincent Jacques
SYNV 1.5	Mon	15:45–16:15	Audimax 2	**Nanoscale magnetic resonance spectroscopy with NV-diamond quantum sensors** — •Dominik Bucher

Invited talks of the joint symposium Multidimensional coherent spectroscopy of functional nanostructures (SYCS)

See SYCS for the full program of the symposium.

SYCS 1.1	Tue	10:00–10:30	Audimax 1	**Multidimensional coherent spectroscopy of perovskite nanocrystals** — •Steven Cundiff, Albert Liu, Diogo Almeida, Gabriel Nagamine, Lazaro Padilha
SYCS 1.2	Tue	10:30–11:00	Audimax 1	**Coherent multidimensional techniques for the characterization of nanomaterials** — •Elisabetta Collini
SYCS 1.3	Tue	11:00–11:30	Audimax 1	**Exciton Dynamics revealed by Multidimensional Coherent Spectroscopies applied to Light-Harvesting Systems** — •Thomas L.C. Jansen
SYCS 1.4	Tue	11:45–12:15	Audimax 1	**Revealing couplings with action-based 2D microscopy** — •Tobias Brixner
SYCS 1.5	Tue	12:15–12:45	Audimax 1	**Low-frequency phonons affect charge carrier dynamics in hybrid perovskites** — •Mischa Bonn

Invited talks of the joint symposium Advanced neuromorphic computing hardware: Towards efficient machine learning (SYNC)

See SYNC for the full program of the symposium.

SYNC 1.1	Wed	10:00–10:30	Audimax 1	**Equilibrium Propagation: a Road for Physics-Based Learning** — •Damien Querlioz
SYNC 1.2	Wed	10:30–11:00	Audimax 1	**Machine Learning and Neuromorphic Computing: Why Physics and Complex Systems are Indispensable** — •Ingo Fischer
SYNC 1.3	Wed	11:00–11:30	Audimax 1	**Photonic Tensor Core Processor and Photonic Memristor for Machine Intelligence** — •Volker Sorger
SYNC 1.4	Wed	11:45–12:15	Audimax 1	**Material learning with disordered dopant networks** — •Wilfred van der Wiel
SYNC 1.5	Wed	12:15–12:45	Audimax 1	**In-memory computing with non-volatile analog devices for machine learning applications** — •John Paul Strachan

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Attosecond and coherent spins: New frontiers (SYAS)

See SYAS for the full program of the symposium.

SYAS 1.1	Thu	10:00–10:30	Audimax 2	**Ultrafast Coherent Spin-Lattice Interactions in Iron Films** — •Steven Johnson
SYAS 1.2	Thu	10:30–11:00	Audimax 2	**Ultrafast spin, charge and nuclear dynamics: ab-initio description** — •Sangeeta Sharma, John Kay Dewhurst
SYAS 1.3	Thu	11:15–11:45	Audimax 2	**Light-wave driven Spin Dynamics** — •Martin Schultze, Markus Münzenberg, Sangeeta Sharma
SYAS 1.4	Thu	11:45–12:15	Audimax 2	**All-coherent subcycle switching of spins by THz near fields** — •Christoph Lange, Stefan Schlauderer, Sebastian Baierl, Thomas Ebnet, Christoph Schmid, Darren Valovcin, Anatoly Zvezdin, Alexey Kimel, Rostislav Mikhaylovskiy, Rupert Huber
SYAS 1.5	Thu	12:15–12:45	Audimax 2	**Ultrafast optically-induced spin transfer in ferromagnetic alloys** — •Stefan Mathias

Invited talks of the joint symposium Physics of van der Waals 2D heterostructures (SYWH)

See SYWH for the full program of the symposium.

SYWH 1.1	Thu	13:30–14:00	Audimax 2	**Spin interactions in van der Waals topological materials and magnets** — •Saroj Dash
SYWH 1.2	Thu	14:00–14:30	Audimax 2	**Exciton optics, dynamics and transport in atomically thin materials** — •Ermin Malic, Samuel Brem, Raul Perea-Causin, Daniel Erkensten, Roberto Rosati
SYWH 1.3	Thu	14:30–15:00	Audimax 2	**Correlated Electrons in van der Waals Superlattices: Control and Understanding** — •Tim Wehling
SYWH 1.4	Thu	15:15–15:45	Audimax 2	**Exciton manipulation and transport in 2D semiconductor heterostructures** — •Andras Kis
SYWH 1.5	Thu	15:45–16:15	Audimax 2	**Chern Insulators, van Hove singularities and Topological Flat-bands in Magic-angle Twisted Bilayer Graphene*** — •Eva Andrei, Shuang Wu, Zhenyuan Zhang

Invited talks of the joint symposium The Rise of Photonic Quantum Technologies – Practical and Fundamental Aspects (SYPQ)

See SYPQ for the full program of the symposium.

SYPQ 1.1	Fri	10:00–10:30	Audimax 2	**Quantum dots operating at telecom wavelengths for photonic quantum technology** — •Simone Luca Portalupi
SYPQ 1.2	Fri	10:30–11:00	Audimax 2	**Photonic graph states for quantum communication and quantum computing** — •Stefanie Barz
SYPQ 1.3	Fri	11:00–11:30	Audimax 2	**Rare-earth ion doped solids at sub-Kelvins: practical and fundamental aspects** — •Pavel Bushev
SYPQ 1.4	Fri	11:45–12:15	Audimax 2	**Quantum Light and Strongly Correlated Electronic States in a Moiré Heterostructure** — •Brian Gerardot
SYPQ 1.5	Fri	12:15–12:45	Audimax 2	**Quantum communication in fibers and free-space** — •Rupert Ursin

Sessions

HL 1.1–1.5	Mon	10:00–12:45	H4	**Focus Session: When theory meets experiment: Hybrid halide perovskites for applications beyond solar**
HL 2.1–2.5	Mon	10:00–12:45	H7	**Focus Session: Exotic Charge Density Wave States of Matter: Correlations and Topology (joint session TT/HL)**
HL 3.1–3.26	Mon	10:00–13:00	P	**Poster Session I**
HL 4.1–4.7	Mon	11:15–13:00	H3	**2D materials and their heterostructures (joint session DS/HL/CPP)**
HL 5.1–5.9	Mon	13:30–16:15	H4	**2D semiconductors and van der Waals heterostructures I (joint session HL/DS)**
HL 6.1–6.8	Mon	13:30–17:00	H5	**Focus Session: Magnon Polarons - Magnon-Phonon Coupling and Spin Transport (joint session MA/HL)**
HL 7.1–7.5	Tue	10:00–11:30	H4	**Semiconductor Lasers**
HL 8.1–8.28	Tue	10:00–13:00	P	**Poster Session II**
HL 9.1–9.3	Tue	11:45–12:30	H4	**Nitride: Preparation, Charakterization and Devices**
HL 10.1–10.5	Tue	13:30–16:15	H3	**Focus Session: Highlights of Materials Science and Applied Physics I (joint session DS/HL)**
HL 11.1–11.7	Tue	13:30–16:30	H4	**Focus Session: Functional Metal Oxides for Novel Applications and Devices**
HL 12.1–12.6	Tue	13:30–16:45	H5	**Focus Session: Spin-Charge Interconversion (joint session MA/HL)**
HL 13.1–13.32	Tue	13:30–16:30	P	**Poster Session III**
HL 14.1–14.9	Wed	10:00–12:45	H4	**Materials and devices for quantum technology (joint session HL/TT)**
HL 15.1–15.5	Thu	10:00–12:45	H4	**Focus Session: Tailored Nonlinear Photonics**
HL 16.1–16.6	Thu	11:15–12:45	H1	**Semiconductors: Optical, Transport and Ultrafast Properties**
HL 17.1–17.5	Thu	13:30–16:15	H1	**Focus Session: Topological Phenomena in Synthetic Matter (joint session DS/HL)**
HL 18.1–18.10	Thu	13:30–16:30	H4	**Quantum Dots and Wires (joint session HL/TT)**
HL 19.1–19.31	Thu	13:30–16:30	P	**Poster Session IV**
HL 20	Thu	18:00–19:00	MVHL	**Annual General Meeting of the Semiconductor Physics Division**
HL 21.1–21.4	Fri	10:00–11:00	H1	**Focus Session: Highlights of Materials Science and Applied Physics II (joint session DS/HL)**
HL 22.1–22.5	Fri	10:00–12:45	H4	**Focus Session: Emerging Semiconductor Laser Concepts**
HL 23.1–23.7	Fri	11:15–13:00	H1	**Focus Session: Highlights of Materials Science and Applied Physics III (joint session DS/HL)**
HL 24.1–24.1	Fri	13:30–15:00	Audimax 2	**Quo Vadis Quantum Technologies? About Promises, Prospects, and Challenges**
HL 25.1–25.5	Fri	13:30–14:45	H4	**2D semiconductors and van der Waals heterostructures II (joint session HL/DS)**

Annual General Meeting of the Semiconductor Physics Division

Thursday 18:00–19:00 MVHL

- Bericht des Vorsitzenden
- Wahl der Leitung des Halbleiterphysik Fachverbandes
- Verschiedenes

Sessions

– Invited, Topical, Contributed Talks, Discussions, and Posters –

HL 1: Focus Session: When theory meets experiment: Hybrid halide perovskites for applications beyond solar

Hybrid halide perovskites are by now well-established solar absorber and emitter materials, with power conversion efficiencies of single-cell devices exceeding 20 percent. We have observed - with notable exceptions - a widening gap between experimental and theoretical efforts in the literature on halide perovskites. Further, a large fraction of the literature focuses on properties relevant for optoelectronic applications, while we envision a much wider scope for these materials, e.g in spintronic and electrochemical applications. The purpose of this focus session is to provide a platform for theorists and experimentalists working in this field, to interact, present state-of-the-art methods, and exchange their ideas on future directions for this technologically relevant class of materials beyond the current focus on optoelectronics.

Organizers: Linn Leppert (University of Twente) and Felix Dreschler (TU München)

Time: Monday 10:00–12:45 Location: H4

Invited Talk HL 1.1 Mon 10:00 H4

Phonon Screening of Excitons in Halide Perovskites and Beyond — •Marina Filip — University of Oxford, Department of Physics

The interaction of photoexcited bound electron-hole pairs (excitons) is screened by both electrons and by polar phonons. For organic-inorganic lead-halide perovskites, theoretical and experimental evidence suggests that ionic vibrations have an important contribution to the dielectric screening [1,2]. However, state of the art GW/BSE methodology for studying electronic and optical excitations does not capture phonon screening effects. In this talk I will present our recently developed framework based on GW/BSE, to include phonon screening effects [3]. I will show that phonon screening contributes to significantly reduce the exciton binding energy, and demonstrate this effect for lead halide perovskites, CsPbX3 (X = Cl, Br, I), as well as other well known semiconductors and insulators. Furthermore, I will show our generalization of the Wannier-Mott model to include phonon screening effects, and discuss general trends for the phonon screening contribution to the exciton binding energy.

[1] Miyata et al, Nat. Phys. 11, 582 (2015) [2] Umari et al, JPCL, 9 , 3 ,620 (2018) [3] Filip, Haber & Neaton, PRL, in press (2021)

This work was supported by the US Department of Energy and the UK EPSRC. Computational resources were provided by the National Energy Research Scientific Computing Center (NERSC) and the Texas Advanced Computing Center (TACC) through the NSF-funded XSEDE program.

Invited Talk HL 1.2 Mon 10:30 H4

Anharmonic semiconductors - Lessons Learned from Halide perovskites — •Omer Yaffe — Weizmann Institute of Science, Rehovot, Israel

In semiconductor physics, the dielectric response, charge carrier mobility and other electronic material properties at finite temperatures, are always treated within the framework of the harmonic approximation. This approach is very successful in capturing the properties of tetrahedrally bonded semiconductors such as silicon and GaAs.

In my talk, I will show that halide perovskites are fundamentally different due to their strongly anharmonic lattice dynamics. Large amplitude, local polar fluctuations induced by lattice anharmonicity localize the electronic states and enhance the screening of electric charge within the material. In other words, in some aspects, halide perovskites behave more like a liquid than a crystalline solid. I will also discuss the implications of these findings on other families of semiconductors such as organic and rock-salt semiconductors.

Invited Talk HL 1.3 Mon 11:00 H4

Exciton structure symmetry analysis for quantum-well layered halide perovskites and charge-energy transfer in presence of π-conjugated organic chromophores — •Claudio Quarti — Laboratory for Chemistry of Novel Materials, University of Mons

2D layered halide perovskites are surging as interesting materials for optoelectronic applications. These systems are characterized by a quantum-well structure, with a semiconducting halide perovskite frame sandwiched between organic insulating spacers, the spatial confinement stabilizing tightly bound excitons. Still, full understanding of the native electronic and excitonic properties of layered halide perovskites is inherently hard to achieve, as many physical mechanisms contribute to complicate the scenario, including dielectric confinement, structural distortions, Spin-Orbit-Coupling (SOC), etc. Here, I review the electronic and excitonic structure of 2D layered halide perovskites, adopting group theory symmetry analysis. This highlights the analogies and differences in the atomic contributions on the single particle band structure, as compared to the 3D case, with SOC inherently included in the analysis. I will then consider the interaction between the organic spacers and the inorganic semiconducting frame in the case of a type II heterointerface, as obtained via incorporation of π-conjugated molecular moieties as organic spacers. With reference to tetrazine-based layered halide perovskite, I discuss several photoexcitation decay channels, with clear distinction between charge, singlet- and triplet-energy transfer.

15 min. break.

Invited Talk HL 1.4 Mon 11:45 H4

Solid state ionics of hybrid halide perovskites: equilibrium situation and light effects — •Alessandro Senocrate[1,2], Gee Yeong Kim[1], Tae-Youl Yang[1], Giuliano Gregori[1], Michael Grätzel[1,2], and Joachim Maier[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

In recent years, hybrid halide perovskites have been attracting great attention due to their exceptional photo-electrochemical properties. When used as light-harvesters in solar cells, device efficiencies exceeding 25 % can be realized. We showed that a deeper understanding of (i) functionality, (ii) stability, as well as (iii) the possibility to improve the performance require a thorough insight into non-stoichiometry and ion transport. In this contribution, we study the nature of the ionic conductivity in methylammonium lead iodide ($MAPbI_3$), the archetypal halide perovskite, by means of a great number of electrochemical and nuclear magnetic techniques. To aid the experimental investigation, we include detailed defect chemical modelling describing the effects of varying iodine partial pressure (stoichiometry) and dopant content. By extending this study to the situation under illumination, we observe a striking enhancement of ionic conductivity by more than 2 orders of magnitude in $MAPbI_3$, alongside the expected increase in electronic conductivity. Such analyses are then extended to other halide perovskite compositions. While discussing these results, a mechanistic explanation of this astonishing phenomenon arises, which has relevance for photo-stability and photo-demixing processes.

Invited Talk HL 1.5 Mon 12:15 H4

Unifying Ultrafast Polarization Responses of Lead Halide Perovskites via Two-Dimensional Optical Kerr Effect — •Sebastian F. Maehrlein — Columbia University, New York, USA — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

The microscopic mechanism behind the outstanding optoelectronic properties of lead halide perovskites (LHPs) may lead to novel design principles for defect tolerant semiconductors, but is still highly debated. Previous studies, investigating the LHPs' ultrafast polarization response by the optical Kerr effect lead to dynamic screening models, which suggest charge carrier protection by large polarons and/or liquid-like screening.

Here, we finally decode the variety of nonlinear polarization signals by developing two-dimensional optical Kerr effect (2D-OKE) spectroscopy. We unveil a surprisingly unified origin: Both (inorganic and hybrid) LHP responses are governed by nonlinear mixing of anisotropic and highly dispersive light propagation near the optical band gap [1]. Based on the 2D-OKE fingerprint, we quantify dispersion anisotropy, follow phase transitions and trace lattice parameters of hybrid alloyed LHPs; supported by a comprehensive four-wave-mixing model. Moreover, our findings raise the awareness in all types of polarization sensitive pump-probe experiments and their modeling, where oscillatory signals are commonly assigned to coherent low-energy excitations (e.g. phonons, magnons, etc.). The presented works were mainly performed with L. Huber, F. Wang, and P.P. Joshi at X.-Y. Zhu group (Columbia U). [1] S. F. Maehrlein et al., DOI:10.1073/pnas.2022268118

HL 2: Focus Session: Exotic Charge Density Wave States of Matter: Correlations and Topology (joint session TT/HL)

The recent observation of charge density waves (CDW) in a variety of topological materials ranging from two-dimensional dichalcogenides, Weyl semimetals and metallic kagome systems has prompted intensive research on the origin and effects of such states. In these systems charge order forms the basis for correlated and topological states of quantum matter: Mott Hubbard correlations, tentative spin-liquid physics and chiral superconductivity in two-dimensional dichalcogenides, the emergence of axionic CDWs in Weyl semimetals and an interplay of Z2 topology, charge order and superconductivity in kagome metals. At the same time topology and electron correlations feed back on the CDW formation and dynamics. In this Focus Session we bring together theorists and experimentalists working in the field to discuss the interplay of charge order, correlations and topology in representative model systems, to identify major open challenges in our understanding of these systems and ultimately reach out for controlling CDW physics in correlated topological states of matter.

Organizers: Roser Valenti (Frankfurt University), Tim Wehling (Bremen University)

Time: Monday 10:00–12:45 Location: H7

See TT 2 for details of this session.

HL 3: Poster Session I

Topics:
- 2D semiconductors and van der Waals heterostructures
- Optical properties
- Quantum transport and quantum Hall effect
- THz and MIR physics in semiconductors

Time: Monday 10:00–13:00 Location: P

HL 3.1 Mon 10:00 P

Biopolymer-templated TiO2 SERS sensors — •Qing Chen[1,2], Marie Betker[1,4,5], Constantin Harder[1,3], Calvin Brett[1,5], Matthias Schwartzkopf[1], Nils Ulrich[7], Maria Eugenia Toimil Molares[7], Christina Trautmann[7], Daniel Söderberg[4,5], Christian Weindl[3], Volker Körstgens[3], Peter Müller-Buschbaum[3,6], Mingming Ma[2], and Roth Stephan[1] — [1]DESY, Notkestraße 85, 22607 Hamburg, Germany — [2]USTC, 230026 Hefei, China — [3]TUM, James-Franck Straße 1, 85748 Garching, Germany — [4]KTH, Teknikringen 56-58, 100 44 Stockholm, Sweden — [5]WWSC, Teknikringen 52-56, 100 44 Stockholm, Sweden — [6]MLZ, TUM, Lichtenbergstraße 1, Garching 85748, Germany — [7]GSI Helmholtz Center, Planckstrße 1, Darmstadt 64291, Germany

Titanium dioxide (TiO2) is an excellent candidate for semiconductor metal oxide-based Surface enhanced Raman scattering (SERS) substrate. We report a novel strategy of the cellulose nanofibril (CNF) - assisted assembly of TiO2/CNF thin-films with a hierarchical three-dimensional network and crystallinity as a SERS substrate. TiO2/CNF thin-films are obtained through the combined action of surface templating and thermal annealing. A high enhancement factor in terms of semiconductor SERS substrates for 4-mercaptobenzoic acid of 1.79 * 106 is obtained in the TiO2/CNF thin-films on ITO substrate with a thickness of 10 nm after thermal annealing. Our approach realizes the improvement of SERS sensitivity of semiconductor metal oxide nanomaterials through a cooperative modulation of the biotemplate morphology and the TiO2 crystalline state.

HL 3.2 Mon 10:00 P

Quantum Theory of Exciton-Plasmon Coupling in Two-Dimensional Semiconductors functionalized with Metal Nanoparticles — •Lara Greten, Robert Salzwedel, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Monolayers of transition metal dichalcogenides (TMDCs) exhibit tigthly bound excitons with large optical amplitudes, originating from a reduced screening of the Coulomb interaction due to the reduced dimensionaly of these ultrathin materials. The latter gives also rise to a high sensivity of such excitons to their environment.

Contrary, the optical response of metal nano-particles is dominated by plasmons which are collective electron oscillations. They facilitate an impressive amplification of the electric near-field and allow to manipulate the electric field on dimensions below the diffraction limit.

In the presented work, we consider theoretically exciton-plasmon coupling in a hybrid structure of a TMDC layer supported by a single metal nano-particle or a two-dimensional array. For this purpose, we develop a Maxwell-Bloch theory where the excitons are described within the Heisenberg equation of motion framework and the metal nano-particles are treated in classical Mie theory.

Our studies reveal new ”plexcitonic” eigenstates of the hybrid system. Furthermore, the results confirm that the configuration allows to reach the strong coupling limit which features a Rabi splitting of tens of meV.

HL 3.3 Mon 10:00 P

Near-field terahertz spectroscopy of flakes of 2D materials — •Ahmad-Reza Etemadi, Sebastian Matschy, Ahana Bhattacharya, and Martin Mittendorff — Department of physics, University of Duisburg-Essen, 47057 Duisburg, Germany

THz spectroscopy is a powerful tool to investigate the carrier dynamics in many materials. Unfortunately, gaining access to the THz conductivities of small samples, e.g. flakes of 2D materials, is rather difficult, as the THz spot size is much larger than the structure of interest. Direct detection in the near-field improves the spatial resolution and can be done by placing the sample directly on top of an electro-optic crystal. A near-infrared (NIR) beam is exploited to probe the THz field in the vicinity of the flake. The spatial resolution of the experiment is mostly determined by the NIR beam size in the electro-optic crystal and the diffraction of the THz beam by the sample. Here we analyze the potential performance of such a THz near-field microscope and present the current stage of our instrument.

HL 3.4 Mon 10:00 P

Optical properties of various crystalline phases of WO_3 — •Felix Bernhardt and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research, Justus- Liebig-Universität Gießen, 35392 Gießen, Germany

Tungsten trioxide (WO_3) is a semiconductor suitable for a wide variety of applications. Due to multiple, temperature-driven phase transitions and an electronic band gap within the optical spectrum [1], it is employed in a multitude of devices, ranging from smart windows [3] to gas sensors [5]. In this work, we investigate the monoclinic (stable at room temperature), the triclinic and orthorhombic phases of WO3 from first principles. Furthermore, we compare them with a hypothetical, simpler cubic configuration, which is often employed to approximate the real structures in theoretical studies.

Ground state properties such as lattice parameters and electronic structures are calculated within density functional theory (DFT). The optical response is modeled within the Bethe-Salpeter equation and time-dependent DFT using a long-range corrected kernel. Our results are in excellent agreement with previous theoretical investigations [1,4] as well as experiments [2,6]. The cubic phase fails to correctly reproduce the dielectric function of the real crystals.

[1] M Mansouri et al, Turk. Journal of Phys. 41(238) (2017) [2] B Loopstra et al, Acta Cryst. 25(1420) (1968) [3] L Liang et al, Sci. Rep. 3(1936) (2013) [4] F Wang et al, Journal Of Phys. Chem. 115(8345) (2011) [5] N. Yamazoe et al, Catalysis Surveys from Asia 7(63-75) (2003) [6] M Vargas et al, Journal of Applied Phys. 115(2014)

HL 3.5 Mon 10:00 P

Theoretical investigations of (non linear) optical properties of [RSi(CH2SnPh)3E3] molecules and molecular crystals on the path to understanding white light generation using molecules containing adamantane-like cores. — •Ferdinand Ziese[1], Irán Rojas-León[2], Christof Dues[1], Stefanie Dehnen[2], and Simone Sanna[1] — [1]Solid State Spectroscopy, Institut für Theoretische Physik Heinrich-Buff-Ring 16, 35392 Gießen — [2]The Dehnen Group, Hans-Meerwein-Straße 4, 35032 Marburg

Recent studies have demonstrated white light generation from molecular clusters with adamantane-like cores and different ligands [1,2]. The mechanism leading to the white light emission is currently under discussion. In order to understand the intertwinement between atomic and electronic structure and optical response, we have modeled the structural, electronic, and (nonlinear) optical properties from first principles. Isolated molecules and molecular crystals with formula unit [RSi(CH2SnPh)3E3], where R=Ph, Tol, and E=S, Se, Te. Both the chemistry of the ligands and of the cluster core have an heavy impact on the optical response of the material. The investigations presented append current and past investigations on the path towards understanding white light generation using molecules containing adamantane-like cores.

[1] N. W. Rosemann, J. P. Eußner, A. Beyer, S. W. Koch, K. Volz, S. Dehnen, S. Chatterjee, Science 2016, 352, 301

[2] N. W. Rosemann, J. P. Eußner, E. Dornsiepen, S. Chatterjee, S. Dehnen, J. Am. Chem. Soc. 2016, 138, 16224.

HL 3.6 Mon 10:00 P

How to Trace Structural Dynamics in Lead Halide Perovskites Using THz Kerr Effect Spectroscopy — •Maximilian Frenzel[1], Marie Cherasse[1,2], Leona Nest[1], Martin Wolf[1], and Sebastian F. Maehrlein[1] — [1]Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]LSI, CEA/DRF/IRAMIS, CNRS, Ecole polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France

The origin of the surprising optoelectronic performance of lead halide perovskite (LHP) semiconductors is still debated. It has been suggested that their highly polar and anharmonic lattice might beneficially govern their optoelectronic properties in the form of dynamic charge carrier screening. To study the LHP's ultrafast lattice polarization when subjected to a transient electric field we employ THz Kerr Effect (TKE) spectroscopy. In particular, we investigate the responses in the organic-inorganic hybrid semiconductor $MAPbBr_3$ and its fully inorganic counterpart $CsPbBr_3$. By comparing our obtained signals to four-wave mixing simulations, we find that it is crucial to account for dispersion and optical anisotropy, as certain features may be misidentified for molecular relaxation dynamics or quasi-particle oscillations. Finally, we show that strong THz fields nonlinearly excite Raman active phonons in both materials, corresponding to distortions of the inorganic lattice. We hope that these findings lead to a more complete understanding of the ultrafast lattice response to transient local fields and its contributions to charge carrier screening.

HL 3.7 Mon 10:00 P

single-photon emission and coherence properties of quantum emitters in WSe_2 monolayers — Martin von Helversen[1], •Bárbara Rosa[1], Chirag Palekar[1], Carlos Antón-Solanas[2], Christian Schneider[3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Institute of Physics,Carl von Ossietzky University, Oldenburg, Germany — [3]Institute of Physics, University of Oldenburg, Oldenburg, Germany

Two-dimensional van der Waals monolayers have arisen as a new plat-form for exploring optical, electronic, and structural properties of semi-conducting materials. Among several unique features of transitionmetal dichalcogenides, the ability of manipulating one or few atomiclayers play an important role in providing a potential two-level single photon emitters (SPEs) by engineering of strain [1,2] or defects [2]. In this work, we explore the quantum properties of SPEs in strained WSe2monolayers [1]. By conducting off- and quasi-resonant optical excitation at cryogenic temperatures, we identify emitters with linewidth sas low as 70 /*mu*eV. Furthermore, throughout second order auto-correlation measurements we observe a multi-photon suppression by achieving $g^{(2)}(0) = 0.05(5)$. Lastly, we investigate the first order of coherence in SPEs WSe_2 when performing scanning Michelson interferometer experiments.

[1] L. N. Tripathi, et al.ACS Photonics8, 5, 1919-1926 (2018).

[2] K. Parto et al.Nat Commun.12, 3585 (2021).

HL 3.8 Mon 10:00 P

Magnetotunneling Spectroscopy of Double Quantum Wells in GaAs/AlGaAs Heterostructures — •Maximilian Mischke[1], Gunnar Schneider[1], Werner Dietsche[2], and Rolf Johann Haug[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik — [2]Max-Planck-Institut für Festkörperfoschung, Stuttgart

In order to investigate the influence of a parallel magnetic field on bilayer phenomena, we performed magnetotunneling measurements on GaAs/AlGaAs double quantum wells. Therefore, the tunneling current between the two quantum wells is measured dependent on applied bias voltage, electron densities in the individual wells and a magnetic field oriented parallel to the 2D layers. We observe a systematic dependence of the tunneling resonance on the energetic difference of the two wells due to imbalanced densities. The applied bias compensates the mismatch. The parallel magnetic field introduces an additional term to the wave vector of the electrons, leading to a shift of the Fermi circles of the two quantum wells against each other [1]. This shift has an influence on the tunneling resonance since 2D-2D-tunneling requires not only energy conservation but also conservation of momentum [2]. The results of the measurements allow for a mapping of the Fermi contours of the two quantum wells [3,4].

[1] G.S. Boebinger et al, Phys. Rev. B 43, 12673 (1991)

[2] J.P. Eisenstein et al, Appl. Phys. Lett. 58, 1497 (1991)

[3] J.P. Eisenstein et al, Phys. Rev. B 44, 6511 (1991)

[4] T. Ihn et al, Phys. Rev. B 54, R2315 (1996)

HL 3.9 Mon 10:00 P

Back Focal Plane Imaging of Interlayer Excitons in $WSe_2/MoSe_2$ Heterostructures — •Lukas Sigl[1], Mirco Troue[1], Mauro Brotons-Gisbert[2], Brian Gerardot[2], Ursula Wurstbauer[3], and Alexander Holleitner[1] — [1]TU Munich, Germany — [2]Heriot-Watt University, United Kingdom — [3]University of Münster, Germany

Transition metal dichalcogenide monolayers exhibit strong light-matter interactions, which promotes them as ideal candidates for novel 2D optoelectronic applications. A vertical stacking into van der Waals heterostacks leads to the formation of long-lived interlayer excitons in adjacent layers.

We experimentally determine the transition dipole orientation of interlayer excitons in $WSe_2/MoSe_2$ heterobilayers at a base temperature of 1.7 K. The far-field photoluminescence is observed in the back focal plane of a microscope objective, such that the angular emission pattern can be resolved. An analytical model, based on source terms and transfer matrices, provides an accurate description of the dipole radiation from the heterobilayers. The obtained dipole orientation gives insight into the nature of interlayer exciton transitions and coincides with theoretical calculations for the ground state configurations in R- and H-type heterobilayers.

HL 3.10 Mon 10:00 P

Terahertz spectroscopy on nanograined Bismuth Telluride pellets — •Ahana Bhattacharya[1], Jeongwoo Han[1], Sepideh Izadi[3,4], Sarah Salloum[2], Stephan Schulz[2], Gabi Schierning[3], and Martin Mittendorff[1] — [1]Department of Physics, University of Duisburg-Essen,47057, Duisburg, Germany — [2]Department of Chemistry, University of Duisburg-Essen, 45141, Essen, Germany — [3]Department of Physics, Experimental Physics, Bielefeld University, 33615, Bielefeld, Germany — [4]Leibniz IFW Dresden, Institute for Metallic Materials, 01069, Dresden, Germany

Topological insulators (TI) host surface carriers with a very high mobility. However, the transport properties of extended crystals are dominated by bulk carriers which outnumber the surface carriers by orders of magnitude. One way to overcome the domination of bulk carriers is to use compacted TI nanoparticles. Bismuth Telluride nanoparticles which are compacted by hot pressing to nanograined bulk samples with a high surface to volume ratio are studied and analyzed.

THz time-domain spectroscopy is used as a tool to elucidate the contribution of surface and bulk carriers to the transport properties. While this is not possible with dc measurements, this can be achieved by measuring the reflection as a function of the frequency. Charge carriers with a high mobility lead to a pronounced frequency dependence of the conductivity, and thus the reflection, while low mobility carriers lead to a rather flat response. Analyzing the experimental results at various temperatures allows us to understand the role of surface and bulk carriers

HL 3.11 Mon 10:00 P

Electrical Investigation of Thin $ZrSe_3$-Films — •Lars Thole[1], Sonja Locmelis[2], Christopher Belke[1], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany

In recent years, 2D materials have garnered a lot of attention. Particularly graphene and transition metal dichalcogenides have been researched extensively [1]. However, there is a continuous interest in different groups of 2D materials because of their potential for new physics. Among these, the transition metal trichalcogenides (TMTC) include a lot of materials showing extraordinary properties [2].

We want to present our research on the TMTC zirconium triselenide ($ZrSe_3$) which we synthesized by a chemical transport method, exfoliated into thin flakes and then contacted by using e-beam lithography. It was possible to determine characteristics similar to that of the bulk material, even in thin layers down to 9 nm. Temperature dependent measurements give a value of about 0.6 eV for the band gap. Looking at the case of infinite thickness by comparing samples with different thicknesses a mean free path for the bulk material was determined.

Thin flakes showed a degradation behavior under ambient condition which was investigated in more detail, showing a growth over several weeks. Furthermore, thin-film transistors show n-type doping when operated with a gate voltage.

[1] A. K. Geim, I. V. Grigorieva, Nature, 499, 419-425 (2013).
[2] J. O. Island et al., 2D Materials, 4, 0220033 (2017).

HL 3.12 Mon 10:00 P

Polarization resolved photoluminescence study of interlayer excitons in a twisted van-der-Waals heterostructure — •Johannes Michl[1], Sergey Tarasenko[2], Frederik Lohof[3], Christopher Gies[3], Martin von Helversen[4], Renee Sailus[5], Sefaattin Tongay[5], Takashi Taniguchi[6], Kenji Watanabe[6], Tobias Heindel[4], Stephan Reitzenstein[3], Tatiana Shubina[2], Sven Höfling[1], Carlos Anton-Solanas[1,7], and Christian Schneider[7] — [1]Technische Physik, Universität Würzburg — [2]Ioffe Institute, St. Petersburg — [3]Institute for Theoretical Physics, University of Bremen — [4]Institute of Solid-State Physics, Technische Universität Berlin — [5]Arizona State University — [6]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [7]Institute of Physics, Carl von Ossietzky University Oldenburg

Two-dimensional monolayers of transition metal dichalcogenides (TMDCs) offer a wide range of possibilities for investigation due to their unique optical properties, resulting from the exotic valley physics and the strong Coulomb interaction. By stacking two different TMDCs with a twist angle, a van der Waals heterostructure is formed that exhibits a spatially periodical Moiré potentials.

We discuss polarization resolved photoluminescence experiments performed on interlayer excitons in a slightly twisted MoSe2/WSe2 heterobilayer. In detail, we focus on the polarization properties of our sample: Our results highlight the observation of a significant degree of circular polarization of excitons, which can be manipulated with an externally applied magnetic field.

HL 3.13 Mon 10:00 P

Magnetotransport Measurements on Folded Twisted Bilayer Graphene-Hexagonal Boron Nitride Heterostructure — •Bei Zheng[1], Lina Bockhorn[1], Christopher Belke[1], Sung Ju Hong[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Division of Science Education, Kangwon National University, Chuncheon, 24341, Republic of Korea

The transport properties of bilayer graphene are strongly depended on rotational mismatch between the two graphene sheets, owing to the energy band modulation from the corresponding Moiré superlattice [1,2]. Here, we focused on the magnetotransport characteristics of folded twisted bilayer graphene (fTBG) which was obtained by mechanical exfoliation and it's heterostructure stacking with hexagonal boron nitride (hBN). The typical Landau fan diagrams from our hBN/fTBG/hBN sample were observed and the corresponding quantum Hall effect was investigated. Additional to the charge neutrality point (CNP), a local resistance peak which is independent of the perpendicular applied magnetic field was also distinguished. This could be attributed to the folded edge [1] that induces strong gauge fields [3] and exhibits different charge carrier densities.

[1] H. Schmidt et al., Nat. Commun. 5, 5742 (2014)
[2] J. C. Rode et al., 2D Mater. 3, 035005 (2016)
[3] D. Rainis et al., Phys. Rev. B 83, 265404 (2011).

HL 3.14 Mon 10:00 P

An ultra-sensitive cavity absorption microscope for hyperspectral imaging of 2D materials — Manuel Nutz[1], •Ines Amersdorffer[1], Florian Sigger[1], Theodor Hänsch[2], Alexander Högele[2], Christoph Kastl[3], and Thomas Hümmer[1] — [1]Qlibri project, Faculty of Physics, Ludwig-Maximilians-Universität Munich, Germany — [2]Faculty of Physics, Ludwig-Maximilians-Universität Munich, Germany — [3]Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany

We use a tunable high-finesse optical micro-cavity as a versatile and powerful tool to measure absorption in transition metal dichalcogenides (TMDs) down to the parts-per-million level. Our scanning-cavity imaging technique [1,2], where a microscopic mirror is scanned across a larger mirror that hosts the sample, allows to collect absorption images of 2D materials with unprecedented sensitivity, spatially resolved with 2*m resolution and in real time. Our approach can be extended to allow for spectrally resolved measurements and reveals polarization-dependent absorption, implanted defects, crystal foldings, and bubbles. Furthermore, we present our progress to extend this absorption measurements to cryogenic temperatures. [1] Mader et al., Nat Commun 6, 7249 (2015) [2] Hümmer et al., Nat Commun 7, 12155 (2016)

HL 3.15 Mon 10:00 P

Detection of correlated noise in quantum rings — C. Riha[1], S. S. Buchholz[1], O. Chiatti[1], A. D. Wieck[2], D. Reuter[3], and •S. F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]Optoelektronische Materialien und Bauelemente, Universität Paderborn, 33098 Paderborn, Germany

Cross-correlated noise measurements in equilibrium at a bath temperature of T_{bath} = 4.2 K are performed in etched AlxGa1-xAs/GaAs-based quantum rings [1], which are of interest to the study of mode control and heat flow at the nanoscale and in quantum systems [2]. The measured white noise exceeds the thermal noise expected from the measured electron temperature T_e and the electrical resistance R. This excess noise is neither observed if one arm of a quantum ring is depleted of electrons nor in 1D-constrictions that have a length and width comparable to the quantum rings. Also, it decreases as T_{bath} increases and vanishes for T_{bath} > 12 K. A model is presented that suggests that the excess noise originates from the correlation of noise sources, mediated by phase-coherent propagation of electrons. The noise measurements at T_{bath} = 4.2 K allow the estimation of a correlation coefficient from the excess noise.

[1] C. Riha *et al.*, Appl. Phys. Lett. **117**, 063102 (2020)
[2] S. S. Buchholz *et al.*, Phys. Rev. B **85**, 235301 (2012); C. Kreisbeck *et al.*, Phys. Rev. B **82**, 165329 (2010); C. Riha *et al.*, Appl. Phys. Lett. **106**, 083102 (2015)

HL 3.16 Mon 10:00 P

Improving the Visibility of Graphene on III-V semiconductors — •Timo Kruck, A.D. Wieck, and Arne Ludwig — Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum

In a first step towards working with graphene on III-V semiconductors the visibility of graphene will be analyzed and improved with an optical microscope in the NIR range.

Each layer of graphene absorbs a certain fraction of light in a wide spectral range from visible to infrared. This fraction is $\pi\alpha \sim 2.3\%$, where α is the fine-structure constant. This absorption can be enhanced by superimposing it on certain photonic structures. For this purpose, a DBR based on GaAs and AlAs with an antireflection layer was grown on a GaAs substrate with MBE and according reflectance spectra are measured. Graphene has been exfoliated on this structure and is observed with an optical microscope illuminated by a NIR VCSEL. The resulting contrast produced by a different number of layers is analyzed and compared with simulations based on the transfer matrix method (TMM). The TMM simulations are supported by reflectometry to account for deviations of the as-grown structure from the intended structure.

HL 3.17 Mon 10:00 P

Temperature and magnetic field dependent noise measurements in quantum rings — •Birkan Düzel[1], Olivio Chiatti[1], Sven S. Buchholz[1], Andreas D. Wieck[2], Dirk Reuter[3], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]Optoelektronische Materialien und Bauelemente, Universität Paderborn, 33098 Paderborn, Germany

Phase-coherent transport of electrons and resulting interference effects offer a way to characterize systems. Noise measurements can be used to determine system properties, such as the electron temperature T_e. White noise exceeding the expected thermal noise has been reported in quantum ring structures [1]. The presented model suggests that the excess noise is caused by a correlation of noise sources in quantum rings, because said excess noise can only be observed when two interfering electron pathes exist. This work investigates the dependence of the excess noise in quantum rings on the bath temperature and applied magnetic field. Noise measurements in Al_xGa_xAs/GaAs-based etched quantum rings are performed in equlibrium with bath temperatures ranging from 15 mK to 12 K and magnetic fields ranging from -50 mT to 50 mT. The aim is to quantify the relationship between the phase coherence length of the electrons and the excess noise in the quantum ring structures.

[1] C. Riha *et al.*, Appl. Phys. Lett. **117**, 063102 (2020).

HL 3.18 Mon 10:00 P

Charge transfer in TMDC-graphene heterobilayers with defects — •Daniel Hernangómez-Pérez and Sivan Refaely-Abramson — Weizmann Institute of Science, Rehovot, Israel

Recent experimental and theoretical studies of charge transport in van der Waals heterostructures have revealed a rich arena of electronic and optical phenomena, that span from tunneling spectroscopy [1] to ultrafast interfacial charge transfer after photoexcitation [2, 3]. We focus here on a theoretical study of charge transfer processes occurring at the interface of XS_2-graphene heterobilayers with isolated chalcogen vacancies (X = Mo, W). We analyze the low-energy subgap features of the defect states in the presence of graphene and propose a perturbation-based theory to describe electronic transport between the defect states mediated by the graphene layer.

[1] N. Papadopoulos, P. Gehring, K. Watanabe et al. Phys. Rev. B 101, 165303 (2020). [2] L. Yuan, T.-F. Chung, A. Kuc et al. Science Advances 4 (2), 10.1126/sciadv.1700324 (2018). [3] S. Aeschlimann, A. Rossi, M. Chávez-Cervantes et al. Science Advances 6 (20), 10.1126/sciadv.aay0761 (2020).

HL 3.19 Mon 10:00 P

A field-effect-transistor based on the carbon allotropes diamond and graphene — •Vasilis Dergianlis, Martin Geller, Dennis Oing, Nicolas Wöhrl, and Axel Lorke — Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

Graphene is the two-dimensional carbon allotrope that exhibits exceptional mechanical strength and electron mobility. Due to its high conductivity, it is considered as one of the best conductors and can also be used as gate electrode in transistor-type devices. A second important carbon allotrope is diamond, which is a wide-bandgap semiconductor in its bulk form, where by hydrogen termination and exposure to ambient atmosphere, a two dimensional hole gas (2DHG) is formed on its surface.

In this work, we have combined the two aforementioned 2D carbon allotropes together with a thin layer of hexagonal Boron Nitride (h-BN) to a diamond-based FET. The sample consists of chemical vapor deposition-grown diamond, where a hydrogen termination induces a 2DHG on the surface as a conductive layer [1]. Graphene and hBN flakes were exfoliated and, using a dry-transfer method, placed onto the functionalized diamond surface. In this transistor-like structure, the h-BN serves as the gate-dielectric. As graphene is an ambipolar two-dimensional semiconductor itself, it can serve as both the gate electrode and tunable conductive channel. We show FET characterization of the graphene-gated structure with a mobility of 5 $cm^2/V \cdot s$ and carrier density of $p = 3.7 \cdot 10^{12} cm^{-2}$ at a gate voltage of $V_g = -9V$ [1] Oing, D., et al. Diamond and Related Materials **97**, 107450 (2019).

HL 3.20 Mon 10:00 P

Proximity control of interlayer exciton-phonon hybridization in van der Waals heterostructures — •Marlene Liebich[1], Philipp Merkl[1], Chaw-Keong Yong[1], Isabella Hofmeister[1], Gunnar Berghaeuser[2,3], Ermin Malic[2,3], and Rupert Huber[1] — [1]Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, Philipps-Universitaet Marburg, 35037 Marburg, Germany — [3]Department of Physics, Chalmers University of Technology, 412 96 Gothenburg, Sweden

Van der Waals stacking has provided unprecedented flexibility in shaping many-body interactions by controlling electronic quantum confinement, orbital overlap and electron-phonon coupling. We introduce proximity-controlled strong-coupling between Coulomb correlations and lattice dynamics in neighbouring van der Waals materials, creating new electrically neutral hybrid eigenmodes, called excitonic Lyman polarons. Specifically, we explore how the internal orbital $1s$–$2p$ transition of Coulomb-bound electron-hole pairs in monolayer tungsten diselenide resonantly hybridizes with lattice vibrations of a polar capping layer of gypsum. Tuning orbital exciton resonances across the vibrational resonances, we observe distinct anticrossing and polarons with adjustable exciton and phonon compositions. Such proximity-induced hybridization can be further tailored by shaping the spatial wavefunction overlap of excitons and phonons, providing a promising new route towards engineering novel ground states of two-dimensional systems.

HL 3.21 Mon 10:00 P

Implementation of the Bethe-Salpeter Equation in the Spex Code — •Jörn Stöhler[1,2], Dmitrii Nabok[1], Christoph Friedrich[1], and Stefan Blügel[1] — [1]Forschungszentrum Jülich and JARA, Germany — [2]RWTH Aachen University, Germany

The Bethe-Salpeter Equation (BSE) and GW approximation are two many-body perturbation theory techniques that together form the state-of-the-art method to include electron-hole interaction in periodic systems. The BSE has proven to be the most accurate tool to compute optical absorption for the valence and core energy region, as well as electron energy loss. In recent developments the BSE has been applied to compute the exciton band dispersion and exciton effective masses, inelastic electron scattering, and many more.

We have implemented the BSE in the SPEX code, a full-potential linearized augmented planewave (FLAPW) code that supports a range of Green function based methods including the GW approximation, optical spectra in the random phase approximation, and more. The BSE is run on top of a one-shot G_0W_0 calculation with SPEX, or directly on top of the underlying density functional theory (DFT) calculations from FLEUR.

Our code has been tested for various bulk, layered and monolayer semiconductors, among them LiF and MoS2, and includes spin-orbit coupling. The results agree with the literature. We also use the crystal symmetries to achieve a significant computational speedup, and maintain good scalability of the code for parallel computing.

HL 3.22 Mon 10:00 P

Excitation-induced quenching and optical amplification in a CDW-phase of a two dimensional material — •Stephan Michael and Hans Christian Schneider — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, P.O. Box 3049, 67653 Kaiserslautern, Germany

The optical excitation of two dimensional materials like transition metal dichalcogenides (TMDs) in connection with their rich electronic phase diagrams offer new ways to manipulate material properties on ultrafast timescales [1,2]. We study theoretically the appearance and the quenching of a CDW phase in a model system of a two dimensional material due to optical excitation with time-dependent interaction matrix elements and screening effects. We describe the excitonic and coherent-phonon effects in the band-dynamics by electron-hole and electron-phonon coupling. The non-equilibrium carrier dynamics includes the optical excitation, the carrier-carrier scattering as well as the carrier-phonon scattering. We discuss how interaction processes affect anomalous expectation values and use projection techniques to illustrate the time-dependent appearance of additional bands. We propose an optical amplification effect in the mid-infrared up to infrared regime with a potential for high-frequency modulation.

[1] S. Mathias et. al., Nat. Commun. **7**, 12902 (2016).
[2] S. Michael and H. C. Schneider, Phys. Rev. B **100**, 035431 (2019).

HL 3.23 Mon 10:00 P

Electric field manipulation of the Zeeman splitting in van der Waals heterostructures — •Paulo E. Faria Junior and Jaroslav Fabian — University of Regensburg, Regensburg, Germany

Under external magnetic fields, the interplay of spin and orbital angular momenta drives the Zeeman splitting, often encoded by the effective g-factors. Here, we explore the electric field control of g-factors in transition metal dichalcogenides (TMDCs) van der Waals heterostructures (vdWHs) of $MoSe_2$ and WSe_2. Using a full ab initio approach for the electronic structure and g-factors, we show that external electric fields introduce strong interlayer hybridization with robust signatures in the g-factors of interlayer and intralayer excitons. Furthermore, different interlayer exciton species can be identified by their characteristic dependence with respect to the electric field, an important information to disentangle the optical spectra observed in experiments. In summary, our study provides fundamental insight on the electric field manipulation of g-factors in TMDC-based vdWHs, benchmarking the relevant physics that must be included to investigate moiré excitons. Supported by SFB 1277 and SPP 2244.

HL 3.24 Mon 10:00 P

InGaAs Based Resonant Tunnelling Diodes By GSMBE — •Begum Yavas Aydin, Sven Höfling, Fauzia Jabeen, and Lukas Worschech — Technische Physik, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany

Resonant Tunneling Diodes (RTD) are promising devices for various applications such as GHz to THz oscillators and high sensitivity photon detectors due to their ultra-high frequency, ultra-high-speed, and low power. High current density (JP) and high peak-to-valley current ratio (PVCR) are required for high-speed RTDs. To obtain high current densities and PVCR, structural parameter's dependence on barrier thickness, the spacer thickness of emitter and collector play key role.

InGaAs-based RTDs are grown by gas sources molecular beam epitaxy (GSMBE). High current density can be achieved by a thin barrier with a high electron transmission [1]. Peak current density reached 75 kA/cm2 with 1.5 nm thin AlAs barriers. Three RTD samples differing in In0.53Ga0.47As collector spacer thickness of 5, 10, and 25 nm are grown. The highest JP of 500 kA/cm2 with PVCR 5.7 is achieved at room temperature for a 1.5 nm thin AlAs barrier and an asymmetric spacer layer.

[1] Moise, T. S., et al. J. of Appl. Phys. 78.10 (1995)
[2] Kanaya, H., et al. J. of Infrared, Millimeter, Terahertz Waves 35.5 (2014)

HL 3.25 Mon 10:00 P

Nonlinear THz spectroscopy at TeraFERMI — •Johannes Schmidt, Paola Di Pietro, and Andrea Perucchi — Elettra - Sincrotrone Trieste S.C.p.A., S.S. 14 km - 163,5 in Area Science Park, I-34149 Basovizza, Trieste, Italy

TeraFERMI is a THz beamline at the Free-electron laser (FEL) FERMI. After passing the undulator of the FEL the electron bunches are refocused on a thin slab and generate coherent transition radiation (CTR) as THz pulses with a spectral range of typically 0.1 to 6 THz. TeraFERMI provides strong single-cycle pulses with MV/cm electric peak fields or magnetic peak fields up to 1 T, which is in combination with the low repetition rate of 50 Hz an ideal source for nonlinear spectroscopy in many sciences from biology to physics. The short ps THz-pulses are phase-envelope stable with a low temporal jitter of about 66 fs (rms) and is therefore perfect for THz-pump probe experiments with different probe colors. Up to now, we focused on THz-pump NIR-probe and fluence-dependent THz spectroscopy. Thereby is the radial polarization of the beam a specialty of the CTR THz-beam and allows for longitudinal spectroscopy. Here, we report about the latest technological advances of TeraFERMI as well as first pilot experiments.

HL 3.26 Mon 10:00 P

Quantum anomalous Hall effect in Bernal-stacked bilayer graphene — Fabian Geisenhof[1], Felix Winterer[1], Anna Seiler[2], Jakob Lenz[1], Tianyi Xu[3], Fan Zhang[3] und •Thomas Weitz[2] — [1]Department of Physics, Ludwig-Maximilians-Universität München, Germany — [2]Department of Physics, University of Texas at Dallas, USA — [3]1st Physical Institute, University of Göttingen, Germany

The anomalous quantum Hall effect is a peculiar state of matter that has been observed in only very few materials systems including artificially engineered Moiré heterostructures [1]. However, the special bandstructure of naturally occurring bilayer graphene, has also been predicted to host an interaction-driven quantum anomalous Hall insulating phase at zero magnetic field [2], which has escaped previous experimental observation. Here, based on advanced sample design of near-field imaging, suspension and dual-gating, we show clear signatures of this quantum anomalous Hall insulating phase in ultra-clean bilayer graphene [3]. Besides the simplicity, diversity, and robustness of the system, the quantum anomalous Hall phase is also distinct from previously observed ones, since it is the first phase that does not only exhibit quantized charge Hall conductance at zero magnetic field, but also spin, valley and spin-valley anomalous quantum Hall effects as well as out-of-plane ferroelectricity.

[1] A.L. Sharpe, et al. Science 365, 605 (2019); M. Serlin, et al. Science 367, 900 (2020),

[2] F. Zhang Synthetic Metals 210, 9 (2015)

[3] F. R. Geisenhof, et al. arXiv:2107.06915 (2021)

HL 4: 2D materials and their heterostructures (joint session DS/HL/CPP)

Time: Monday 11:15–13:00 Location: H3

See DS 2 for details of this session.

HL 5: 2D semiconductors and van der Waals heterostructures I (joint session HL/DS)

Time: Monday 13:30–16:15 Location: H4

Invited Talk HL 5.1 Mon 13:30 H4

The role of chalcogen vacancies for atomic defect emission in MoS_2 — Elmar Mitterreiter[1], Bruno Schuler[2], Daniel Hernangómez-Pérez[3], Julian Klein[4], Jonathan Finley[1], Sivan Refaely-Abramson[3], Alexander Holleitner[1], Alexander Weber-Bargioni[5], and •Christoph Kastl[1] — [1]Walter Schottky Institute, TU Munich — [2]nanotech@surfaces Laboratory, Empa — [3]Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science — [4]Massachusetts Institute of Technology — [5]Molecular Foundry, Lawrence Berkeley National Laboratory

The microscopic understanding of defect-related modifications in 2D materials requires correlation between atomic structure and resulting macroscopic electronic, optical or excitonic properties. Combing controlled defect engineering with optical spectroscopy as well as atomic imaging and ab-initio theory, we identify the optical signature of pristine chalcogen vacancies in single layer MoS_2. [1] Vacancies introduce a narrow optical emission, markedly different from previously observed broad luminescence bands. Comparing annealed vs. He-ion treated MoS_2, we establish that the recently discovered single-photon emitters in He-ion irradiated MoS_2 originate from chalcogen vacancies. Using focused ion beam irradiation, the latter can be created site-selectively [2] with a spatial precision better than 10 nm [3], which is important for a prospective integration of defect-based single photon emitters into quantum photonic circuits. [1] E. Mitterreiter et al., Nat. Commun. 12, 3822 (2021). [2] J. Klein et al. ACS Photonics 8, 669-677 (2021). [3] E. Mitterreiter et al., Nano Lett. 20, 4437 (2020).

HL 5.2 Mon 14:00 H4

Coherent light emission of exciton-polaritons in an atomically thin crystal at room temperature — •Hangyong Shan[1], Lukas Lackner[1], Bo Han[1], Evgeny Sedov[2], Falk Eilenberger[4], Sebastian Klembt[3], Sven Höfling[3], Alexey V. Kavokin[2], Christian Schneider[1], and Carlos Anton-Solanas[1] — [1]Institute of Physics, Carl von Ossietzky University, 26129 Oldenburg, Germany. — [2]School of Science, Westlake University, 310024 Hangzhou, People's Republic of China. — [3]Technische Physik, Universität Würzburg, D-97074 Würzburg, Am Hubland, Germany. — [4]Institute of Applied Physics, Abbe Center of Photonics, Friedrich Schiller University, 07745 Jena, Germany.

We experimentally study the coherence of exciton-polaritons in a Fabry-Perot microcavity loaded with an atomically thin WSe2 layer. Via Michelson interferometry, we capture clear evidence of increased spatial and temporal coherence of the emitted light from the spatially confined system ground-state. The coherence build-up is accompanied by a threshold-like behaviour of the emitted light intensity, which is a fingerprint of a polariton condensation effect. Valley-physics is manifested in the presence of an external magnetic field, which allows us to manipulate K and K* polaritons via the Valley-Zeeman-effect. Our findings are of high application relevance, as they confirm the possibility to use atomically thin crystals as simple and versatile components of coherent light-sources, and in valleytronic applications at room temperature.

HL 5.3 Mon 14:15 H4

Bosonic condensation of exciton-polaritons in an atomically thin crystal — •Carlos Anton-Solanas[1,2], Maximilian Waldherr[1], Martin Klaas[1], Holger Suchomel[1], Tristan H. Harder[1], Hui Cai[3], Evgeny Sedov[4], Sebastian Klembt[1], Alexey V. Kavokin[4], Sefaattin Tongay[5], Kenji Watanabe[6], Takashi Taniguchi[6], Sven Hoefling[1], and Christian Schneider[2] — [1]Univ. Wuerzburg, Germany — [2]Univ. Oldenburg, Germany — [3]Univ. California, USA — [4]Westlake Univ., China — [5]Arizona State Univ., USA — [6]Nat. Institute for Materials Science, Japan

Semiconducting monolayer crystals have emerged as a new platform for studies of tightly bound excitons and many-body excitations in ultimately thin materials. Their giant dipole coupling to optical fields makes them very appealing for (nano-) photonic devices, and for fundamental investigations in the framework of cavity quantum electrodynamics.

Our experiments demonstrate the strong light-matter coupling and, for the first time, the bosonic condensation of exciton-polaritons in an atomically thin layer of $MoSe_2$ coupled to a hybrid micro-cavity [1].

We demonstrate the emergence of long-range first-order spatial coherence, via interferometric $g^{(1)}(\tau)$ measures, and we have investigated the Zeeman splitting effects of condensed polaritons under strong magnetic fields.

[1] Anton-Solanas, C., Waldherr, M., Klaas, M. et al. Bosonic condensation of exciton polaritons in an atomically thin crystal. Nat. Mater. (2021).

HL 5.4 Mon 14:30 H4

Hybridization between monolayer transition-metal dichalcogenides and conjugated molecular adsorbants — •Jannis Krumland[1] and Caterina Cocchi[1,2] — [1]Humboldt-Universität zu Berlin — [2]Carl von Ossietzky Universität Oldenburg

We present a first-principles study on electronic hybridization in inorganic-oraganic interfaces composed of monolayer transition-metal dichalcogenides (TMDCs; molybdenum and tungsten disulfide and diselenide) and exemplary carbon-conjugated molecules such as pyrene and perylene. By means of band-structure unfolding techniques applied to hybrid density-functional theory calculations including spin-orbit coupling, we achieve an intuitive and clear description of electronic interaction between the inorganic and organic components of the heterostructures. From atom-projected band structures, we are able to rationalize the strong mixing between the valence states of the TMDC and the molecular orbitals. We additionally clarify why the highest occupied orbital couples with the TMDC bands only very weakly, regardless of the composition of the interface. The proposed analysis based on band structure unfolding lends itself for computationally efficient and yet reliable predictions of electronic interactions in more complex hybrid interfaces including larger molecules harvesting visible radiation.

HL 5.5 Mon 14:45 H4

Tunable Polymer/Air Bragg Optical Microcavity Configurations for Light-Matter Coupling with Transition-Metal Dichalcogenides and their Heterostructures — •Chirag Palekar[1,2], Stephan Reitzenstein[1], and Arash Rahimi-Iman[2] — [1]Present address: Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany

Light-matter interactions (LMI) in semiconducting materials is being studied extensively with the help of optical microcavities. Specifically, tunable microcavities provide a versatile platform to control the LMI between the material excitation and cavity photons. Here, we explore a new resonator approach which can be employed to achieve microscopic photonic Fabry-Pérot (FP) cavities with mechanically- tunable resonator modes and polymer/air Bragg mirrors [1], directly on a chip or device substrate in combination with active materials. Moreover, our simulations based on the transfer matrix method show, compression-induced mode control of the air-Bragg cavities enables tuning between the weak and strong coupling regime. Using this unique cavity configurations, LMI experiments with 2D semiconductors such as transitionmetal dichalcogenides (TMDC) are very attractive. Additionally, incorporation of TMDC heterostructures in FP cavities will provide a platform to understand the new regimes of Dicke superradiance as well as Bose-Einstein condensation of Moiré exciton-polaritons. Ref.: [1] Phys. Status Solidi RRL 2021, 15, 2100182

15 min. break

HL 5.6 Mon 15:15 H4

Phonon-assisted exciton dissociation in transition metal dichalcogenides — •Raul Perea-Causin[1], Samuel Brem[1], and Ermin Malic[1,2] — [1]Chalmers University of Technology, Gothenburg, Sweden — [2]Philipps-Universität, Marburg, Germany

Monolayers of transition metal dichalcogenides (TMDs) have been established in the last years as promising materials for novel optoelectronic devices. However, the performance of such devices is often limited by the dissociation of tightly bound excitons into free electrons and holes. While previous studies have investigated tunneling at large electric fields, we focus in this work on phonon-assisted exciton dissociation that is expected to be the dominant mechanism at small fields.

We present a microscopic model based on the density matrix formalism providing access to time- and momentum-resolved exciton dynamics including phonon-assisted dissociation [1]. We track the pathway of excitons from optical excitation via thermalization to dissociation, identifying the main transitions and dissociation channels. Furthermore, we find intrinsic limits for the quantum efficiency and response time of a TMD-based photodetector and investigate their tunability with externally accessible knobs, such as excitation energy, substrate screening, temperature and strain.

Our work provides microscopic insights in fundamental mechanisms behind exciton dissociation and can serve as a guide for the optimization of TMD-based optoelectronic devices.

[1] R. Perea-Causin et al., Nanoscale 13, 1884 (2021)

HL 5.7 Mon 15:30 H4

Lattice Configurations of Self-Assembled Folded Graphene — •Lina Bockhorn, Johannes C. Rode, Lucas Gnörich, Pengfei Zuo, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The stacking- and folding angle of 2D materials to 3D structures has emerged as an important, novel tuning parameter for the tailoring of optical, mechanical, electronic and magnetic properties. Therefore, it is highly desirable to gather insight into the mechanical formation of these structures on the nano-scale.

Here, we focus on the evolution of self-assembled folded graphene generated via atomic force microscopy technique, which could give a deep insight into its underlying growth energy [1, 2, 3]. The self-assembly process involves the folding-over of the graphene layer and the subsequent growth of a twisted graphene bilayer. We conclude, that these self-assembled structures move not only forward during the growth process but also appear to rotate and lock in at specific commensurate twist angles.

[1] J. C. Rode et al., Ann. Phys. 529, 1700025 (2017).
[2] J. C. Rode et al., 2D Mater. 6, 015021 (2018).
[3] L. Bockhorn et al., Appl. Phys. Lett. 118, 173101 (2021).

HL 5.8 Mon 15:45 H4

All-optical polarization and amplitude modulation of second harmonic generation in atomically thin semiconductors — •Sebastian Klimmer — Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany

Nonlinear optics is of paramount importance in several fields of science and technology. This is particularly true in the case of second harmonic generation (SHG), which is commonly used for frequency conversion, self-referencing of frequency combs, crystal characterization, sensing, and ultra-short pulse characterization. Large efforts have been devoted in the last years to realizing electrical and all-optical modulation of SHG in atomically thin materials, which are easy to integrate on photonic platforms and thus ideal for novel nano-photonic devices. Here, we propose a new approach to broadband all-optical modulation of SHG in 2D materials. Our concept is based only on symmetry considerations and thus is applicable to any material of the D3h symmetry group and with deep sub-wavelength thickness, such as all monolayer transition metal dichalcogenides. With this approach we demonstrate a 90° rotation of the polarization of the emitted SH on a time-scale limited only by the fundamental pulse duration. In addition, this ultrafast polarization switch can be immediately applied to realize all-optical SH amplitude modulation with depth of 100 %. Our results outperform any previous work on all-optical SHG modulation [1,2] in terms of modulation speed, modulation depth and SHG bandwidth.

[1] Taghinejad M. *et al.*, Small **16**, 1906347 (2020)
[2] Cheng Y. *et al.*, Nano Lett. **20**, 11 (2020) 8053-8058

HL 5.9 Mon 16:00 H4

Microscopic Theory of Exciton-Exciton Annihilation in Two-Dimensional Semiconductors — •Alexander Steinhoff, Matthias Florian, and Frank Jahnke — Institute for Theoretical Physics, University of Bremen, Bremen, Germany

Auger-like exciton-exciton annihilation (EEA) is considered the key fundamental limitation to quantum yield in devices based on excitons in two-dimensional (2d) materials. Since it is challenging to experimentally disentangle EEA from competing processes, guidance of a quantitative theory is highly desirable. The very nature of EEA requires a material-realistic description that is not available to date.

We present a many-body theory of EEA based on first-principle band structures and Coulomb interaction matrix elements that goes beyond an effective bosonic picture. Applying our theory to monolayer MoS_2 encapsulated in hexagonal BN, we obtain an EEA coefficient in the order of 10^{-3} cm^2s^{-1} at room temperature, suggesting that carrier losses are often dominated by other processes, such as defect-assisted scattering.

Our studies open a perspective to quantify the efficiency of intrinsic EEA processes in various 2d materials in the focus of modern materials research.

HL 6: Focus Session: Magnon Polarons - Magnon-Phonon Coupling and Spin Transport (joint session MA/HL)

The coupling of spin waves and atomic lattice vibrations in solid magnetic states, so-called magnon polarons (MPs), can have large impact on spin transport properties as recently explored for spin Seebeck effect, spin pumping and nonlocal spin transport. This resonant enhancement can be reached when the magnon dispersion is shifted by a magnetic field and crosses the phonon dispersion with sufficient overlap. While initially observed at low temperatures and large magnetic fields, further material and device developments have led to MPs at room temperature and moderate magnetic fields. Thus, MPs become important for the manipulation and amplification of spin currents in spintronic and spin caloritronic devices, e.g. by carrying the spins much further than using uncoupled magnons. This focus session highlights the main important research outcomes for MPs, state-of-the-art techniques to detect MPs, such as Brillouin light scattering, and to study MP transport, e.g. by spin Seebeck effect and nonlocal spin transport, as well as the investigation of MPs in different material classes such as garnets, ferrites and antiferromagnets. In addition, the excessive theoretical work on MPs performed recently is addressed in this focus session.

Organizer: Timo Kuschel (Bielefeld University)

Time: Monday 13:30–17:00 Location: H5

See MA 2 for details of this session.

HL 7: Semiconductor Lasers

Time: Tuesday 10:00–11:30 Location: H4

Invited Talk HL 7.1 Tue 10:00 H4

Ultrafast Spin-Lasers — Natalie Jung[1], Markus Lindemann[1], Tobias Pusch[2], Rainer Michalzik[2], Martin R. Hofmann[1], and •Nils C. Gerhardt[1] — [1]Photonics and Terahertz Technology, Ruhr-University Bochum, 44780 Bochum, Germany — [2]Institute of Functional Nanosystems, Ulm University, 89081 Ulm, Germany

Current-driven intensity-modulated semiconductor lasers are key optical sources for short-distance data transmission, but their modulation bandwidth is usually limited to values below 50 GHz. By exploiting the coupling between carrier spin and light polarization in semiconductor spin-lasers, the modulation frequencies can be increased to values above 200 GHz [1]. These high frequencies are achievable by increasing the resonance frequency of the coupled spin-photon system using strong birefringence in the laser cavity. Birefringent spin-lasers are capable to provide polarization modulation bandwidths and digital data transmission rates of more than 240 GHz and 240 Gbit/s respectively [1]. In contrast to intensity modulation in conventional lasers, polarization modulation in spin-lasers is largely independent of the pumping level and less sensitive to temperature increase [2]. This makes spin-lasers perfect candidates for future ultrafast communication systems as well as for many other emerging applications such as radio-over-fiber [3], neuromorphic computing [4] or THz generation [5].

[1] M. Lindemann et al., Nature 568, 212 (2019). [2] M. Lindemann et al., AIP Adv. 10, 035211 (2020). [3] N. Yokota et al., IEEE Photon. Technol. Lett. 33, 297 (2021). [4] K. Harkhoe et al., Appl. Sci. 11, 4232 (2021). [5] M. Drong et al., Phys. Rev. Appl. 15, 014041 (2021).

HL 7.2 Tue 10:30 H4

Extraction of silver permittivity at cryogenic temperatures through the optical characterization of Ag-coated plasmonic nanolasers — •Georgios Sinatkas[1,2], Aris Koulas-Simos[2], Jianxing Zhang[3], Jia-Lu Xu[3], Cun-Zheng Ning[3,4], and Stephan Reitzenstein[2] — [1]School of Physics, Aristotle University of Thessaloniki, 54124, Greece — [2]Institut für Festköperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany — [3]Department of Electronic Engineering, Tsinghua University, Beijing, 100084, China — [4]School of Electrical, Computer and Energy Engineering, Arizona State University, Tempe, AZ 85287, USA

Plasmonic nanolasers hold great promise for compact, low threshold opto-electronic devices [1, 2]. For the development and design of such lasers, often operating at cryogenic temperatures, it is important to know the temperature dependence of the involved materials with high accuracy. Here, we report the extraction of silver permittivity in the range 10 K–230 K by performing temperature-dependent μPL measurements in conjunction with numeric simulations on silver-coated nanolasers in the near-infrared regime. By mapping the changes in Q-factor, measured at transparency, into silver-loss variations, we extract the imaginary part of silver permittivity, estimating an order of magnitude shift in the examined temperature range. This data is missing from the literature and it could be useful for theoretically validating experimental observations and evaluating thermal effects.

[1] S. I. Azzam et al., *Light: Science & Applications* **9**(1) (2020).
[2] S. Kreinberg et al., *Laser Photonics Rev.* **14**(12), 2000065 (2020).

HL 7.3 Tue 10:45 H4

Linewidth transition at the laser threshold of quantum-well nanolasers — •J. Buchgeister[1], M. L. Drechsler[1], F. Lohof[1], C. Gies[1], F. Jahnke[1], A. Koulas-Simos[2], K. Laiho[2], G. Sinatkas[2], S. Reitzenstein[2], T. Zhang[4], J. Xu[4], C.-Z. Ning[3,4], and W. W. Chow[5] — [1]Universität Bremen, Germany — [2]Technische Universität Berlin, Germany — [3]Arizona State University, USA — [4]Tsinghua University, China — [5]Sandia National Laboratories, USA

Semiconductor nanolasers as small-scale sources of coherent light have become increasingly important for applications in the data and medical industry for their size, power-efficiency, and modulation speed. Determining the presence of lasing, however, is challenging due to the near-thresholdless behaviour of ultra-efficient devices, which requires going beyond input-output characteristics. The research presented here focuses on a quantum-optical study of a silver-coated InGaAsP nanolaser, accompanied by a full quantum-mechanical semiconductor laser theory; this gives access to the time-resolved single-photon and zero-time-delay two-photon correlation function that holds information about the photon statistics, allowing to identify the onset of coherent emission with confidence. Our theoretical model can match the experimentally obtained data using a single set of realistic parameters that holds not just in a stationary regime, but also when focusing on the temporal dynamics for the investigation of the coherence time. This procedure presents a comprehensive strategy for the identification of lasing while being extensible to those gain materials requiring a more pronounced focus on quantum-material aspects, like TMDCs.

HL 7.4 Tue 11:00 H4

Electro-optical switching of a topological polariton laser — •Philipp Gagel[1], Tristan H. Harder[1], Simon Betzold[1], Oleg A. Egorov[2], Johannes Beierlein[1], Holger Suchomel[1], Monika Emmerling[1], Adriana Wolf[1], Ulf Peschel[2], Sven Höfling[1], Christian Schneider[3], and Sebastian Klembt[1] — [1]Technische Physik, Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Condensed Matter Theory and Solid State Optics, Abbe Center of Photonics, Friedrich-Schiller-Universität Jena, D-07743, Germany — [3]Institute of Physics, University of Oldenburg, D-26129 Oldenburg, Germany

Here we implement a topological domain boundary defect in an orbital Su-Schrieffer-Heeger geometry by etching coupled pillars into an AlGaAs based microcavity. We show exciton-polariton lasing from the topologically non-trivial domain boundary defect in the bandgap of the P-bands under optical excitation. A gold back and top contact is used to apply a reverse bias to the structure allowing to tune the exciton-polariton detuning due to a shift in the energetic position of the exciton based on the quantum confined Stark effect. This way, we demonstrate control of the energetic position polariton condensation and lasing takes place. Furthermore, we show that this effect can be used to switch the polariton lasing from the topological defect on and off. These findings are an important step towards the realization of an electrically driven, topological polariton laser.

HL 7.5 Tue 11:15 H4

Investigation of the bimodal behavior of microlasers with a two-channel photon number-resolving transition edge sensor system — •Marco Schmidt[1,2], Isa Hedda Grothe[3], Sergej Neumeier[3], Lucas Bremer[1], Martin von Helversen[1], Wenera Zent[1], Boris Melcher[3], Jörn Beyer[2], Christian Schneider[4,5], Sven Höfling[4], Jan Wiersig[3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin — [2]Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin — [3]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg — [4]Technische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg — [5]Universität Oldenburg, 26129 Oldenburg

A two-channel photon-number-resolving (PNR) transition-edge sensor (TES) is used to measure the photon-number distribution of a bimodal quantum-dot micropillar laser [1]. The TES system simultaneously detect light emission of two orthogonal components of the fundamental emission mode of the bimodal microlaser. The applied cross-correlation scheme provides an unprecedented access to the joint PNR and allows an insight into the photon statistics and dynamics of the coupled mode components. Especially, the measurements reveal an optical bi-stability of the anti-correlated mode components, which can be interpreted as a temporal hopping between emission with coherent and thermal-like emission statistics. Our studies clearly demonstrate the great advantage of investigating nanophotonic devices via TESs.

[1] M. Schmidt et al, Phys. Rev. Res. 3, 013263 (2021)

HL 8: Poster Session II

Topics:
- Functional semiconductors for renewable energy solutions
- Heterostructures, interfaces and surfaces
- Nitrides: Preparation and characterization
- Organic semiconductors
- Oxide semiconductors
- Perovskite and photovoltaics
- When theory meets experiment: Hybrid halide perovskites for applications beyond solar

Time: Tuesday 10:00–13:00 Location: P

HL 8.1 Tue 10:00 P

Design optimization for bright electrically-driven quantum dot single-photon sources emitting in telecom O-band — Sergey Blokhin[1], Mikhail Bobrov[1], Nikolai Maleev[1], •Jan Donges[2], Lukas Bremer[2], Alexey Blokhin[3], Alexey Vasil'ev[3], Alexander Kuzmenkov[3], Evgenii Kolodeznyi[4], Vitaly Shchukin[2,5], Nikolay Ledentsov[5], Stephan Reitzenstein[2], and Victor Ustinov[3] — [1]Ioffe Institute, Politekhnicheskaya 26, St. Petersburg 194021, Russia — [2]Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [3]Research and Engineering Center for Submicron Heterostructures for Microelectronics, Politekhnicheskaya 26, St. Petersburg 194021, Russia — [4]ITMO University, Kronverksky pr. 49, St. Petersburg 197101, Russia — [5]VI Systems GmbH, Hardenbergstr. 7, 10623 Berlin, Germany

To enable long distance quantum communication, electrically-driven single-photon sources with almost ideal optical properties are desired. Through 3D finite-difference time-domain modelling, we present a design based on self-assembled quantum dots which delivers promising results in the telecom O-band by employing a broadband bottom distributed Bragg reflector (DBR) and a top DBR formed in a dielectric micropillar with an additional circular Bragg grating in the lateral plane. The design provides broadband emission enhancement (8-10nm) with an overall photon-extraction efficiency of 83% into the upper hemisphere, while photon coupling into single-mode fibers reaches efficiencies up to 40% for a HNA fiber (NA = 0.42). Blokhin et al., Opt. Express 29, 6582-6598 (2021)

HL 8.2 Tue 10:00 P

Examination of time-energy-entanglement on the biexciton-exciton-system under resonant two-photon driving via Franson interferometry — •Marcel Hohn, Matthias Kunz, Samir Bounouar, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany

We investigate the degree of time-energy entanglement from the XX-X-system under resonant two-photon driving. The dressing of this "three-level ladder" system leads to new eigenstates and previous experiments showed correlated emission of paired photons with manipulatable time ordering of the cascade [1]. In addition, a recent theoretical treatment indicated possibilities and limitations for the visibility of two-photon interference using Franson interferometry [2]. We measured the degree of time-energy-entanglement of the emitted pairs by Franson interferometry and observed a strong dependence of the visibility on excitation power and detuning. In particular, our measurements show that the degraded energy time entanglement of the XX-X-system under off-resonant excitation can be enhanced via strictly resonant two-photon-excitation.

[1] S. Bounouar et al., Physical Review Letters 118 (2017).
[2] K. Barkemeyer et al., Physical Review A 103 (2021).

HL 8.3 Tue 10:00 P

Focused ion beam implantation of rare-earth ions in semiconductor nanostructures — •Christian Düputell, Arne Ludwig, and Andreas D. Wieck — Chair of Applied Solid State Physics, Ruhr University, Bochum

We report on focused ion beam (FIB) implantation of rare-earth ions in semiconductor nanostructures. Semiconductor nanostructures have attracted a lot of attention due to their unique optical, electrical and mechanical properties. To use nanostructures for a certain purpose, often very specific properties have to be achieved. An elegant method to tune the electrical and optical properties of semiconductor nanostructures is focused ion beam implantation. Using ion beams offers high-resolution lateral engineering, local band gap modulation due to ion-induced intermixing as well as local doping applications and even isotopic resolution. To carry out implantation of rare-earth ions in semiconductor nanostructures, we especially focus on the incorporation of erbium ions into GaAs. Erbium shows two unique properties. First, it has a huge magnetic moment, which could lead to a rich spectrum of possible spin coupling processes in the host material. And second, the optical transitions of erbium should lead to an emission of electromagnetic radiation at the important telecom-C-band wavelength of 1.54 μm, which has minimal absorption in glass fibres. We are presenting the current status of our studies on both of these properties as a function of the implantation pattern, the ion fluence and the used annealing parameters. We also report on the preparation and composition of the corresponding liquid metal alloy sources for FIB.

HL 8.4 Tue 10:00 P

Using a novel scanning probe technique to strongly couple a single quantum dot to a tunable plasmonic nanogap antenna at room temperature — •Michael A. Becker[1], Hsuan-Wei Liu[1], Korenobu Matsuzaki[1], Randhir Kumar[1], Stephan Götzinger[2,1], and Vahid Sandoghdar[1,2] — [1]Max Planck Institute for the Science of Light — [2]Friedrich Alexander University of Erlangen-Nürnberg

Scanning probe techniques are indispensable methods for optical investigations of structures smaller than the diffraction limit. Moreover, techniques like atomic force microscopy and scanning near-field optical microscopy can be utilized to measure electrical and thermal conductance and probe near-field light-matter interactions. However, these types of experiments typically require sensitive and expensive state-of-the-art equipment. Here, we report on a novel and simple press-roll scanning probe technique (PRoScan) capable of performing optical near-field measurements with remarkable stability, even in the absence of any stabilization mechanism. We demonstrate its performance by a precise coupling of an individual quantum dot to a gold nanoparticle, where we can control the Purcell enhancement with nanometer-resolution. Next, we utilize the technique to create an open and tunable nanogap antenna. By tuning the resonance of the nanogap antenna and controlling the position of the single quantum dot, we can drive the system from the weak to the strong light-matter coupling regime, evidenced by a vacuum Rabi splitting and a characteristic anticrossing behaviour.

HL 8.5 Tue 10:00 P

Capacitance-voltage spectroscopy on quantum dots without electronic wetting layer states — •Ismail Bölükbasi, Sven Scholz, Andreas D. Wieck, and Arne Ludwig — Ruhr-Universität Bochum, D-44780 Bochum, Germany

Quantum dots have interesting physical properties and allow research in zero dimensional systems. They are used in modern displays and may become important for the progress of semiconductor and information technology in the form of qubits in quantum computers and quantum memories or sources of high-fidelity single photons in quantum communication applications.

Quantum dots are created by molecular-beam-epitaxy (MBE) in the so-called Stranski-Krastanov growth mode. InAs arranges epitaxially on GaAs in a strained layer of up to 1.5 monolayers without relaxation before nucleation of coherently strained islands takes place. This layer remains between the islands and is called the wetting layer.

We find that a monolayer of AlAs deposited after the growth of the quantum dots can suppress certain states in this wetting layer [1], allowing to purify their photoluminescence spectra from electronic contributions such as for example a two-dimensional-electron gas would induce. Capacitance-voltage and photoluminescence measurements are carried out to investigate the effects of this monolayer of AlAs on the physical properties of the quantum dots and the modified charging behaviour around flat band conditions.

[1] Löbl, M. C. et al. Excitons in InGaAs quantum dots without electron wetting layer states. Commun. Phys. 2, 93 (2019).

HL 8.6 Tue 10:00 P

Surface Morphology of Self-Assembled InAs/GaAs Quantum Dots and Pattern Definition Layers grown by Molecular Beam Epitaxy — •Peter Zajac, Nikolai Bart, Andreas D. Wieck, and Arne Ludwig — Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum

The nucleation of self-assembled InAs/GaAs Quantum Dots (QDs), grown by molecular beam epitaxy, can be locally influenced by growing them on gradient pattern definition layers. Macro Photoluminescence Spectroscopy (PL) mapping reveals a modulation of QD density in a striped pattern along the gradient direction. Automated Atomic Force Microscopy (AFM) was employed to study the morphology of pattern definition layers over several millimeters, revealing a sinusoidal behavior of the monolayer step density. Local PL contrast is used to

locate areas of highest QD density modulation. It is proposed that the periodic variation of roughness locally modifies the QD nucleation condition leading to the observed pattern [1].
[1] Bart et al., arXiv:2011.10632 (2020).

HL 8.7 Tue 10:00 P

Wafer Scale Density Modulation of Self-Assembled Quantum Dots by Epitaxial Surface Roughness Control — •Nikolai Bart, Nikolai Spitzer, Peter Zajac, Marcel Schmidt, Andreas D. Wieck, and Arne Ludwig — Ruhr-Universität Bochum, Lehrstuhl für Angewandte Festkörperphysik, Universitätsstraße 150, 44801 Bochum, Germany

The effect of nanoscale roughness of GaAs surfaces on the nucleation of self-assembled InAs quantum dots (QD) is investigated with photoluminescence (PL) spectroscopy. We control the roughness in-situ by simple epitaxial layer-by-layer growth: Depositing integer (fractional) values of GaAs monolayer thicknesses yields a smooth (rough) surface. We report significant differences in both PL intensity and QD surface density at the critical threshold of nucleation. By growing GaAs thickness gradients, we create and control various density modulation patterns on whole 3-inch wafers. Moreover, we investigate the influence of surface annealing time and temperature on the modulation and demonstrate how to utilize this mechanism for density control of high quality single QD photonic device wafers.

HL 8.8 Tue 10:00 P

Semiconductor nanophotonic light sources with site- and number- controlled quantum dots for the investigation of collective effects — •Ching-Wen Shih, Jan Grosse, Imad Limame, Chirag Palekar, Yuhui Yang, Lasse Kosiol, Sebastian Krüger, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany

Sub- and superradiance are intriguing collective radiative emission processes which occur when coherence is built up among the emitters spontaneously via exchange of photons. Semiconductor quantum dots (QDs) are attractive candidates to study these collective emission processes. However, a systematic study of the collective effects in these semiconductor nanostructures requires a control over the position, number, and emission energy of the quantum dot emitters. We report on the development of nanophotonic light sources via a buried-stressor approach, which enables a precise position control of the InGaAs QDs by tailoring the strain induced by an oxidation aperture. Furthermore, the number of such site-controlled QDs is successfully varied from 0 to 20 across each device via a careful balance between the aperture size and the MOCVD growth condition. Finally, electron beam lithography is implemented to pattern micro-mesa cavity structures, which enhance the photon extraction efficiency of the QDs to facilitate the observation of sub- and superradiance.

HL 8.9 Tue 10:00 P

A Master Equation centered foundation for an open-source project for quantitative simulation of the transition dynamics in finite state quantum systems. — •Arn Baudzus, Andreas Wieck, and Arne Ludwig — Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum

We present a novel approach and status on the implementation of a program to quantitatively simulate the electronic, photonic and phononic behaviour of a quantum dot that is embedded in a semiconductor device. Our main aim is to start an open-source project, everyone can expand and contribute to.

We outline a theoretical framework that is developed to break this complex system down into modules that can be treated one at a time.

The framework is centered around the generation and solution of master equations with constant or time dependent coeffitients. The coeffitients in the master equation and the information of the relevant states can be calculated by different programs, each governing another kind of interaction.

We use a graph data structure to manage the system states and interface with the other program parts in an intuitive way. A C++ implementation for this structure has been developed.

At the moment we are mainly focusing on the simulation of electron tunneling dynamics between a single quantum dot and a two dimensional electron gas. We illustrate how the tunnel dynamics can be simulated using our framework.

HL 8.10 Tue 10:00 P

Spatially resolved multi-probe electrical characterization of GaAs-based nanowire structures — •Juliane Koch[1], Lisa Liborius[2], Peter Kleinschmidt[1], Werner Prost[2], and Thomas Hannappel[1] — [1]Fundamentels of energy materials, Ilmenau University of Technology, Germany — [2]Components for High Frequency Electronics (BHE), University of Duisburg-Essen, Germany

To achieve high performance optoelectronic devices with III-V semiconductor nanowire (NW) heterostructures sophisticated junctions with controlled properties are required. In order to study microscopic details of the NW structure and its composition, we investigated upright standing p-GaAs/i-GaInP/n-GaInP core-shell-shell NWs on the growth substrates. Cores of the NWs were grown via the vapor-liquid-solid mode followed by epitaxial shell growth in a low-pressure horizontal metalorganic vapor-phase epitaxy reactor. We employ a combination of material-selective wet chemical etching of as-grown coaxial NWs and a multi-tip scanning tunnelling microscope operated as a four-point nano-prober to obtain spatially resolved I-V analysis. These revealed a leakage mechanism causing degraded core-shell pn-junction performance, which is localized at the NW base where a buried contact of the n-GaInP shell to the p-GaAs substrate is formed. Furthermore, the combination of SEM with EDX and XRD measurements reveal the contrast of NW shell and planar layer growth. Our high-end characterization methods enable a direct relation between the NW structures and the electronic properties of as-grown coaxial NWs, which provides precise advice for future NW core-shell pn-junction optimization.

HL 8.11 Tue 10:00 P

Examination of self-assembled quantum dots in a density-modulated pattern with capacitance-voltage and photolulminescence spectroscopy — •Nikolai Spitzer, Nikolai Bart, Arne Ludwig, and Andreas Wieck — Ruhr-Universität Bochum

Self-assembled InAs quantum dots (QDs) on GaAs with a QD density modulation upright to the growth direction were grown by molecular beam epitaxy. The QDs can be arranged in stripe patterns whose properties can be changed by a gradient in the GaAs sublayer beneath the QDs. We suspect that the formation of QDs is favoured by atomic rough areas as opposed to flat areas during molecular epitaxial growth. The differences in the sublayer are due to the profile of the molecular beam. Capacitance-voltage spectroscopy and photoluminescence spectroscopy are used to investigate the properties of the quantum dots arranged in this way at different densities.

HL 8.12 Tue 10:00 P

Design and fabrication of waveguide-based nanobeam cavity for on-chip single photon source — •Yuhui Yang[1], Uğur Meriç Gür[1,2], Johannes Schall[1], Ronny Schmidt[1], Arsenty Kaganskiy[1], Michael Mattes[2], Samel Arslanagić[2], Stephen Reitzenstein[1], and Niels Gregersen[3] — [1]Institut für Festkörperphysik, TU Berlin, Germany — [2]Department of Electrical Engineering, Technical University of Denmark, Denmark — [3]Department of Photonics Engineering, Technical University of Denmark , Denmark

In quantum technology, the two-photon interference acts as an important role related to the indistinguishability of single-photon. One approach to improve the indistinguishability of single-photon is to enhance the spontaneous emission into cavity mode by Purcell effect. In this regard, nanobeam cavities, are promising candidates because they can easily be integrated with other on-chip components. In this contribution, we optimize the geometrics of nanobeam cavities. A numerically optimized nanobeam cavity design yields a high directional spontaneous emission β factor of 0.73 with broadband enhancement of 9 nm. The nanobeam cavity containing embedded InGaAs/GaAs quantum dots fabricated structures demonstrates the cavity effect. By micro-photoluminescence (μPL) characterization, three distinct Fabry-Pérot resonance peaks as well as cavity effects are observed. Due to the Purcell enhancement from the cavity, the spontaneous emission rate of a resonance (non-resonance) peak is (1.59 * 0.09) ns^{-1} [(1.14 * 0.14) ns^{-1}], indicating the potential of nanobeam cavity for full on-chip single-photon source.

HL 8.13 Tue 10:00 P

Frequency Shift of Electronic Resonances in Self Assembled InAs Quantum Dots — •Ibrahim Azad Engin, Ismail Bölükbaşı, Sven Scholz, Andreas D. Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-UniversitätBochum, D-44780 Bochum, Germany

Self-assembled InAs quantum dots (SAQD) proved promising semiconductor structures as single-photon sources and provide possibilities for quantum memories. Therefore understanding the physical properties is important and in progress. We investigate electronic resonances in InAs SAQDs by using C(V)-spectroscopy.

The thermal shift of the s-states has been reported and described with a master equation [1], which has been improved further to model excitonic and non-equilibrium states in such SAQD [2]. The model shows contrarily shifting in dependence of frequency and temperature.

Here we investigate both s- and p-states in dependence of temperature and frequency to measure the shifting characteristics of p-peaks and observe the dominancy of the frequency shift for s-states. The superposition of thermal and frequency shift are being analyzed. Adjustments to the master equation model are needed.

[1] Brinks, F. et al., "Thermal shift of the resonance between an electron gas and quantum dots: what is the origin?" New J. Phys. 18, 123019 (2016).

[2] Valentin, S. et al., "Illumination-induced nonequilibrium charge states in self-assembled quantum dots", Phys. Rev. B 97, 045416 (2018).

HL 8.14 Tue 10:00 P

Metamorphic buffer layer based single-photon sources for application in quantum telecommunications — •Piotr Andrzej Wronski, Sven Höfling, and Fauzia Jabeen — Technische Physik, University of Würzburg and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Am Hubland, D-97074 Würzburg, Germany

Obtaining single-photon sources requires them not only to characterize by low FSS, low g(2)(0), and high emission rate, it is also essential for them to be built-in telecommunication network. Ideally, obtained sources should emit at spectral range aligned with the lowest attenuation window (C-band) for silicon fibers. So far, such emitters are reported only on InP, but the low refractive contrast of lattice-matched materials makes it difficult to obtain complete photonic structures with efficient outcoupling.

Metamorphic buffer layer on GaAs substrate as a base for InAs QDs leads to strain relaxation and induces required emission shift. Past attempts in this matter lacked low surface roughness required for development of top DBRs and fabricating micropillars

By implementing our approach of introducing a stepwise increase of "In" composition inside a digitally alloyed superlattice, we can observe a shift of emission wavelength, improvement of surface quality, and observation of single-photon emission in 1550 nm spectral range from InAs QDs grown on GaAs (001) substrate, confirmed by autocorrelation experiments. The incorporation of AlAs/GaAs DBRs improved the emission intensity.

HL 8.15 Tue 10:00 P

Purcell-enhanced single-photon emission from a strain-tunable quantum dot in a cavity-waveguide device — •Florian Hornung[1], Stefan Hepp[1], Stephanie Bauer[1], Erik Hesselmeier[1], Xueyong Yuan[2,3], Michael Jetter[1], Simone Luca Portalupi[1], Armando Rastelli[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, 4040 Linz, Austria — [3]School of Physics, Southeast University, Nanjing, 211189, China

The miniaturization of optical elements to chip-size in so-called photonic integrated circuits has attracted a lot of attention in recent years. Due to its great scalability, the approach seems highly promising for the efficient realization of photon-based quantum technologies.

In this study, we show the coupling of an In(Ga)As quantum dot (QD) to a waveguide-integrated cavity. The chip is bonded to a piezoelectric actuator, enabling the strain-tuning of both the emission energy of the QD and the cavity mode. As the QD is more sensitive to the applied strain, a differential tuning factor of four is obtained, allowing to compensate the initial energy mismatch of the QD and the cavity. A clear Purcell-enhancement as well as the single-photon emission of the device are demonstrated. This combination of a strain-tunable quantum emitter and a waveguide-integrated cavity represents an important building block for large scale quantum photonic circuits.

HL 8.16 Tue 10:00 P

Full Wafer Property Control of Local Droplet Etched GaAs Quantum Dots — •Hans-Georg Babin, Nikolai Bart, Marcel Schmidt, Andreas D. Wieck, and Arne Ludwig — Ruhr-Universität Bochum, Germany

Local droplet etched GaAs quantum dots (LDE-QDs) are a promising candidate for excellent single and entangled photon sources. Taking further steps towards application, this requires structures of increasing complexity, engineering the electronic and photonic environments of the QDs. Therefore, it is important to get perfectly matched QDs for the required photonic structures. In this submission, we show a way to compensate for non-perfectly adjusted growth conditions and to accelerate required parameter studies.

We induce certain flux gradients by stopping sample rotation and using the parallax of the effusion-cells. This results in a gradual change of deposited material and cell flux, as well as an induced surface roughness modulation. By this we can vary properties of the QDs like density and emission wavelength over the hole wafer range. Additionally, we induce a stripe patterned density modulation, which was shown before with Stranski-Krastanov QDs. As an example, the widest achieved wavelength shift of the ground state emission energy at 100 K, measured by photoluminescence spectroscopy, extends over the range of 795 nm to 737 nm. The change in surface roughness leads to an additional periodical modulation of the ground state of approximately 3 nm on a mm scale.

HL 8.17 Tue 10:00 P

Changes of transport properties in individual carbon nanotubes due to MOF growth — •Marvin J. Dzinnik[1], Benedikt Brechtken[1], Hendrik A. Schulze[2], Adrian Hannebauer[2], Enes Akmaz[1], Peter Behrens[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, Callinstrasse 9, 30167 Hannover, Germany

Metal-organic frameworks (MOF) are porous structures with tunable pore size and adsorption sites but mostly non-conducting. In combination with carbon nanotubes (CNTs) these hybrid structures preserve porosity of the MOFs while gaining conductivity through the CNTs [1,2]. The mechanism of MOF growth on CNTs is accountable to the functionalization of the carbon nanotubes [1]. To study the interaction between MOF and CNTs and the influence of the synthesis, we prepared samples of contacted multi-walled CNTs. We drop-casted CNTs from ethanol solution on a silicon dioxide surface and contacted them with Cr and Au by electron beam lithography and lift-off. DC transport measurements were performed. In a second step, the sample with the contacted CNT was given into a UiO-66 MOF synthesis. Later transport measurements show drastically increased two-terminal resistance.

[1] H. A. Schulze et al., ChemNanoMat, 5, 1159-1169, (2019).
[2] M.-Q. Wang et al., Electrochimica Acta, 190, 365-370, (2016).

HL 8.18 Tue 10:00 P

Optimal Bandwidth in Quantum Event Measurements Using Post-Processing — •Jens Kerski[1], Hendrik Mannel[1], Pia Lochner[1], Eric Kleinherbers[1], Annika Kurzmann[2], Arne Ludwig[3], Andreas D. Wieck[3], Jürgen König[1], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]2nd Institute of Physics, RWTH Aachen University, Germany — [3]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

The realization of novel applications, such as quantum computing or quantum sensing, is largely limited by the time resolution and accuracy with which individual quantum events can be measured. For the measurement of single electron tunneling, radio-frequency single-electron transistors and quantum point contacts have been the most successful detection methods. A promising alternative to this is to exploit an optical transition. For this purpose, resonance fluorescence of the excitonic transition is detected at 4.2 K from a self-assembled quantum dot embedded in a tailored diode structure.

In this work, we use single photon signal post-processing to identify the optimal time resolution for the analysis of our data. We show how the bandwidth affects both the determination of the tunneling rates and the statistical evaluation by full counting statistics, and demonstrate that we can evaluate our data with sampling rates up to 340 kHz. Using a simple model, we discuss the limiting factors for reaching the highest time resolution and propose how a time resolution of more than 1 MHz could be achieved.

HL 8.19 Tue 10:00 P

Topological superconductivity in (3D) topological insulator-based hybrid devices — •Dennis Heffels[1], Declan Burke[2], Malcolm R. Connolly[2], Peter Schüffelgen[1], Kristof Moors[1], and Detlev Grützmacher[1] — [1]Peter Grünberg Institut (PGI-9), FZ Jülich — [2]Imperial College London

Topological insulator (TI) nanostructures have been proposed as a host system for one-dimensional topological superconductivity. This is made possible by the special properties of the TI surface states in combination with an external magnetic field and proximity-induced superconductivity. Recently, however, it was shown that specific conditions are required to realize fully gapped topological superconductivity. In this talk, I will report on tight-binding simulations with Kwant that allow for a detailed investigation of the formation of a topological band gap in experimentally realizable hybrid devices. We model the TI hybrid device in full three-dimensional detail which allows us to compare different device layouts and proximitization schemes. In general, we find that a topological gap can be opened by breaking the transverse symmetry of the system. One possibility for such a symmetry breaking is the consideration of a ribbon which is only proximitized via the top surface. Our simulation approach also allows us to optimize the device layout in order to maximize the size of the gap. I will also comment on related experimental activities on TI nanostructure-based hybrid devices and tunnel junctions as well as magnetic TI-based hybrid devices.

HL 8.20 Tue 10:00 P

Deterministically fabricated GaAs quantum dot based single-photon sources with emission at Cs wavelengths — •Monica Pengerla[1], Lucas Bremer[1], Jin Dong Song[2], Sven Rodt[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Center for Opto-Electronic Materials and Devices, Korea Institute of Science and Technology, Seoul 02792, Republic of Korea

In this work, we investigate GaAs based quantum dot (QD) single photon sources at 894 nm. The goal is to control the emission of single photon sources time delay with Cs vapor. To increase the photon extraction efficiency, the device design includes a gold mirror on back side. Numerical simulations reveal a photon extraction efficiency of approximately 52% with numerical aperture NA = 0.4. The flip chip gold bonding process results in a thin QD membrane, which includes wet etching of AlGaAs and GaAs layers. The preliminary low temperature micro photoluminescence and cathodoluminescence results of Au bonded samples are fair enough to pursue further device fabrication steps. With In-situ electron-beam lithography (EBL), QDs at target wavelength, based on their intensity can be selected prior to the structure patterning. We are planning to deterministically integrate quantum dots at 894 nm into mesa and one ring structure with in-situ electron beam lithography. Later, the emitted single photon properties of fabricated structures will be studied with photon autocorrelation measurements.

HL 8.21 Tue 10:00 P

Structural and Optical Properties of Hexagonal Pyramids Containing GaInN Quantum dots Formed by Wet Etching of GaInN/GaN Quantum Wells — •Samar Hagag, Sidikejiang Shawutijiang, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Technische Universität Braunschweig, Institut f. Angewandte Physik, 38106 Braunschweig,Germany

We present first results from our studies of the structural and optical properties of hexagonal pyramids containing GaInN Quantum Dot(QD)-like structures located close to the tip of pyramids with a smooth side facets of the type (1-10-1) and very sharp tips obtained through the wet chemical etching of GaInN/GaN Quantum Well(QW)structures grown on N-face GaN. The photoluminescence spectrum of the QD's shows the intuitive additional quantum confinement manifested by a blue shift of the photoluminescence peak and narrow emission lines have been observed in the microphotoluminescence spectra. A comparison between the peak energy separation observed in the microphotoluminescence spectrum of pyramidal structures containing several quantum disks and calculations of the quantization energy of the quantum disks shows that the top most QD has a diameter of 18.5nm. In a further attempt to control the position and size of the hexagonal pyramids a Focused Ion Beam-deposited etch mask was used and regular array of pyramidal structures were formed. While the QD thickness and indium contents are given by the QW structure,an optimization of the etching process to control the pyramid size is required to enable the control of the QD lateral extension.

HL 8.22 Tue 10:00 P

Kondo effect in a few-electron quantum dot — •Olfa Dani[1], Johannes C. Bayer[1], Timo Wagner[1], Gertrud Zwicknagl[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Institut für Mathematische Physik, Technische Universität Braunschweig, Germany

The Kondo effect is a many particle entangled system, that involves the interaction between a localized spin in the quantum dot and free electrons in the electron reservoirs. This entanglement can be however exactly calculated for models adopting simplifying assumptions concerning the electronic structure of the quantum dot.

The investigated quantum dot device is based on a flat two-dimensional electron gas (2DEG) formed in a GaAs/AlGaAs heterostructure. A single quantum dot is formed in this 2DEG using top-gates and a quantum point contact (QPC) is operated as sensitive charge detector, allowing the real-time detection of electrons tunneling through the system [1].

The Kondo effect dominates at a strong coupling between dot and leads. It gives rise to a finite conductance in the otherwise Coulomb-blockaded regime, and has a characteristic temperature dependence. Here we study the Kondo effect as a function of the tunnel coupling and its symmetry. For small number of electrons, we see that the shell structure[2] of the electronic states in the quantum dot influence the Kondo effect.

[1] T. Wagner, et. al., Nat. Nanotech. 12, 218-222 (2017).

[2] L. P. Kouwenhoven, Rep. Prog. Phys. 64, 701-736 (2001).

HL 8.23 Tue 10:00 P

Theoretical description of higher excited quantum dot states in an external magnetic field — •Jan Kaspari, Matthias Holtkemper, Tilmann Kuhn, and Doris Reiter — Institut für Festkörpertheorie, WWU Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

The influence of a magnetic field on the quantum dot states is usually reduced to the interaction of the external magnetic field with the spins of electrons and holes. Based on the envelope function approximation and minimal coupling we derive additional interaction terms of the magnetic field with the envelope functions and treat the magnetic field interaction, direct and short-range exchange Coulomb interactions as well as the four-band Luttinger theory within a configuration interaction approach. The quantum dot confinement is approximated by an anisotropic harmonic potential. We show that the magnetic field interaction with the envelope functions crucially depends both on the geometry of the quantum dot as well as on the orientation of the magnetic field. In the case of a magnetic field in the growth direction of a cylindrically symmetric quantum dot we find that the interaction with the envelopes results in the mixing of states of the same type which leads to a partial splitting of higher excited energy levels, while for a broken cylindrical symmetry an additional mixing with other orbital states and further energy shifts can be noted. We discuss in detail the observed dependencies on geometric parameters and analyze whether the common approximation to describe the interaction of the external magnetic field solely with spins is applicable for higher excited states.

HL 8.24 Tue 10:00 P

Ultra-high quality factor Ta2O5-on-insulator microring resonators with cryogenic temperature stability — •Julian Rasmus Bankwitz, Martin A. Wolff, Adrian Abazi, Alexander Eich, and Carsten Schuck — Institute of Physics University of Münster, Germany

Tantalum pentoxide (Ta2O5) on insulator is an emerging nanophotonic material system that benefits applications in nonlinear and quantum technology due to its outstanding optical properties [1]. As many implementations of quantum technology require cryogenic environments a need for low loss photonic integrated circuits with high temperature stability has arisen. Here we demonstrate ultra-high quality factor Ta2O5-on-insulator microring resonators with minimal temperature-dependent wavelength shift (TDWS). Through careful tuning of design and nanofabrication parameters, we achieve critically coupled devices with loaded quality factors of up to 1.8 Mio., observed over the entire range from room to cryogenic temperatures. The TDWS of ring resonances is as low as 237 pm from 1.74 K to 286 K and, remarkably, vanishes in the 110 K to 140 K range as it changes sign. Our Ta2O5-on-SiO2 devices will thus enable athermal operation of ultra-stable resonators as desired for wavelength division multiplexing, on-chip frequency stabilization and low-noise optical frequency combs.

[1] G. Moody et al. "Roadmap on Integrated Quantum Photonics," arXiv preprint arXiv:2102.03323, 2021.

HL 8.25 Tue 10:00 P

Magnetic Field Dependence of the Auger Recombination Rate in a Self-Assembled Quantum Dot — •Fabio Rimek[1], Hendrik Mannel[1], Marcel Ney[1], Arne Ludwig[2], Andreas D. Wieck[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

A quantum dot (QD) is an ideal system to study electron-electron interaction in a confined nanostructure [1]. The Auger recombination is a special case, where the recombination energy is transferred to third charge carrier that leaves the dot or is excited to an higher energy level. Therefore the Auger effect destroys the radiative trion transition - an effect, which should be minimized for future applications of QDs using the spin states as stationary qubit that should be transferred to a photon via this trion transition.

**In this work, we investigate how the Auger rate is affected by an external magnetic field, applied along the growth direction of the sample. In the magnetic field, the trion state of a QD is no longer spin degenerate and splits up. We use two-color, time-resolved resonance fluorescence spectroscopy to investigate the quenching of the trion recombination by the Auger effect. Two-color excitation allows us to symmetrically excite both trion resonances and thus neglect spin relaxation as well as spin-flip Raman scattering. We observe a suppression of the Auger recombination by almost a factor of three, when increasing the field up to B = 10T.

[1] A. Kurzmann et al., Nano Lett. **16, 3367-3372 (2016)

HL 8.26 Tue 10:00 P

Halogen vacancy migration at a surface of CsPbBr3: Insights from Density Functional Theory — •Raisa-Ioana Biega[1] and Linn Leppert[1,2] — [1]Institute of Physics, University of Bayreuth, Bayreuth 95440, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

Migration of mobile halogen ions is ubiquitous in lead-halide perovskites, and has been studied in detail experimentally and with computational modelling techniques. However, the question whether and how surfaces affect ion migration in these materials is still debated. Here we contribute to this debate by using density functional theory to compute bromine vacancy migration in the bulk and at the (001) surface of cubic CsPbBr3. We find that the migration barrier at the surface is approximately half of that in the bulk due to larger structural distortions at the surface. The targeted choice of an alkali-halide passivation layer can suppress this undesirable effect and leads to an increase of migration barrier to almost the bulk value.

HL 8.27 Tue 10:00 P

Polarons and Dynamic Disorder in Halide Perovskites: a Tight Binding Approach — •Maximilian. J. Schilcher[1], Matthew. Z. Mayers[2], Paul. J. Robinson[2], David. J. Abramovitch[3], Liang. Z. Tan[4], Andrew. M. Rappe[5], David. R. Reichman[2], and David. A. Egger[1] — [1]Technical University of Munich, Germany — [2]Columbia University, USA — [3]University of California Berkeley, USA — [4]Lawrence Berkeley National Laboratory, USA — [5]University of Pennsylvania, USA

Unusual experimental observations of halide perovskites (HaPs) are often explained by polaronic effects. However, the standard polaron picture in its simplest form cannot properly rationalize some of the key carrier-transport features of HaPs. We propose to augment it by a complementary concept based on dynamic disorder [1], taking into account the slow, anharmonic lattice dynamics and incoherent nature of carrier relaxation in HaPs. This approach can be tackled computationally in the framework of a tight-binding (TB) model [2], allowing for modeling large-scale system sizes and temperature-dependent optoelectronic properties. We demonstrate that in this way, we can, e.g., elucidate on the influence of dynamic disorder around room temperature on the band gaps in a variety of HaPs.

[1] M. J. Schilcher et al., ACS Energy Lett. 6, 2162-2173 (2021).

[2] M. Z. Mayers et al., Nano Lett. 18, 8041-8046 (2018).

HL 8.28 Tue 10:00 P

Disorder in halide perovskites: anharmonicity and dynamically shortened correlations — •Christian Gehrmann and David A. Egger — Technical University Munich, Germany

Small Urbach energies, important for an effective collection of sunlight in photovoltaic devices, imply a short range correlated disorder potential [1]. Halide perovskites (HaPs), however, are discussed to show a long-range bonding mechanism, anharmonic nuclear dynamics, disorder, and small Urbach energies all at the same time. We show that correlations in the disorder potential for electronic states, calculated using density functional theory (DFT) and DFT-based molecular dynamics simulations, are dynamically shortened in HaPs [2]. This dynamic shortening of the disorder correlation, which we attribute to the motion of A-site and, in particular, X-site ions, results in narrow band-edge energy distributions as we show explicitly. Our findings about correlations in the disorder potential due to nuclear motion is complemented by data showing considerable anharmonicity in the lattice dynamics of $CsPbBr_3$. With this, we conclude that besides showing complex nuclear dynamics, a mechanism of dynamic shortening of the disorder potential promotes a sharp optical absorption edge in HaPs.

[1] C. W. Greeff & H. R. Glyde, Phys. Rev. B 51, 1778-1783 (1995).
[2] C. Gehrmann & D. A. Egger, Nat. Commun. 10, 3141 (2019).

HL 9: Nitride: Preparation, Charakterization and Devices

Time: Tuesday 11:45–12:30 Location: H4

HL 9.1 Tue 11:45 H4

AlPN on GaN: A new barrier material for HEMTs — •Markus Pristovsek and Yuto Ando — IMaSS, Nagoya University, Japan

We report on the ternary alloy wurzite AlP_yN_{1-y} on (0001) GaN, grown by metal-organic vapor phase epitaxy. AlPN is lattice matched to GaN at about 11% P content, while having a larger bandgap than AlInN. Furthermore, AlPN is grown in H_2 at similar temperatures as GaN, avoiding long growth interruptions and temperature ramping. Unlike AlInN, Ga carry over is not an isssue. Finally, there is tertiary-butylphosphine (tBP), a proven metal-organic precursor with a high vapor pressure which is not available for AlScN. Therefore, AlPN looks like a promising material to replace AlGaN as barrier layer in high electron mobility transistors (HEMT) especially for high frequency applications. First results confirmed high sheet carrier densities, and highlighted the crucial influence of strain to avoid point defects. As with any new material there are new challenges, most notably the growth transitions between the binary GaN and the group V alloy AlPN and avoiding detrimental effects on growth and background doping from residual P in GaN.

HL 9.2 Tue 12:00 H4

Low-temperature internal quantum efficiency of GaInN/GaN quantum wells under steady state conditions — •Shawutijiang Sidikejiang[1], Philipp Henning[1,2], Philipp Horenburg[1], Heiko Bremers[1,2], Uwe Rossow[1], Dirk Menzel[3], and Andreas Hangleiter[1,2] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig — [2]Laboratory for Emerging Nanometrology, Technische Universität Braunschweig — [3]Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig

In this work, we compared the low-temperature PL intensities of a range of QW samples under identical conditions, mounting the samples side by side. Normalizing the measured intensity to the absorbed power density in the QWs, we find that the PL efficiencies of several samples, which the 100% internal quantum efficiency (IQE) can be confirmed by the temperature-dependent lifetime measurements from time-resolved PL (TRPL), are identical under steady-state PL excitation. On the other hand, for samples with a reduced low-temperature IQE observed in TRPL, the PL efficiencies saturate at significantly lower values. The experimental results confirm a unity IQE at low temperature for those efficient samples, but also allow to estimate the absolute IQE of samples with a lower efficiency by a direct comparison. The latter case is investigated by studying the influence of point defects due to Ar implantation on the low-temperature PL efficiency of the QWs.

HL 9.3 Tue 12:15 H4

Structural analysis of novel orientations of AlN grown on *m*-plane sapphire — •Jochen Bruckbauer[1], Gergely Ferenczi[1], Humberto Foronda[2], Sarina Graupeter[2], Ben Hourahine[1], Aimo Winkelmann[1,3], Zhi Li[4], Ling Jiu[4], Jie Bai[4], Tao Wang[4], Tim Wernicke[2], Michael Kneissl[2], and Carol Trager-Cowan[1] — [1]University of Strathclyde, UK — [2]Technische Universität Berlin, Germany — [3]AGH University of Science and Technology, Poland — [4]University of Sheffield, UK

Heteroepitaxial III-nitrides can be grown with a wide range of orientations on a range of substrates. Determination of the epitaxial orientation relationship of the nitride film with its substrate is often necessary. Here, we report on the determination and observation of novel orientations in AlN grown on *m*- or $(1\bar{1}00)$ plane sapphire using electron backscatter diffraction (EBSD). An electron backscatter diffraction pattern is recorded for each spatial point in an EBSD map from which crystal structure, orientation and misorientation can be determined with a spatial resolution of around 50 nm and a relative angular precision of around 0.1°. The AlN thin film exhibits twinned regions where the normal to a $\{1\bar{2}13\}$ plane for each twin is within 9° of the $[1\bar{1}00]$ sapphire direction. The twins share a common $\{1\bar{1}00\}$ plane. Furthermore for each twin, the normal to a $\{11\bar{2}2\}$ AlN plane is within 3.5° of the $[11\bar{2}0]$ sapphire direction and a $\langle\bar{4}312\rangle$ AlN direction is within 2° of the [0001] sapphire direction. These orientations, together with the usually observed $(1\bar{1}00)$ and $(11\bar{2}2)$ cases, form a family of related growth directions for nitride thin films.

HL 10: Focus Session: Highlights of Materials Science and Applied Physics I (joint session DS/HL)

Jointly organized on the occasion of the 60th anniversary of the *physica status solidi* journals (*pss*, http://www.pss-journals.com), this Focus Session features several invited presentations, talks and posters from key contributors on core condensed matter and applied physics topics. Highlights comprise the latest results on diamond, nitride semiconductors, organic materials, two-dimensional and quantum systems, oxides, magnetic materials, solar cells, thermoelectrics and more.

physica status solidi was launched by Akademie-Verlag Berlin in July 1961 and is published by Wiley-VCH Berlin and Weinheim today, supported by Wiley colleagues in China and the US. While in its first three decades it served as an East-West forum for solid state physics, since 1990 it has evolved into a family of journals with international author- and readership in a globalized scientific world. Its professional editorial services include topical curation, peer review organization, technical editing, special issue and hybrid open access publication.

The Focus session celebrates the numerous close collaborations and the steady support which the journals receive from their Advisory Board members, authors, reviewers and guest editors, including many members of the DPG and the condensed matter physics community in Germany.

(More information on '60 years of *pss*' is available at http://bit.ly/60_years_pss)

Organizers: Stefan Hildebrandt (Editor-in-Chief, pss), Norbert Esser (TU Berlin, ISAS) and Stephan Reitzenstein (TU Berlin)

Time: Tuesday 13:30–16:15 Location: H3

See DS 5 for details of this session.

HL 11: Focus Session: Functional Metal Oxides for Novel Applications and Devices

Metal oxides exhibit a myriad of fascinating physical properties that enable a large variety of potential applications such as sensors and detectors, solar energy harvesting, transparent and potentially bendable electronics, power electronics, high-electron-mobility transisitors, memristors, topological quantum computation and so on. These functionalities typically require homo- or heteroepitaxial layers of high crystallinity with bendable amorphous semiconducting oxides as an exception. This session sets a focus on growth of bulk and thin films, experimental and theoretical investigation of their physical properties as well as fabrication and characterization of demonstrator devices.

Organizers: Oliver Bierwagen (Paul-Drude-Institut für Festkörperelektronik, Berlin), Holger Eisele (TU Berlin), Jutta Schwarzkopf (Leibniz-Institut für Kristallzüchtung, Berlin) and Holger von Wenckstern (Universität Leipzig).

Time: Tuesday 13:30–16:30 Location: H4

Invited Talk HL 11.1 Tue 13:30 H4

Modulation Doping in High-Mobility Alkaline-Earth Stannates — •Bharat Jalan — University of Minnesota, Twin Cities, USA

The vast majority of work concerning a conducting oxide interface focus on the LaAlO3/SrTiO3 (LAO/STO) interfaces including some on Al2O3/STO and ReTiO3/STO (Re refers to the rare-earth elements) interfaces among others. Amazingly, all these heterostructures involve the use of STO as an active layer where electron transport occurs. Attempts to synthesize non-STO based modulation-doped heterostructure have been unsuccessful so far despite theoretical predictions. Nor has any appreciable level of control been gained over the electron density at the interface, which is critical to device applications. In this talk, we will report the first demonstration of true modulation doping in a wider bandgap perovskite oxides without the use of STO. We show that the La-doped SrSnO3/BaSnO3 system precisely fulfills the theoretical criteria for electron doping in BaSnO3 using electrons from La-doped SrSnO3, and we demonstrate how rearrangement of electrons can be used to control the insulator-to-metal transition in these heterostructure. We further show the use of angle-resolved HAXPES as a non-destructive approach to not only determine the location of electrons at the interface but also to quantify the width of electron distribution in BaSnO3. The transport results are in good agreement with the results of self-consistent solution to one-dimensional Poisson and Schrödinger equations.

Invited Talk HL 11.2 Tue 14:00 H4

Ultrathin oxides on InGaN nanowires: Hybrid nanostructure photoelectrodes and optical analysis of chemical processes — P. Neuderth[2], J. Schörmann[2], M. Coll[3], M. de la Mata[4], J. Arbiol[4], R. Marschall[5,6], and •M. Eickhoff[1,2] — [1]Inst. of Solid State Physics, Univ. of Bremen, Germany — [2]Inst. of Exp. Phys. I, JLU Giessen, Germany — [3]Inst. de Ciencia de Materials de Barcelona, Spain — [4]ICN2, Barcelona, CAT, Spain — [5]Inst. of Phys. Chem., JLU Giessen, Germany — [6]Phys. Chem. III, Univ. of Bayreuth, Germany

We demonstrate an experimental strategy for systematically assessing the influence of surface passivation layers on the photocatalytic properties of nanowire (NW) photoanodes by combining photocurrent analysis, photoluminescence spectroscopy and high resolution transmission electron microscopy. We apply this approach to separate the influence of different mechanisms on recombination and transport processes of photogenerated carriers and to compare the effect of TiO2, CeO2 and Al2O3 coatings deposited by atomic layer deposition (ALD). Due to efficient charge transfer from the InGaN NW core a stable TiO2-covered photoanode with visible light excitation is realized. As further applications we demonstrate the quantitative optical analysis of oxygen diffusion in ultrathin CeO2 and of the Li intercalation in TiO2 using hybrid nanostructures. In both cases the optical properties of the InGaN NWs are used as a probe for chemical processes in the ultrathin oxide layer that was deposited by ALD. Further potential applications of advanced hybrid nanostructures are discussed.

Invited Talk HL 11.3 Tue 14:30 H4

Doping and charge compensation mechanisms in semiconducting oxides — •Andreas Klein — Technical University of Darmstadt

Different charge compensation mechanisms are known for ionic solids. Among them are the formation of compensating defects such as electronic or ionic defects, the valence changes of atoms and the segregation of dopants. In principle, the introduction of positive charges by donor doping or reduction results either in the compensation by electrons, negatively charged intrinsic acceptors as metal vacancies, the reduction of a one of the species in the compound, or in the segregation of the dopant species. The situation is reversed for the addition of negative charges. While the different mechanisms are well-documented for different materials, predicting the prevailing compensation mechanism in a material is hardly possible. It is well known that the Fermi energy is determined by the defect concentrations but it is equivalent to describe the concentration of defects as a function of the Fermi energy. This enables a direct comparison of the different compensation mechanisms. The challenges in discriminating the different compensation mechanisms are discussed using the example of Sn-doped indium oxide.

Invited Talk HL 11.4 Tue 15:00 H4

Oxide Memristors for edge computing and secure electronics — •Heidemarie Schmidt — Leibniz-IPHT, Jena, Germany — Friedrich-Schiller-Universität Jena, Jena, Germany — Fraunhofer ENAS, Chemnitz, Germany

In the future, new hardware components will determine the power and strength of artificial intelligence and manchine learning. These components are called memristors [1]. The first memristor with unified analog data storage and information processing is the BiFeO3 (BFO) memristor. BFO is an electroforming-free, bipolar memristor and its potential has been shown in in-memory information processing [2], edge computing [3], and hardware cryptography. Another electroforming-free memristor is the unipolar memristor YMnO3 (YMO) [4]. In order to develop memristor technology and applications further, it is more than ever necessary to understand the underlying resistive switching mechanisms when a write voltage is applied. We discuss results from quasi-static test measurements on BFO [5] and from temperature dependent transport measurements on YMO [6].

[1] Leon Chua, IEEE Transactions on Circuit Theory 18, 507, 1971
[2] T. You et al., Adv. Funct. Mat. 24, 3357-3365, 2014.
[3] N. Du et al., Front. Neurosci. 15, 660894, 2021.
[4] H. Schmidt, 118, 140502, 2021.
[5] N. Du et al., Phys. Rev. Applied 10, 054025, 2018.
[6] V.R. Rayapati et al., J. Appl. Phys. 126, 074102, 2019.

Invited Talk HL 11.5 Tue 15:30 H4

Integration of 33°Y-$LiNbO_3$ films with high-frequency BAW resonators — Sondes Boujnah[1], Mihaela Ivan[2], Vincent Astié[3], Samuel Margueron[1], Mario Constanza[1], Jean-Manuel Decams[3], and •Ausrine Bartasyte[1] — [1]FEMTO-ST Institute, University of Bourgogne Franche-Comté Besançon, France — [2]SATT-Sayence, Dijon, France — [3]Annealsys, Montpellier, France

The next generation telecommunications require RF filters operating at frequencies of 6-9 GHz. $LiNbO_3$ (LN) films were identified as one of the materials with sufficient electromechanical coupling, K^2, for these applications. To attain 6-9 GHz frequencies in bulk acoustic wave (BAW) devices, LN film thickness has to be below 200 nm, which makes challenging their fabrication by popular smart-cut process. This motivates further development of integration of deposited highly-coupled LN films with BAW resonators. Several challenges have to be overcome in the case of LN direct growth on electrodes/mirrors/sacrificial layers used in BAW devices: (i) heterostructure has to be stable chemically/structurally at LN growth temperature/atmosphere, (ii) eliminate interaction between Li_2O and SiO_2, (iii) bottom electrode with good conductivity.

The aim of this work is to optimize SMR and HBAR structures adapted to high-deposition temperatures, and chemically not interacting with LN thin films. The Bragg mirror with a reflection coefficient of 0.98 and a stopband width of 3.1 GHz, centered at 6 GHz, for the longitudinal mode was designed. Deposition parameters were optimized to fabricate the Bragg reflectors with small roughness, without defaults and good stability and Pt bottom electrode with low resistivity ($4\mu\Omega\cdot$cm). The SMR resonator based on 125 nm thick 33°Y-LN film allows attain pure longitudinal mode with K^2 as high as 14.5 % at 5.9 GHz. 33°Y-LN films grown on seed layer/Pt bottom electrode presented single orientation, and dielectric constant close to bulk LN. After electrical poling, the pyroelectric coefficient increased from 11 μC$\cdot$m$^{-2}\cdot$K^{-1} to the value of bulk 33°Y-LN indicating single domain state of the film. The acoustical performance of BAW devices will be presented, as well.

HL 11.6 Tue 16:00 H4

Observation and control of improper ferroelectric nano-domains in Gd2(MoO4)3 — •Ivan Ushakov[1], Theodor Holstad[1], Didier Perrodin[2], Edith Bourret[2], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Norway — [2]Materials Science Division, Lawrence Berkeley National Laboratory, USA

Gd2(MoO4)3 is a classical example of an improper ferroelectric material and has been extensively studied with respect to its ferroic properties and ferroelectric/ferroelastic domains. Here, we revisit the ferroelectric domain structure and expand previous optical investigations to the nanoscale. By using Piezoresponse Force Microscopy (PFM), we resolve the established pattern of ferroelectric and anti-phase domains in Gd2(MoO4)3. In addition, we discover stripe-like nanodomains with a periodicity of about 50 nm. The response of the ordered nanodomains to locally applied electric fields, pressure, and temperature is presented. Our findings provide new insight into the physics of Gd2(MoO4)3 at the level of the domains and introduce novel opportunities for property engineering at the local scale.

HL 11.7 Tue 16:15 H4

Electronic Raman scattering study of Ir4+ ions in beta-Ga2O3 — •Palvan Seyidov[1], Manfred Ramsteiner[2], Zbigniew Galazka[1], and Klaus Irmscher[1] — [1]Leibniz-Institut für Kristallzüchtung, Max- Born-Str. 2, 12489 Berlin, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

Currently, beta-Ga2O3 is in the research focus as a material for power electronic devices because of its anticipated high electric break down field (~8MV/cm). For such applications, unintentional impurities in bulk crystals can lead to detrimental effects in device performance. Here we study electronic Raman scattering (ERS) of Ir4+ ions in bulk crystals grown by the Czochralski method. The optical excitation energy was varied between 1.95eV to 3.81eV by using Ar+ ion and HeCd lasers. Conventionally, Raman scattering is used to investigate vibrational modes of molecules and crystals. In contrast, inelastic light scattering due to electronic transitions can be studied by ERS. We observed an ERS feature at 5152 cm-1 (1.94 um, 0.639 eV) in room-temperature spectra from bulk beta-Ga2O3. The observed spectral feature is attributed to Ir4+ ions incorporated on Ga sites and assigned to an intra-center d-d transition within the t2g orbitals. The ERS efficiency is found to strongly depend on the photon energy used for optical excitation. The observed maximum at 2.8 eV can be explained by a resonance enhancement involving an electron transfer from Ir3+ to the conduction band at ~2.2 eV and an Ir4+ intra-center transition at ~0.6 eV.

HL 12: Focus Session: Spin-Charge Interconversion (joint session MA/HL)

While classical spintronics has traditionally relied on ferromagnetic metals as spin generators and spin detectors, a new approach called spin-orbitronics exploits the interplay between charge and spin currents enabled by the spin-orbit coupling (SOC) in non-magnetic systems. Efficient spin-charge interconversion can be realized through the direct and inverse Edelstein effects at interfaces where broken inversion symmetry induces a Rashba SOC. Although the simple Rashba picture of split parabolic bands is usually used to interpret such experiments, it fails to explain the largest conversion effects and their relation to the actual electronic structure.

Organizer: Ingrid Mertig (University Halle-Wittenberg)

Time: Tuesday 13:30–16:45 Location: H5

See MA 6 for details of this session.

HL 13: Poster Session III

Topics:
- Materials and devices for quantum technology
- Quantum dots and wires
- Functional Metal Oxides for Novel Applications and Devices
- Advanced neuromorphic computing hardware: Towards efficient machine learning

Time: Tuesday 13:30–16:30 Location: P

HL 13.1 Tue 13:30 P

Universal short-time response and formation of correlations after quantum quenches — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

The short-time evolutions of two distinct systems, the pump and probe experiments with a semiconductor and the sudden quench of cold atoms in an optical lattice, are found to be described by the same universal response function. This analytic formula at short time scales is derived from the quantum kinetic-theory approach observing that correlations need time to form. The demand of density conservation leads to a reduction of the relaxation time by a factor of 4 in quench setups. The influence of the finite-trapping potential is derived and discussed along with Singwi-Sjølander local-field corrections including the proof of sum rules. The quantum kinetic equation allows to understand how two-particle correlations are formed and how the screening and collective modes are build up. Phys. Rev. B 90 (2014) 075303, Phys. Rev. E 66 (2002) 022103, Phys. Rev. E 63 (2001) 20102, Phys. Lett. A 246 (1998) 311

HL 13.2 Tue 13:30 P

Synchronization Properties in Coupled Mode-Locked Lasers — •Clara Rodríguez Roca-Sastre, Stefan Meinecke, and Kathy Lüdge — Institut für Theoretische Physik, Technische Universität, Berlin, Deutschland

Passively mode-locked semiconductor lasers (PMLLs) are simple and compact sources of high-frequency ultrashort light pulses. These devices can be used in novel secure communication schemes and for optical clock synchronization. However, due to the lack of an external reference clock, this class of MLLs exhibits higher timing jitter than their active counterparts [1]. To overcome this detrimental effect, mutual all-optical coupling can be introduced to reduce the timing jitter [2]. This technique also allows access to different synchronization regimes of the laser outputs. To better understand the synchronization regime, we numerically model a coupled system using delay differential equations [1]. Two coupled identical lasers pumped differently can operate with a high degree of in-phase and localized synchronization if one of them is driven in stable FML operation and the detuning between the devices is not too pronounced. Otherwise, the ML output collapses and complex dynamics such as multi-pulse dynamics may arise. The lasers then exhibit mode-locked pulses with a finite number of different intensities. In addition, regions of anti-phase dynamics appear at delay times around fractional integers of the laser resonance round-trip time.

[1] Otto et al., New J. Phys. 14, 113033 (2012).
[2] Simos et al., IEEE JQE 54, 2001106 (2018).

HL 13.3 Tue 13:30 P

Off-resonant excitation swing up of a quantum emitter — •Thomas Bracht[1], Michael Cosacchi[2], Tim Seidelmann[2], Moritz Cygorek[3], Alexei Vagov[2,4], Martin Axt[2], Tobias Heindel[5], and Doris Reiter[1] — [1]Institut für Festköpertheorie, Universität Münster,Germany — [2]Theoretische Physik III, Universität Bayreuth, Germany — [3]Heriot-Watt University, Edinburgh, United Kingdom — [4]ITMO University, St. Petersburg, Russia — [5]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany

Controlled preparation of a quantum emitter is key for many of its applications, for example as a single photon source. Here, we present a scheme which uses pulses detuned significantly below the excited-state energy that lead to a swing up of the quantum emitter occupation. We show that a two-color excitation leads to high final excited-state occupation and discuss the conditions under which the scheme works. Applied to semiconductor quantum dots, the proposed swing-up scheme results in the emission of high-quality single photons. The main advantage of our scheme compared to Rabi rotations is that no filtering is needed in order to separate the resulting signal from the laser source. Another advantage is that in contrast to off-resonant schemes relying on phonon-assisted transitions, our scheme does not depend on any auxiliary quasi-particles. In summary, we are proposing an experimentally feasible swing-up scheme to excite a quantum emitter yielding high-quality photon emission for quantum technology.

HL 13.4 Tue 13:30 P

On the Advantage of Sub-Poissonian Single Photon Sources in Quantum Communication — •Daniel Vajner, Timm Gao, and Tobias Heindel — Institute of Solid State Physics, Technical University Berlin, 10623 Berlin

Quantum Communication in principle enables a provably secure transmission of information. While the original protocols envisioned single photons as the quantum information carrier [1], nowadays implementations and commercial realizations make use of attenuated laser pulses. There are, however, a number of advantages of using single photon sources. They are not limited by the Poisson statistics and suffer less under finite-key length corrections [2]. In addition, the second order interference visibility of true single photons can exceed the classical value of 50% which will be benefitial for all quantum information processing schemes, as well as measurment device independent QKD schemes, that rely on Bell state measurements of photons from different sources [3]. Given recent advances in the development of engineered semiconductor QD-based light sources, harnessing these advantages is within reach. We present an overview of different scenarios in which employing single photon sources improves the communication rate and distance.

[1] Bennett et al. *Proceedings of the IEEE International Conference on Computers, Systems and Signal Processing* (1984)
[2] Cai et al. *New Journal of Physics* 11.4 (2009): 045024
[3] Mandel, L. *Physical Review A* 28.2 (1983): 929

HL 13.5 Tue 13:30 P

Diameter dependent whispering gallery mode lasing effects in quantum dot micropillar cavities — •Imad Limame, Ching-Wen Shih, Johannes Pietsch, Aris Koulas-Simos, Leo Roche, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin

Whispering-gallery modes (WGMs) were first theorized by Lord Rayleigh in 1878 at the St. Paul cathedral. WGMs with lateral emission characteristics occur also in micropillar cavities which is of great interest for integrated quantum nanophotonics. In this work, we present an in depth study of WGM emission in micropillars ranging between 2 and 20 μm in diameter. The samples were grown by mean of metal organic chemical vapor deposition and include multi layers of InGaAs quantum dots as active region. The pillars were processed using electron beam lithography, using a Ni hard mask. This hard mask is only partially removed to create a highly obsorbant surface on the top of the pillar, which suppresses emission through standard vertically emitting micropillar modes. The optical properties were studied by means of micro-photoluminescence spectroscopy (μPL). Investigating the input-output characteristics, the free spectral range, the Q-factor and the beta-factor as function of the pillar diameter provides deep insight into the underlying physics and paves the way for the applicaiton of the developed WGM microlasers as coherent excitation sources in integrated quantum photonic circuits.

HL 13.6 Tue 13:30 P

Continuum of quantized bound quasinormal modes — •Robert Fuchs, Sebastian Franke, Andreas Knorr, and Marten Richter — Technische Universität Berlin, Berlin, Germany

Quasinormal modes (QNMs) have proven to be a useful and intuitive way to define modes for open cavities. They have been calculated for a variety of problems both in classical electrodynamics, and recently used in a fully quantized description for three dimensional geometries.

However, so far, a quantized description of multi-cavity-structures using QNMs with substantial propagation delays is missing. We show that an extension of the QNM quantization is possible if the cavities are far away from each other so that retardation effects are important.

The related quantization approach leads to a set of non-bosonic operators with a continuous spectrum. In the multi-cavity theory, this continuum serves as a bath which can be used to describe photon propagation between the separately quantized cavities. Using multi-time correlation functions we are able to construct a systematic formulation to describe the inter-cavity transfer determined by QNM parameters.

HL 13.7 Tue 13:30 P

Fiber-pigtailing quantum-dot cavity-enhanced light emitting diodes — Lucas Rickert[1], •Frederik Schröder[1], Timm Gao[1], Christian Schneider[2,3], Sven Höfling[2], and Tobias Heindel[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Technische Physik, Physikalisches Institut, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Würzburg, Germany — [3]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany

Semiconductor quantum dots embedded in engineered microcavities are considered key building blocks for photonic quantum technologies [1]. The direct fiber-coupling of respective devices would thereby offer many advantages for practical applications [2]. Here, we present a method for the direct and permanent coupling of electrically operated quantum-dot micropillar-cavities to single-mode fibers [3]. The fiber-coupling technique is based on a robust four-step process fully carried out at room temperature, which allows for the deterministic coupling of a selected target device. Using the cavity mode electroluminescence as feedback parameter, precise fiber-to-pillar alignment is maintained during the whole process. Permanent coupling is achieved in the last process step using UV curing of optical adhesive. Our results are an important step towards the realization of plug-and-play benchtop electrically-driven single-photon sources.

[1] T. Heindel et al., Appl. Phys. Lett. 96, 011107 (2010)
[2] T. Kupko et al., arXiv.2105.03473 (2021)
[3] L. Rickert et al., arXiv.2102.12836 (2021)

HL 13.8 Tue 13:30 P

Hyperspectral imaging for deterministic quantum dot microcavities — •Quirin Buchinger[1], Magdalena Moczała-Dusanowska[1], Łukasz Dusanowski[2], Tobias Huber[1], and Sven Höfling[1] — [1]Technische Physik, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Electrical and Computer Engineering, Princeton University, 08544 Princeton (NJ), USA

For many photonic quantum communication schemes, including quantum networks, indistinguishable single photons or entangled photon pairs are required. Semiconductor quantum dots (QDs) in microcavities are a promising source due to their high quantum efficiency [1], photon indistinguishability [2], and outcoupling efficiency. As a disadvantage these self-assembled QDs are randomly distributed over the sample and have inhomogeneosly distributed emission wavelengths.

Here, we present an approach using hyperspectral imaging to locate self-assembled QDs and to integrate them deterministically into microcavities. We image InGaAs-QDs in a GaAs-Membrane and perform subsequent processing of Circular-Bragg-grating cavities. We show possibilities and solutions to improve the spatial accuracy through marker design, data acquisition and image processing. Further, we discuss the combination of imaging and acquisition of single spectrums at thereby identified QDs to reduce the needed time compared to hyperspectral imaging without a trade-off on spectral and spatial information.

[1]Michler et al. Science, 290, 2282-2285 (2020)
[2]Santorio et al. Nature, 419, 594-597 (2002)

HL 13.9 Tue 13:30 P

Mobility spectrum analysis on three-dimensional topological insulator $BiSbTeSe_2$ — •Jimin Wang[1], Alexander Kurzendorfer[1], Lin Chen[1], Zhiwei Wang[2], Yoichi Ando[2], Yang Xu[3], Ireneusz Miotkowski[3], Yong P. Chen[3], and Dieter Weiss[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, German — [2]Physics Institute II, University of Cologne, Zülpicher Str. 77, 50937 Köln, Germany — [3]Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907, USA

We conducted mobility spectrum analysis on a high quality 3D topological insulator film of $BiSbTeSe_2$ to extract mobility μ, and carrier density n. Top and bottom gates were applied to tune the carrier density on top and bottom surfaces independently. At 1.5 K, when conduction is entirely dominated by the Dirac surface states, we always find two dominant conduction channels (top and bottom surfaces), with $\mu = 500 - 3000\,\mathrm{cm}^2/(\mathrm{Vs})$, and n on the order of $10^{12}\,\mathrm{cm}^{-2}$. However, at sufficiently high temperature ($T = 85$ K), when the bulk contributes, a third channel with maximum mobility $\mu \sim 400\,\mathrm{cm}^2/(\mathrm{Vs})$, and n on the order of $10^{11} - 10^{13}\,\mathrm{cm}^{-2}$ opens. Our data show the feasibility of the method to analyze the different conduction channels in a topological insulator, being also promising for other similar material systems.

HL 13.10 Tue 13:30 P

Feedback-induced chaotic emission from a GaAs-QW high-contrast grating microcavity structure — •Aris Koulas-Simos[1], Melanie Hoeschele[1], Jiaqi Hu[2], Hui Deng[2,3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Applied Physics Program, University of Michigan, Ann Arbor, Michigan 48109, USA — [3]Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA

We investigate the optical and quantum optical properties of a high-contrast grating microcavity structure based on GaAs multiple quantum wells subject to optical feedback. Power-dependent microphotoluminescence (μPL) studies reveal the typical s-shaped form in the I/O curve with a pronounced kink signifying the lasing onset, accompanied by an abrupt linewidth narrowing. The effect of the optical feedback is visible in the shift of the threshold to lower excitation powers. Additional angle-resolved PL measurements show a condensation to lower k-states and spectrally narrower emission. In power-dependent photon-autocorrelation, enhanced bunching and revival peaks with a period equal to the round-trip time of the external cavity are pronounced, indicating chaotic emission as a result of the optical feedback [1]. This is again verified by calculating the photon-autocorrelation function $g^{(2)}(\tau)$ through single-shot intensity trace measurements with a streak camera.

[1] F. Albert et al., *Nat. Comm.* **2**, p. 1-5 (2011)

HL 13.11 Tue 13:30 P

Spectral manipulation of coherent acoustic phonons in a graphite nanofilm observed by ultrafast electron diffraction — •Arne Ungeheuer, Ahmed Hassanien, Mashood Mir, Arne Senftleben, and Thomas Baumert — University of Kassel, Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), D-34132 Kassel, Germany

Femtosecond-laser-excited nanomechanical strain-waves in thinfilm-structures allow for a series of quantized resonant modes with amplitudes that depend on the photoinduced spatiotemporal strain-distribution in the material [1]. We investigate the possibilities to amplify specific higher harmonic modes in a graphite nanofilm, employing a NIR femtosecond-laser double pulse excitation-scheme. We present results from ultrafast electron diffraction studies for different relative pulse-delays within the double-pulse sequence, yielding constructive or destructive interference for selected coherent acoustic phonon harmonics.

[1] F. Hudert et al.: Phys. Rev. B 79, 2009.

HL 13.12 Tue 13:30 P

Laser controlled charge-carrier dynamics in pyrene-doped $MoSe_2$ monolayer — •Matheus Jacobs[1], Jannis Krumland[1], and Caterina Cocchi[1,2] — [1]Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Institute of Physics, Carl von Ossietzky Universität Oldenburg,26129 Oldenburg, Germany

In the last years, the interest in transition metal dichalcogenide monolayers have grown enormously due to their unique electronic structure and light-matter coupling properties. Combining these materials with carbon conjugated molecules can give rise to new materials with enhanced opto-electronic performance, specially when excited by coherent radiation. In the framework of real-time time-dependent density functional theory, we investigate the ultrafast charge-carrier dynamics at the interface formed by pyrene molecules physisorbed on a $MoSe_2$ monolayer. By monitoring the effect of the incident pulse intensity on the energy and the electron transfer on the hybrid heterostructure, we identify a striking nonlinear response of the system, which in turn impacts the charge-carrier dynamics and the nature of cahrge transfer from the inorganic to the organic components.

HL 13.13 Tue 13:30 P

Validity of the Siegert relation in partially-coherent regimes — •Monty Drechsler, Frederik Lohof, and Christopher Gies — Institute for Theoretical Physics, University of Bremen, Bremen, Germany

With increasing miniaturization of coherent light sources to the diffraction limit and below, their emission properties change and new effects appear. Therefore, a description in the context of quantum optics is required. An objective in studying such nano light sources is their classification. In this context, the investigation of the statistical nature of photon correlations plays a major role. We are able to access information about photon correlations quantified by $g^{(1)}(\tau)$ and $g^{(2)}(\tau)$ using a master-equation or a cluster-expansion approach. We discuss the temporal behavior of these correlation functions in different device regimes from the quantum limit of a single emitter to larger systems. When combining the theoretical prediction with experiments we are confronted with the limited time resolution of detectors used in the measurement of correlations function. To treat this issue, a generalized Siegert relation has been used previously [1][2]. Here, we quantify when such an approach is justified.

[1] Kreinberg et al., Light Sci Appl 6, e17030 (2017)
[2] Kreinberg et al., Laser & Photonics Reviews 14, Nr. 12, 2000065 (2020)

HL 13.14 Tue 13:30 P

Top-down fabrication of silicon nanophotonic structures for hosting single-photon emitters — •Nagesh S. Jagtap[1,2], Michael Hollenbach[1,2], Ciaran Fowley[1], Woo Lee[3], Manfred Helm[1,2], Georgy V. Astakhov[1], Artur Erbe[1], and Yonder Berencén[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Korea Research Institute of Standards and Science (KRISS), Yuseong, 305-340 Daejeon, Republic of Korea

Silicon, the ubiquitous material for computer chips, has recently been shown to be instrumental for hosting sources of single-photons emitting in the strategic optical telecommunication O-band (1260-1360 nm)[1], the so-called G center. To increase the brightness and the photon extraction efficiency of single G center, the coupling of these centers into photonic structures is strong.

This work presents a top-down approach avoiding the use of ion beam-based etching methods for fabricating high-quality defect-free photonic structures such as silicon nanopillars, which can host single-photon emitters. This method builds upon a wet-chemical process known as metal-assisted chemical etching. We report the successful fabrication of two-dimensional arrays of vertically-directed waveguiding silicon nanopillars. We also show the etch chemistry dependence on the Si wafer resistivity along with its effect on the etch rate and the sidewall roughness of pillars for a variety of pillar diameters.

References:[1] M. Hollenbach, et al. Opt. Express 28,26111-26121

HL 13.15 Tue 13:30 P

Sensitivity to high energy Proton irradiation of 670 nm VCSELs in emitter and receiver mode — •Heinz-Christoph Neitzert — Salerno University - DIIn, Fisciano (SA), Italy

Vertical Cavity Surface Emitting Lasers (VCSELs) have recently found increasing interest also for space applications, for example for ultra-compact atomic clocks and intra-satellite data-links. Besides their application as efficient emitters also their application as resonant-cavity type photo-receiver has been demonstrated. The radiation stability of commercial VCSELs emitting at 670nm bas been tested with the exposition to 68 MeV protons with different fluence values up to 10^13 protons/cm^2. Besides the conventional electrical and electro-optical characterization under forward bias conditions, also the reverse bias characteristics up to device breakdown and the receiver characteristics under white light LED illumination have been investigated. Even for the highest proton fluence value only a very small change of the laser threshold current and slope efficiency values has been observed, confirming that these VCSELs can be operated successfully in space or in a high energy physics environment. Regarding their optical receiver properties up to 10^12 protons/cm^2, only a minor decrease of the primary photocurrent was observed. Only for the highest proton fluence a more substantial decrease in open circuit voltage and primary photocurrent and also a increase of the reverse bias current due to defect related tunnelling, before the inset of avalanche breakdown, has been found.

HL 13.16 Tue 13:30 P

Carrier dynamics and modulation properties in tunnel- injection based quantum-dot structures — •Michael Lorke[1], Igor Khanonkin[2], Stephan Michael[1], Gadi Eisenstein[2], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen, Germany — [2]Andrew and Erna Viterbi Department of Electrical Engineering, Technion, Haifa, Israel

For tunnel-injection (TI) quantum-dot (QD) lasers record high small signal modulation bandwidth and improved performance of 1.55μm InAs QDs on InP-based hetero-structures were reported, which underscores their application potential for high-speed optical communication networks. However, large signal modulation, which really is the fingerprint of applicability in optical communication, is much less investigated. We present a theoretical analysis of TI laser and amplifier devices by combining material realistic electronic structure calculations with a detailed description of the carrier dynamics. Based on these investigations, we can give design guidelines to optimize the modulation bandwidth and turn-on delay.

HL 13.17 Tue 13:30 P

Wave Digital Emulation of Hydra's Neuronal Activity — •Sebastian Jenderny[1], Karlheinz Ochs[1], Christoph Giez[2], Alexander Klimovich[2], and Thomas Bosch[2] — [1]Ruhr University Bochum, Chair of Digital Communication Systems, Bochum, Germany — [2]Christian-Albrechts University Kiel, Zoological Institute, Kiel, Germany

Modeling real neuronal networks by electrical circuits is especially interesting as it can reveal novel design principles. A promising model organism for this purpose is Hydra, a freshwater polyp with rich behavioral patterns despite its neuronal network only consisting of roughly 3000 neurons. Modeling Hydra's nerve net by an electrical circuit is, however, challenging as only calcium imaging measurements instead of electrophysiology are available. The neuronal activity associated to these calcium imaging measurements are difficult to mimic by electrical circuits as they are based on fluorescence traces instead of voltage and current measurements. In this work, we present a circuit-based approach to mimic these fluorescence traces utilizing the fact that the latter can be used to determine the intracellular calcium concentration. For this purpose, we make use of the Morris-Lecar model already accounting for calcium currents and hence allowing to calculate a calcium concentration comparable to the one inferred from the fluorescence traces. A wave digital emulation of our circuit approach shows the successful mimicking of exemplary neuronal activity of Hydra.

HL 13.18 Tue 13:30 P

Light-sensitive Resonant Tunneling Diodes for single photon detection — •Sebastian Krüger[1], Andreas Pfenning[2], Fabian Hartmann[1], Fauzia Jabeen[1], and Sven Höfling[1] — [1]Technische Physik, Julius-Maximilians Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z4

Double barrier resonant tunneling diodes (RTDs) are versatile optoelectronic devices with a multitude of possible applications. The focus of interest is the application for terahertz oscillation and the detection of single photons. Especially the downtime-free photodetection has an advantage compared to the state-of-the-art techniques, which are using avalanche multiplication. The capability of single-photon detection has been demonstrated in [1]. The low efficiency of around 10% is limiting. We present our work on RTD photodetectors based on AlGaAs/GaAs DBQW with GaAsSb quantum well (QW) close to the double barrier structure [2]. The strained ternary alloy, GaAsSb, is grown on GaAs. The type II band alignment leads to better *hole* confinement compared to InGaAs-QW or quantum dots (QD). The photodetection based on minority charge carrier accumulation at the DBS in RTDs, is sensed by the influence of their electrostatic potential. It leads to an additional voltage drop over the DBS and shifts the I(V) characteristics towards lower voltages [2]. [1] J. C. Blakesley, et al., Physical Review Letters 94, 067401 (2005). [2] A.Pfenning, et al., Applied Physics Letters 107, 081104 (2015).

HL 13.19 Tue 13:30 P

Towards Scalable Reconfigurable Electronics: Fabrication of Schottky Barrier Field-Effect Transistors using Flash Lamp Annealing — •Muhammad Bilal Khan, Sayantan Ghosh, Slawomir Prucnal, Rene Hübner, Artur Erbe, and Yordan M. Georgiev — Institute of Ion Beam Physics And Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden

To complement the scaling down of complementary metal-oxide-semiconductor (CMOS), new device concepts have been introduced. One such concept is the reconfigurable field-effect transistor (RFET). In the most general case, an RFET is a silicon nanowire (SiNW) based device. The SiNW is silicided at both ends, which results in silicide-Si-silicide Schottky junctions. Typically, two distinct gate electrodes are placed on silicide-Si junctions. By controlling the electrostatic potential on the gate electrodes, the RFET is programmed to the *p*- or *n*- polarity. We report on the fabrication and electrical characterization of top-down fabricated SiNW based RFETs. Flash lamp annealing based silicidation process is developed, which enables control over the silicidation process. Uni-polar transfer characteristics are obtained using two top-gates. The effect of implementing various gate dielectric materials (SiO_2, Al_2O_3 and hBN) is studied to enhance device electrostatics.

HL 13.20 Tue 13:30 P

Space-charge effects in high-coherence electron pulses — •Alexander Schröder, Christopher Rathje, Niklas Müller, Jonathan Weber, Nora Bach, and Sascha Schäfer — Institute of Physics, University of Oldenburg, Germany

Ultrafast transmission electron microscopy (UTEM) enables the imaging of ultrafast nanoscale dynamics, utilizing an optical-pump/electron-probe approach within a high-resolution transmission electron microscope [1]. The spatio-temporal resolution in this technique sensitively depends on the phase-space structure of the employed ultrashort electron pulses. Whereas needle-shaped photoemitters were demonstrated to deliver high-coherence electron pulses in the single-electron regime, at larger bunch charges significant Coulomb interactions within the pulse need to be considered [2].

Using the newly constructed Oldenburg UTEM, we investigate the impact of Coulomb interactions on the longitudinal phase-space structure of electron pulses. Depending on the illumination intensity on the photoemitter, we observe a fluence-dependent shift and broadening of the electron energy distribution which is compared to a multiparticle simulation taking into account the expanding electron pulse close to the emitter tip. The impact of the initial electron energy after photoemission, the acceleration field and the bunch charge on the spatio-temporal electron pulse structure at the sample are discussed.

[1] A. Feist et al., Ultramicroscopy, 176, 63 (2017)
[2] N. Bach et al., Structural Dynamics 6, 014301 (2019)

HL 13.21 Tue 13:30 P

Solving the Vertex Cover Problem with a Wave Digital Model of an Ising Machine — •Bakr Al Beattie and Karlheinz Ochs — Ruhr University Bochum, Bochum, Germany

The efficient solution of NP-problems is an unresolved computational challenge with many real-world applications. Ising machines are promising for solving these types of problems. The idea is to map a problem onto the Ising Hamiltonian and let an Ising machine find the ground state, which corresponds to the solution of the problem. These machines are designed so they have the natural tendency to converge to the ground state of the Hamiltonian. Multidimensional wave digital algorithms are known to be massively parallel, and they are additionally robust for emulating large electrical networks, like the coupled oscillator network of an Ising machine. In this work, a wave digital model mimicking the phase dynamics of an ideal Ising machine is derived and generalized to support solving Ising problems containing the Zeeman term. To prove usefulness and quality of this wave digital Ising machine, we solve a vertex cover problem.

HL 13.22 Tue 13:30 P

Decision-Making Processes by a Kuramoto Model with Hebbian Learning: Circuit Synthesis and Wave Digital Emulation — •Sebastian Jenderny, Dennis Michaelis, and Karlheinz Ochs — Ruhr University Bochum, Chair of Digital Communication Systems, Bochum, Germany

Decision-making processes are an interesting topic often studied in synchronizing oscillatory networks. Here, synchronization is, on an abstract level, related to learning. In this context, the Hebbian learning rule can be interpreted as the increasing and decreasing coupling strength between oscillators with a small and a large phase difference, respectively. This can for example be implemented by the Kuramoto model, being a simple and well-studied model for oscillatory networks. Our aim is to synthesize an electrical circuit of the Kuramoto model with Hebbian learning with which decision-making processes can be mimicked. For this purpose, we derive a memristor model accounting for the Hebbian learning rule. We then develop a corresponding wave digital model and utilize it to mimic the decision-making process associated with the observation of optical illusions.

HL 13.23 Tue 13:30 P

A Memristive Circuit for a Delay-Based Supervised Classifier — Dennis Michaelis, •Sebastian Jenderny, and Karlheinz Ochs — Ruhr University Bochum, Chair of Digital Communication Systems, Bochum, Germany

Supervised learning based on artificial neural networks is a major principle for many pattern recognition tasks. Corresponding circuit implementations are often based on implementing synaptic weight changes. In this work, we propose a different approach based on learning delays instead of synaptic weights. For this purpose, we synthesize an electrical circuit for a dynamic axon model. The resulting circuit is based on memristive Jaumann structures in combination with delay elements. We utilize this circuit to design a neural network for the supervised learning of gait patterns. Here, the learning is based on the circuit selecting delay lengths in a self-organized way, which further introduces an additional degree of freedom compared to the synaptic weight approach. A wave digital emulation verifies our approach by showing that the axonal delays associated with the trained gait patterns are successfully learned, leading to correct classification results.

HL 13.24 Tue 13:30 P

Mimicking Delay-Based Self-Sustaining Gait Pattern Generators — Dennis Michaelis, •Sebastian Jenderny, and Karlheinz Ochs — Ruhr University Bochum, Chair of Digital Communication Systems, Bochum, Germany

Hardware implementations of gait pattern generators are an active field of research especially in robotics, where recent approaches are based on neural networks. Most of the latter implementations, however, only consider synaptic weight changes. In contrast to this, we design a gait pattern generator being able to learn and generate self-sustaining gait patterns based on a neural network adjusting its axonal delays. For this purpose, we synthesize a memristive circuit of a dynamic axon model serving as the basis for the neural network. Here, the circuit realization of the axon is based on Jaumann structures with memristors. A wave digital emulation of the resulting complete circuit verifies our approach by showing the successful learning and generation of self-sustained gait patterns of a dog.

HL 13.25 Tue 13:30 P

Towards an Improved Anticipation Circuit with Self-Organized Resonance-Frequency-Adaption — Karlheinz Ochs and •Sebastian Jenderny — Ruhr University Bochum, Chair of Digital Communication Systems, Bochum, Germany

Inspired by the ability of an amoeba to anticipate environmental changes, an RLC circuit with a memristor in parallel has been proposed as an anticipation circuit. Here, the memristor enables a self-organized Q-factor adaption. Since this circuit's functionality is limited to an excitation with its resonance frequency, further research has been done to achieve an additional self-organized resonance-frequency adaption. Existing approaches are based on utilizing memcapacitors instead linear capacitors, where the memcapacitor models are very sophisticated. In contrast to this, in this work we develop a physically more meaningful memcapacitor to use it for an improved anticipation circuit. A wave digital emulation of the resulting circuit shows a self-organized resonance-frequency adaption, supporting the Q-factor adaption of the memristor.

HL 13.26 Tue 13:30 P

Optimal Topology Formation of Memristive Neuronal Networks — Dennis Michaelis, •Sebastian Jenderny, and Karlheinz Ochs — Ruhr University Bochum, Chair of Digital Communication Systems, Bochum, Germany

The topology formation of neuronal networks during their ontogenesis is of great importance since it lays the foundation for the neuronal networks being well adapted for future tasks. While the synapse formation is the most popular part of this aspect, it is also important to take axon growth into account. This is because the latter can be assumed to play a key role in the emergence of optimal communication paths of neuronal networks in terms of delays. In this work, we synthesize an electrical circuit abstractly mimicking the topology formation of neuronal networks with respect to delays by making use of memristors. The resulting circuit can be used to find the optimal communication paths of a neuronal network by finding its minimal spanning tree, which is verified by LTspice simulations.

HL 13.27 Tue 13:30 P

CMOS back-end compatible Metal-$Hf_{0.5}Zr_{0.5}O_2$-Al_2O_3-Metal ferroelectric tunnel junction devices for neuromorphic applications — •Keerthana Nair[1,2], Marco Holzer[1,2], Sourish Banerjee[1], Catherine Dudourdieu[1,2], and Veeresh Deshpande[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Freie Universität Berlin, Physical Chemistry, Arnimallee 22, 14195 Berlin, Germany

$Hf_{0.5}Zr_{0.5}O_2$ (HZO) ferroelectric layer provides an opportunity for CMOS back-end-of-line integrable devices owing to low crystallization temperature (around 400°C). Ferroelectric tunnel junction (FTJ) memory devices based on HZO feature ultra-low power consumption and have potential for multiple resistance states necessary for neuromorphic applications. FTJ architecture based on the Metal-Ferroelectric-Dielectric-Metal stack allows high ON/OFF ratio with thicker ferroelectric layer (10-12nm). In this work, we demonstrate 400°C-crystallized Metal-HZO-Al_2O_3-Metal FTJ architecture with TiN and W metals. Utilizing the coercive field distribution of the domains, we demonstrate multiple resistance states through partial switching operations and switching pulse-width modulations. The influence of cycling waveform on the ON/OFF ratio (which directly impacts achievable multiple resistance states) will be discussed. The intermediate resistance state stability will also be discussed. Our study also investigates the role of the process conditions, dielectric thickness and metal placement on attaining high ON/OFF ratio back-end compatible FTJ devices.

HL 13.28 Tue 13:30 P

Epitaxial BaSnO3 thin films without extended defects on lattice matched LaInO3 substrates — •Daniel Pfützenreuter, Zbigniew Galazka, Robert Schewski, Klaus Irmscher, Martin Albrecht, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

BaSnO3 is a semiconducting perovskite material offering an electron mobility of 320 cm2/Vs at a carrier density of 8E19 cm-3 at room temperature in a bulk crystal. Epitaxial thin films however, always have a much lower electron mobility, which is ascribed to a high density of threading dislocations emerging in the films as a consequence of a large lattice mismatch between substrate and film.

LaInO3 crystals with (110) surface orientations were applied as a novel orthorhombic substrate for the epitaxial growth of BaSnO3 thin films due to its negligible lattice mismatch. We revealed by means of reflection high energy electron diffraction, energy dispersive x-ray analysis and atomic force microscopy that a slight Ba-doping in the LaInO3 substrates helps to stabilize the substrate surface at elevated temperatures and under reducing atmosphere, which are the typically used pulsed laser deposition conditions for the growth of BaSnO3 thin films. Transmission electron microscopy measurements confirm the growth of fully strained BaSnO3 thin films without extended defects on LaInO3:Ba substrates. Temperature dependent Hall-effect measurements of a BaSnO3 film doped with 0.5 % La exhibit a Hall-mobility of 69 cm2/Vs at room temperature and 99 cm2/Vs at 20 K at a constant charge carrier density of 3.8E19 cm-3.

HL 13.29 Tue 13:30 P

β-Ga2O3 material for vertical power devices: challenges to the epitaxy process — •Ta-Shun Chou, Saud Bin Anooz, Raimund Grüneberg, Vi Tran Thi Thuy, Zbigniew Galazka, Klaus Irmscher, Palvan Seyidov, Martin Albrecht, and Andreas Popp — Leibniz-Institut für Kristallzüchtung, Berlin, Germany

β-Ga2O3 is a promising ultra-wide bandgap (~4.8 eV) semiconductor material. A breakdown field strength up to 8 MV/cm is expected from theoretical calculation, which makes it attractive for power electronic applications and a competitor to SiC and GaN. Especially a vertical architecture for β-Ga2O3-based transistors can exploit the high potential of this material and will benefit from a low on-resistance at a given breakdown voltage in combination with less power losses within a transistor switching operation. To fulfill the requirements of the vertical device, extremely low doped homoepitaxial thin films with thicknesses of several um and high crystallinity are necessary.

In this contribution, we present the growth development to achieve step-flow β-Ga2O3 grown layer by MOVPE on Mg-doped β-Ga2O3 (100) substrates with a thickness above 1 um by applying a high growth rate. This improvement can be related to the possible formation of a Ga adlayer which is widely reported already for the GaN system. In addition low, Si doping concentrations down to and below 1E17 cm^-3 were demonstrated while maintaining mobilities comparably high as previous results based on low growth rate and low thickness layers. The developed epitaxy process is a key enabler for the growth of (100) β-Ga2O3 material for vertical power device applications.

HL 13.30 Tue 13:30 P

Influence of group III dopants on the properties of SnO(001) films grown via plasma-assisted molecular beam epitaxy — •Kingsley Egbo, Georg Hoffmann, Andrea Ardenghi, Alexandra Papadogianni, Jonas Laehnemann, and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany

Most metal oxides show a propensity for n-type conductivity, few oxides show p-type character. Metastable tin monoxide (SnO) is among the few p-type oxide semiconductors and its unintentional p-type conductivity is believed to be controlled by Sn-vacancies. Few studies have also suggested the possibility for bipolar doping in SnO. In this study, the growth of SnO(001) doped with the group III La, In and Ga on YSZ(100) substrates by plasma-assisted MBE is investigated. Structural properties of the doped SnO(001) films were studied by x-ray diffraction, Raman spectroscopy and scanning electron microscope. Detailed electrical properties of the doped films are obtained from Hall Effect measurements. Hole concentration, p of ~0.8-2.0 x 1019 cm-3 and resistivity, ρ of 0.15-0.30 Ω-cm respectively is obtained from room temperature hall measurement of unintentionally doped SnO (001). We find that p increases to ~ 4.0-5.0 x 1019 cm-3 and ρ decreased to 0.04-0.063 Ω-cm for Ga doped films. In contrast, thin films doped with In and La show reduction in p and remarkable increase in ρ with increasing dopant concentration. Our results reveal that p-type conductivity in SnO can be improved by Ga acceptors while La and In likely acts as compensating donors in SnO. These results offer an opportunity for exploring bipolar doping in SnO.

HL 13.31 Tue 13:30 P

The role of Sr deficiency in SrTiO3 thin films grown by metal-organic vapor phase epitaxy — •Aykut Baki, Julian Stöver, Tobias Schulz, Houari Amari, Carsten Richter, Jens Martin, Klaus Irmscher, Martin Albrecht, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 in 12489 Berlin

SrTiO3 is widely studied due to interesting physical properties such as its high permittivity at room temperature, resistive switching and strain induced ferroelectricity. However, the underlying physical origin of these effects is not fully understood. In order to investigate the influence of structural defects on the physical properties, we performed the growth of SrTiO3 films by liquid-delivery spin metal-organic vapor phase epitaxy, which takes place nearby the thermodynamic equilibrium and at high oxygen partial pressures ensuring growth of films with high quality and negligible amount of oxygen vacancies. In this study, homoepitaxial SrTiO3 thin films were grown on 0.5 wt.% niobium doped SrTiO3 (100) substrates with varying Sr/Ti ratio in the gas phase. This provides single-phase stoichiometric and deliberately off-stoichiometric thin films with an intentionally incorporated Sr deficiency. Even films with Sr deficiency of up to 20 % were grown without the formation of any extended defects or foreign phase. In-situ high-resolution x-ray diffraction and transmission electron microcopy measurements verified a negligible amount of oxygen vacancies in the films and the absence of conductive oxygen filaments at typically applied switching voltages in a metal-oxide-semiconductor structure. The observed physical properties are Sr-deficiency related.

HL 13.32 Tue 13:30 P

Doping of β-Ga2O3 in a plasma assisted MBE using a SiO source. — •Andrea Ardenghi[1], Georg Hoffmann[1], Oliver Bierwagen[1], Piero Mazzolini[2], Andreas Falkenstein[3], and Manfred Martin[3] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Department of Mathematical, Physical and Computer Sciences, Parma University, Italy — [3]Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany

β-Ga2O3 is the most likely candidate for the next generation of power electronic devices but, achieve high quality doped sample is still challenging. To obtain n-doping for Ga2O3 the main candidate are Sn, Ge and Si. Between them Si-doped samples showed the higher mobility, making Si the most interesting doping source. Using a silicon source as dopant in PAMBE can be difficult since, due to the oxygen plasma, the source will be oxidized. In Kalarickal work[1], the flux from the Si source were highly influenced by the oxygen pressure, due to the formation and desorption of SiO. In order to avoid this problem a study similar to the one reported by Hoffmann et al[2]. was carried on a SiO source. Another advantage of the SiO source is the low cell temperature in comparison with Si and SiO2. From our results temperatures between 600-800°C should give us doping concentration in the range of 10e17 to 10e20 cm-3. The SiO source will be used for the growth of Si-doped Ga2O3 layers by PAMBE and the results will be reported.

[1]Kalarickal, Nidhin Kurian, et al. Applied Physics Letters 115.15 (2019).
[2]Hoffmann, Georg, et al. APL Materials 8.3 (2020).

HL 14: Materials and devices for quantum technology (joint session HL/TT)

Time: Wednesday 10:00–12:45 Location: H4

Invited Talk HL 14.1 Wed 10:00 H4

Quantum Interference of Identical Photons from Remote Quantum Dots — •Giang N. Nguyen[1], Liang Zhai[1], Clemens Spinnler[1], Julian Ritzmann[2], Matthias C. Löbl[1], Andreas D. Wieck[2], Arne Ludwig[2], Alisa Javadi[1], and Richard J. Warburton[1] — [1]Department of Physics, University of Basel, Switzerland — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr- Universität Bochum, Germany

Photonic quantum technology provides a viable route to quantum communication, quantum simulation, and quantum information processing. Scaling the complexity requires photonic architectures containing a large number of single photons, multiple photon-sources and photon-counters. Semiconductor quantum dots are bright and fast sources of coherent single-photons. For applications, a significant roadblock is the poor quantum coherence upon interfering single photons created by independent quantum dots.

Here, we present two-photon interference with near-unity visibility using photons from remote quantum dots. We show a Hong-Ou-Mandel visibility of 93% between photons from quantum dots separated in two cryostats. Exploiting the quantum interference, we demonstrate a photonic controlled-not circuit and a high-fidelity entanglement between photons of different origins. These results provide a long-awaited solution to the challenge of creating coherent single photons in a scalable way.

HL 14.2 Wed 10:30 H4

Natural heavy-hole flopping mode qubit in germanium — •Philipp M. Mutter and Guido Burkard — University of Konstanz, Konstanz, Germany

Flopping mode qubits in double quantum dots allow for coherent spin-photon hybridization and fast qubit gates when coupled to either an alternating external or a quantized cavity electric field. To achieve this, however, electronic systems rely on synthetic spin-orbit interaction by means of a magnetic field gradient as a coupling mechanism. Here we theoretically show that this challenging experimental setup can be avoided in heavy-hole systems in germanium by utilizing the sizable cubic Rashba spin-orbit interaction. We argue that the resulting natural flopping mode qubit possesses highly tunable spin coupling strengths that allow for qubit gate times in the nanosecond range when the system is designed to function in an optimal operation mode which we quantify.

HL 14.3 Wed 10:45 H4

On-chip Stark tuning of deterministically fabricated quantum dot waveguide systems — Peter Schnauber, Jan Grosse, Arsenty Kaganskiy, Maximilian Ott, Pavel Anikin, Ronny Schmidt, •Sven Rodt, and Stephan Reitzenstein — Institute of Solid State Physics, Technische Universit́at Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

On-chip quantum photonic circuits based on monolithic waveguides structures provide a compact and robust solution for setting up quantum logics and processors. The required structuring has already reached a very high level in different material systems but the monolithic integration of a number of single-photon emitters with identical emission wavelength is still a crux of the matter. We tackle this issue by deterministically integrating single InGaAs/GaAs quantum dots (QDs) into pin-doped GaAs/AlGaAs waveguides by in-situ electron-beam lithography (iEBL) [1]. This approach promises the integration of QDs with quasi-identical emission wavelength in combination with a fine-tuning mechanism via the quantum confined Stark effect. The wavelength accuracy in the pre-selection step of iEBL was about 0.2 nm which is nicely covered by tuning-range of about 0.4 nm when applying a bias voltage of up to 1.2 V. This paves the way for the fabrication of scalable quantum photonic circuits that rely on photon interference from multi emitters.

[1] P. Schnauber et al., APL Photonics 6, 050801 (2021)

HL 14.4 Wed 11:00 H4

Integration of NV-centers in nanodiamond in 1D photonic crystal cavities — •Jan Olthaus[1], Philip P.J. Schrinner[2], Carsten Schuck[2], and Doris E. Reiter[1] — [1]Institute of Solid State Theory, University of Münster, Germany — [2]Institute of Physics, Center for NanoTechnology - CeNTech and Center for Soft Nanoscience - SoN, University of Münster, Germany

The scalable integration of single-photon emitters with photonic circuits remains a major hurdle for the realisation of quantum information technologies. Efficient integration requires an interface, combining low losses and high coupling strength between these components. Here, we show results for the coupling of nitrogen vacancy centers in nanodiamond to 1D on-substrate photonic crystal cavities. In the first step, we use 3D FDTD simulations to optimise the geometry of a on-substrate photonic crystal cavity based on tantalum pentoxide waveguides. Based on the optimised structures, we then analyse the coupling conditions, if a nanodiamond cluster of varying sizes is placed in different positions around the cavity center. We find that for a deterministic air-mode design, optimal coupling is achieved when placing the nanodiamond at the air-waveguide interface within the central air-hole. Then, we validate our results experimentally by placing nanodiamonds close to the determined optimal position. We measure antibunching of the integrated photoluminescence signal proving single-photon emission. The scalability of our approach is demonstrated by simultaneous readout of the electron-spin of two neighbouring devices in a optical detected magnetic resonance measurement.

HL 14.5 Wed 11:15 H4

Optoelectronic sampling of ultrafast electric transients with single quantum dots — •Sebastian Krehs[1], Alex Widhalm[1,2], Dustin Siebert[2], Nand Lal Sharma[1,3], Timo Langer[1], Björn Jonas[1], Dirk Reuter[1], Andreas Thiede[2], Jens Förstner[2], and Artur Zrenner[1] — [1]Paderborn University, Physics Department, Warburger Straße 100, 33098 Paderborn, Germany — [2]Paderborn University, Electrical Engineering Department, Warburger Straße 100, 33098 Paderborn, Germany — [3]Institute for Integrative Nanosciences, Leibniz IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

The use of quantum systems as sensors promises high sensitivity, high precision and access to nanoscale applications. In our work, we have pioneered optoelectronic sampling of ultrafast electric signals with low capacitance single quantum dots photodiodes as sensor devices [1]. Our concept exploits the Stark effect to convert a time-dependent electric signal into a time-dependent shift of the QD transition energy. Time resolved measurements of the shift can be measured by resonant ps laser spectroscopy with spectrally tunable photocurrent detection. With our method we are able to sample the laser synchronous output pulse of an ultrafast CMOS circuit at cryogenic temperatures. We demonstrate an impressive sub-20 ps time resolution and an amplitude resolution in the mV-range. Theoretical calculations show that the accuracy of our method is not affected or limited by a moderate timing jitter or the optical pulse width.

[1] http://arxiv.org/abs/2106.00994

15 min. break.

HL 14.6 Wed 11:45 H4

Bright Electrically Controllable Quantum-Dot-Molecule Devices Fabricated by In Situ Electron-Beam Lithography — •Johannes Schall[1], Marielle Deconinck[1], Nikolai Bart[2], Matthias Florian[3], Martin von Helversen[1], Christian Dangel[4], Ronny Schmidt[1], Lucas Bremer[1], Frederik Bopp[4], Isabell Hüllen[3], Christopher Gies[3], Dirk Reuter[5], Andreas D. Wieck[2], Sven Rodt[1], Jonathan J. Finley[4], Frank Jahnke[3], Arne Ludwig[2], and Stephan Reitzenstein[1] — [1]IFKP, TU Berlin, Germany — [2]LS AFP, Ruhr-Universität Bochum, Germany — [3]ITP, University of Bremen, Germany — [4]WSI, TU München, Germany — [5]Department Physik, Universität Paderborn, Germany

In quantum repeater networks it is of central importance to temporarily store and retrieve quantum information. Concepts based on quantum dot molecules (QDMs) promise storage times in excess of 1 ms. To make use of QDM based quantum memories, efficient coupling to flying qubits needs to be realized while maintaining precise electrical control. We report on the development of electrically tunable single-QDM devices with strongly enhanced broadband photon extraction efficiency. The quantum devices are based on stacked quantum dots in a pin-diode structure underneath a deterministically defined circular Bragg grating using in situ electron beam lithography. We determine the photon extraction efficiency, demonstrate bias voltage dependent spectroscopy and measure excellent single-photon emission properties. The metrics make the developed QDM device an attractive building block for use in future photonic quantum networks.

HL 14.7 Wed 12:00 H4

Photon-number entanglement generated by sequential excitation of a two-level atom — Stephen C. Wein[1], Juan C. Loredo[2], Maria Maffei[3], Paul Hilaire[2], Abdou Harouri[2], Niccolo Somaschi[4], Aristide Lemaitre[2], Isabelle Sagnes[2], Loic Lanco[2,5], Olivier Krebs[2], Alexia Auffeves[3], Christoph Simon[1], Pascale Senellart[2], and •Carlos Anton-Solanas[2,6] — [1]Univ. of Calgary, Canada — [2]C2N-CNRS, France — [3]Inst. Neel-CNRS, France — [4]Quandela SAS, France — [5]Univ. Paris-Diderot, France — [6]Carl von Ossietzky Univ., Germany

During the spontaneous emission of light from an excited two-level atom, the atom briefly becomes entangled with the photonic field, producing the entangled state $\alpha|e,0\rangle + \beta|g,1\rangle$, where g and e are the ground and excited states of the atom, and 0 and 1 are the vacuum and single photon states [1].

We experimentally show that the spontaneous emission can be used to deliver on demand photon-number entanglement encoded in time [2]. By exciting a charged quantum dot (an artificial two-level atom) with two sequential π pulses, we generate a photon-number Bell state $\alpha|00\rangle + \beta|11\rangle$. We characterize the quantum properties of this state using time-resolved photon correlation measurements. We theoretically show that applying longer sequences of π pulses to a two-level atom can produce multipartite time-entangled states with properties linked to the Fibonacci sequence.

[1] V. Weisskopf, E. Wigner, Zeitschrift für Physik 63, 54 (1930). [2] S. C. Wein, et al., arXiv:2106.02049 (2021).

HL 14.8 Wed 12:15 H4

Evaluating Atomically Thin Quantum Emitters for Quantum Key Distribution — •Timm Gao[1], Martin v. Helversen[1], Carlos Anton-Solanas[2], Christian Schneider[2], and Tobias Heindel[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

Single photon sources are considered key building blocks for future quantum communication networks. In recent years, atomic monolayers of transition metal dichalcogenides (TMDCs) emerged as a promising material platform for the development of compact quantum light sources. In this work, we evaluate for the first time the performance of a single photon source based on a strain-engineered WSe_2 monolayer [1] for quantum key distribution (QKD). Employed in a QKD-testbed emulating the BB84 protocol, we analyze the single-photon purity in terms of $g^{(2)}(0)$ and secret key rates as well as quantum bit error rates to be expected in full implementations of QKD. Furthermore, we exploit routines for the performance optimization previously applied to quantum dot based single-photon sources [2]. Our work represents a major step towards the application of TMDC-based devices in quantum technologies.

[1] L. Tripathi et al., ACS Photonics 5, 1919-1926 (2018)
[2] T. Kupko et al., npj Quantum Inform. 6, 29 (2020)

HL 14.9 Wed 12:30 H4

Single Photon Emission from a topological cavity — •Jonathan Jurkat[1], Sebastian Klembt[1], Tristan H. Harder[1], Johannes Beierlein[1], Monika Emmerling[1], Tobias Huber[1], Christian Schneider[2], and Sven Höfling[1] — [1]Technische Physik, Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Physics, University of Oldenburg, 26129 Oldenburg, Germany

We measured the emission enhancement as well as single photon emission of a In(Ga)As quantum in spectral resonance with a topological defect mode. The emission was measured in a micro-photoluminescence setup under quasi resonant pumping with a pulsed laser. Spectral resonance was achieved by means of temperature tuning. The photonics lattice and topologically protected defect mode was implemented in an orbital Su-Schrieffer-Heeger chain. This zigzag chain of coupled micropillar devices was fabricated using molecular beam epitaxy in combination with an etch and overgrowth technique. These coupled resonators offer the exciting opportunity to combine a complex band structure formation with the emission of single localized quantum emitters.

HL 15: Focus Session: Tailored Nonlinear Photonics

The research field of nonlinear photonics is driven by the tailoring and control of nonlinear light-matter interactions and by the application of nonlinear concepts for advanced light management. Current research activities are driven by concepts from quantum optics, coherent optics, and solid-state physics. The progress in the field strongly benefits from advanced solid-state materials, nanostructures, and photonic structures, as well as from extremely intense and efficient ps and fs laser sources. The application of new concepts paves technically viable routes towards advanced nonlinear photonic devices, which are indispensable for the implementation of efficient frequency conversion, conditional photonic functionalities, and photonic quantum technologies.

Organizers: Artur Zrenner (Uni Paderborn), Thomas Zentgraf (Uni Paderborn), Manfred Bayer (TU Dortmund)

Time: Thursday 10:00–12:45 Location: H4

Invited Talk HL 15.1 Thu 10:00 H4

Quasi-instantaneous switch-off of deep-strong light-matter coupling — •Christoph Lange[1], Joshua Mornhinweg[2], Maike Halbhuber[2], Viola Zeller[2], Cristiano Ciuti[3], Dominique Bougeard[2], and Rupert Huber[2] — [1]Department of Physics, TU Dortmund University, 44227 Dortmund, Germany — [2]Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [3]Université de Paris, laboratoire Matériaux et Phénomènes Quantiques, CNRS, F-75013 Paris, France

Optical microresonators facilitate custom-tailored quantum states of matter by dressing electronic excitations with virtual cavity photons. Once the rate of energy exchange between light and matter modes exceeds the carrier frequency of light, "deep-strong coupling" emerges, which profoundly modifies the vacuum ground state and gives rise to novel phenomena including cavity-mediated superconductivity and other phase transitions. While the exploration of the equilibrium properties of deep-strong coupling has just started, yet more unusual effects are expected on subcycle scales. Here, we explore the dynamics that arises when deep-strong coupling is switched off abruptly. The experiments employ cyclotron resonances of two-dimensional electron gases coupled to light modes of custom-cut THz nanoresonators, which can be switched off by femtosecond photoexcitation. The polariton states are extinguished more than an order of magnitude faster than the polariton cycle duration, leading to sub-polariton-cycle oscillations as confirmed by a quantum model. Our experiments introduce time as a new control parameter for deep-strong light-matter coupling.

Invited Talk HL 15.2 Thu 10:30 H4

Lithium niobate nonlinear nanophotonics — •Frank Setzpfandt — Institute of Applied Physics, Abbe Center of Photonics, Friedrich Schiller University Jena

Lithium niobate is one of the most interesting optical materials, owing to its high transparency in a wide spectral range, high second-order nonlinearity, and the ability for quasi-phase matching. These enticing properties have been utilized many times in nonlinear optics, in particular for nonlinear parametric frequency conversion. However, lithium niobate is also a material that is challenging to structure on the nanoscale, which is only done regularly since a short time.

In this talk, I will discuss our recent progress in the implementation of nanoscale structures in lithium niobate and their application for the generation of classical and quantum light by parametric frequency conversion. In particular, I will focus on our realization of lithium niobate metasurfaces and their use in experimental demonstrations of second-harmonic and photon-pair generation.

Invited Talk HL 15.3 Thu 11:00 H4

Quadratic nanomaterials for integrated photonic devices — •Rachel Grange — ETH Zurich, Switzerland

Nonlinear and electro-optic devices are present in our daily life with many applications: light sources for microsurgery, green laser pointers, or modulators for telecommunication. Most of them use bulk materials such as glass fibres or high-quality crystals, hardly integrable or scalable due to low signal and difficult fabrication. Generating nonlinear or electro-optic effects from materials at the nanoscale can expand the applications to biology and optoelectronics. However, the efficiency of nanostructures is low due to their small volumes. Here I will show several strategies to enhance optical signals by engineering metal-oxides at the nanoscale with the goal of developing nonlinear and electro-optic photonics devices for a broad spectral range. We use metal-oxides such as barium titanate (BTO) and lithium niobate (LNO) as an alternative platform for nanoscale nonlinear photonics. BTO and LNO are non-centrosymmetric materials with high refractive index and high energy band gaps. We already demonstrated linear Mie resonances in BTO and LNO nanostructures, such as nanospheres or nanocubes. Recently, we focused on bottom-up assemblies of BTO nanoparticles to obtain electro-optic metasurfaces and quasi phase matching effects. We measured an electro-optic response in assembled nanostructures as strong as certain other perfect crystalline structure. The field of metal-oxides at the nanoscale has a huge potential of applications in nanophotonics, integrated optics and telecommunication.

15 min. break.

Invited Talk HL 15.4 Thu 11:45 H4

Topological plasmonics: Ultrafast vector movies of plasmonic skyrmions on the nanoscale — •Harald Giessen[1], Pascal Dreher[2], David Janoschka[2], Frank Meyer zu Heringdorf[2], Tim Davis[1,3], and Bettina Frank[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]CENIDE, University of Duisburg-Essen, Duisburg, Germany — [3]University of Melbourne, Melbourne, Australia

Plasmonic skyrmions are topological defects in the electromagnetic near-field on thin metal films, recently observed using scanning near-field optical microscopy. However, only one spatial component of the electric field was measured and one of the most intriguing features of skyrmions, namely their dynamics, was not assessed.

Two-photon photoemission electron microscopy was previously able to image the local plasmon fields with femtosecond time resolution. Still, the vector information about the local electric fields was missing. Here we introduce a new technique, time-resolved vector microscopy, that enables us to compose entire movies on a sub-femtosecond time scale and a 10 nm spatial scale of the electric field vectors of surface plasmon polaritons [1]. Specifically, we image complete time sequences of propagating surface plasmons that demonstrates their spin-momentum-locking as well as plasmonic skyrmions on atomically flat single crystalline gold films that have been patterned using gold ion beam lithography.

[1] T. Davis et al., Science 367, eaba6415 (2020).

Invited Talk HL 15.5 Thu 12:15 H4

Supercontinuum second-harmonic generation spectroscopy of 2D semiconductors — •Steffen Michaelis de Vasconcellos — Institute of Physics and Center for Nanotechnology, University of Münster, Germany

The emergence of 2D materials has opened up a wealth of new research topics for a wide variety of applications. The intensive research efforts on 2D materials were initially ignited by the groundbreaking work on graphene. Since then, the family of 2D crystals and their heterostructures has been expanding rapidly. The research has been focusing not only on their unique electrical properties, but also on their fascinating optical, mechanical, thermal, and chemical properties. Several of the materials are particularly suited for establishing nonlinear light-matter interactions. The strong optical nonlinearity, broadband and tunable optical absorption, and ultrafast response of these materials have been successfully employed in all-optical modulators, saturable absorbers used in passive mode locking and Q-switching, wavelength converters, and optical limiters.

A powerful tool to gain insight into nanoscale materials is the prototypical nonlinear process second-harmonic generation (SHG) due to its dependence on crystal symmetry and electronic structures. We developed a new method to perform ultra-broadband SHG spectroscopy, which provides access to the frequency-dependent nonlinear susceptibility $\chi^{(2)}$ of atomically thin materials and allows for the identification of the prominent excitonic resonances.

HL 16: Semiconductors: Optical, Transport and Ultrafast Properties

Time: Thursday 11:15–12:45 Location: H1

HL 16.1 Thu 11:15 H1

A Koopman's compliant exchange correlation potential for semiconductors — •Michael Lorke, Peter Deak, and Thomas Frauenheim — Universität Bremen

Density functional theory is the workhorse of theoretical materials investigations. Due to the shortcoming of (semi-)local exchange correlation potentials, hybrid functionals have been established for practical calculations to describe surfaces, molecular adsorption, and defects. These functionals operate by mixing between semi-local and Hartree-Fock exchange semi-emprically. However, their parameters have to be optimized for every material separately. To treat materials with a more physics driven approach and without the need of parameter optimization is possible with many-body approaches like GW, but at an immense increase in computational costs and without the access to total energies and hence geometry optimization. We propose a novel exchange correlation potential[1] for semiconductor materials, that is based on physical properties of the underlying microscopic screening. We demonstrate that it reprocuduces the low temperature band gap of several materials. Moreover, on the example of defects in semiconductors, it respects the required linearity condition of the total energy with the fractional occupation number, as expressed by the generalized Koopman's theorem. It is shown, that alloys can be treated with a common choice of the functional. We also show that this novel functional can be used as a kernel in linear response TDDFT to reproduce excitonic effects in optical spectra

[1] Physical Review B 102 (23), 235168 (2020)

HL 16.2 Thu 11:30 H1

Kerr and Faraday rotations of two-dimensional topological flat bands — Alireza Habibi, Johan Ekström, Thomas Schmidt, and •Eddwi Hasdeo — Department of Physics and Materials Science, University of Luxembourg, Luxembourg, Luxembourg

Flat-band systems are one of main subjects of research in condensed-matter physics especially after the discovery of a strongly correlated phase in twisted bilayer graphene. Flat bands can be observed directly via angle-resolved photoemission spectroscopy. However, due to the band flatness and the close proximity to the Fermi energy, a flat band is usually difficult to characterize. Here, we propose an alternative characterization method for topological flat bands using photon absorption. In topological bands, the anomalous Hall conductivity can rotate the incident light polarization, resulting in a rotated polarization of the transmitted light (Faraday effect) and the reflected light (Kerr effect). In this work, we employ a model featuring nearly flat bands, for which the bandwidth is much smaller than the band gap. We investigate the dynamical (ac) conductivities of the model in the presence of an external electric field. We contrast how flat bands and dispersive bands can be detected sensitively via Kerr and Faraday rotations. These results can serve as a simple characterization tool to determine the bandwidth or band flatness of topological materials.

HL 16.3 Thu 11:45 H1

Benchmarking the accuracy of screened range-separated hybrids for bulk properties of semiconductors — •Stefan A. Seidl, Bernhard Kretz, Christian Gehrmann, and David A. Egger — Technical University of Munich

A recently developed class of functionals, the so called screened range-separated hybrid (SRSH) functionals, only use one empirical parameter to fit the band gap to the accurately calculated band gap from the GW approach. After the tuning procedure of the range-separation parameter, SRSH functionals have been shown to provide accurate electronic-structure and optical properties of semiconductors [1]. This is an advantage over conventional semilocal and hybrid functionals in density functional theory (DFT), where it is known that they predict the structural properties well, but fail in the accurate description of electronic and optical properties. Here, we assess the accuracy of the SRSH functional to compute static and dynamic bulk properties (lattice constants, bulk moduli, atomization energies as well as phonon dispersion relations) of inorganic semiconductors [2]. We find that for these quantities, SRSH is similarly accurate as the two well-established functionals PBE and HSE. This demonstrates that the superior performance of SRSH for electronic-structure and optical calculations does not come at a cost of reduced accuracy for calculations of bulk properties.

[1] D. Wing et al, Phys. Rev. Materials 3, 064603 (2019)

[2] S. A. Seidl et al, Phys. Rev. Materials 5, 034602 (2021)

HL 16.4 Thu 12:00 H1

Hydrogen-Bonding Ability of the GaAs (001) Surface — •MARSEL KARMO and ERICH RUNGE — Weimarer Str.32

Thin films of direct-band gap III-V-semiconductors are widely used in optoelectronic devices such as lasers or solar cells. Their production via MOVPE/MOCVD involves hydrogen, which may or may not bind to the semiconductor surface. We study the hydrogen-bonding ability of the paradigmatic GaAs (001) surface via DFT using the VASP code. From the calculated thermodynamic potentials, we derive the phase diagram for the surface reconstructions as function of the availability of hydrogen and arsenic. Furthermore, we calculate the potential surface energy (PES) for a single adsorbed hydrogen which gives information about potential hydrogen bonding sites. For a wide range of the surface chemical potentials the (2x2)-surface with one hydrogen adsorbed to each As-dimer is energetically favored.

HL 16.5 Thu 12:15 H1

Size-dependent electrical characteristics of highly doped Germanium nanowires — •ahmad echresh, slawomir prucnal, yordan georgiev, and lars rebohle — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Germanium (Ge) is the most compatible material with silicon (Si)-based complementary metal-oxide-semiconductor processes. Ge has a higher electron and hole mobility compared to Si, leading to improved device performance. Moreover, Ge nanowires (GeNWs) are promising nanostructures for future nano- and optoelectronics due to their unique properties. In this work, ion beam implantation and flash lamp annealing (FLA) were used to dope phosphorous into the top Ge layer of Ge-on-insulator (GeOI) substrates, achieving a highly n-type doped semiconductor. Raman spectroscopy and Rutherford backscattering spectrometry were performed to characterize the crystallinity of the Ge layers after ion beam implantation and FLA. Subsequently, doped GeNWs were fabricated using electron beam lithography and inductively coupled plasma reactive ion etching. Electrical characterization of the GeNWs was conducted using an innovative Hall bar configuration. The effect of nanowire width on transport parameters such as resistivity and carrier mobility was investigated. Moreover, a nickel germanide layer was made using Ni deposition, followed by FLA to create ohmic contacts on n-type GeNWs.

HL 16.6 Thu 12:30 H1

Extreme ultraviolet laser source for time resolved experiments including a terahertz driver laser — Torsten Golz, Gregor Indorf, Mihail Petev, Jan-Heye Buss, Michael Schulz, and •Robert Riedel — Class 5 Photonics GmbH, Luruper Hauptstraße 1, 22547 Hamburg

The investigation of ultrafast dynamics in condensed matter and interfaces requires high repetition rates and multiple wavelength laser sources, together with femtosecond resolution. To meet these needs, we have therefore designed an extreme-ultraviolet laser source with output within the range of 21.7 to 50 eV (total flux of 3×10^{12} photons/sec), together with a tunable output from 750 - 950 nm with 10 μJ pulse energy and a pulse duration of <40 fs, as well as, a third output for terahertz generation (2 mJ, <600 fs at 1030 nm). All three outputs are optically synchronized and can be used, for example, in time- and angle-resolved photoemission spectroscopy (trARPES) experiments.

HL 17: Focus Session: Topological Phenomena in Synthetic Matter (joint session DS/HL)

Topological insulators are a striking example of materials in which topological invariants are manifested in robustness against perturbations. Topology has emerged as an abstract, yet surprisingly powerful, new paradigm for controlling the flow of an excitation, e.g. the flow of electrons or light. This interdisciplinary Focus Session aims at discussing the latest experimental and theoretical results in the fast developing field of topological phenomena in synthetic matter. The recent merging of topology and cold atoms, photonics, mechanics and many more fields promises a considerable impact on these disciplines. We bring together leading theoretical and experimental experts from the fields of topological phenomena in synthetic matter to discuss recent progress and interdisciplinary synergy emerging at the interface of these fields. Furthermore, we give an overview to young scientists of exciting possibilities of interdisciplinary research in these fields with the special focus on the practical applications of fundamental science.

Organizer: Sebastian Klembt (Julius-Maximilians-Universität Würzburg)

Time: Thursday 13:30–16:15 Location: H1

See DS 6 for details of this session.

HL 18: Quantum Dots and Wires (joint session HL/TT)

Time: Thursday 13:30–16:30 Location: H4

Invited Talk HL 18.1 Thu 13:30 H4

Telecom wavelength quantum dot-based single-photon sources for quantum technologies — •Anna Musial — Department of Experimental Physics, Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology, Wybrzeze Wyspianskiego 27, 50-370 Wroclaw, Poland

Important building blocks for quantum technology applications are non-classical light sources, in particular those emitting single photons on demand. Among pursued approaches to realize them semiconductor epitaxial quantum dots (QDs) stand out in terms of single-photon purity, compatibility with semiconductor technology including deterministic fabrication of photonic structures, integration into photonic circuits and fiber infrastructure as well as unprecedented possibilities of engineering their electronic structure and optical properties. The current status, recent developments and future prospects of the single-photon sources based on single GaAs-based and InP-based epitaxial QDs emitting in the telecommunication spectral range will be given. Reviewed aspects include thermal stability of emission, energies for efficient quasi-resonant excitation, optimization of photon extraction efficiency, approaches to maximize coupling to a single mode telecom fiber, single-photon emission purity as well as tests of a fully operational plug&play fiber-based single-photon source.

HL 18.2 Thu 14:00 H4

Electric-field induced tuning of electronic correlation in weakly confining quantum dots — Huiying Huang[1], Diana Csontosová[2,3], Santanu Manna[1], Yongheng Huo[4], Rinaldo Trotta[5], Armando Rastelli[1], and •Petr Klenovský[2,3] — [1]Johannes Kepler University Linz, Linz, Austria — [2]Masaryk University, Brno, Czech Republic — [3]Czech Metrology Institute, Brno, Czech Republic — [4]University of Science and Technology of China, Hefei, Anhui, China — [5]Sapienza University of Rome, Rome, Italy

We conduct a combined experimental and theoretical study of the quantum confined Stark effect in GaAs/AlGaAs quantum dots obtained with the local droplet etching method. In the experiment, we probe the permanent electric dipole and polarizability of neutral and positively charged excitons weakly confined in GaAs quantum dots by measuring their light emission under the influence of a variable electric field applied along the growth direction. Calculations based on the configuration-interaction method show excellent quantitative agreement with the experiment and allow us to elucidate the role of Coulomb interactions among the confined particles and – even more importantly – of electronic correlation effects on the Stark shifts. Moreover, we show how the electric field alters properties such as built-in dipole, binding energy, and heavy-light hole mixing of multiparticle complexes in weakly confining systems, underlining the deficiencies of commonly used models for the quantum confined Stark effect.

HL 18.3 Thu 14:15 H4

Towards deterministic generation of time-bin entangled photons from GaAs quantum dots — •Florian Kappe[1], Yusuf Karli[1], Vikas Remesh[1], Santanu Manna[2], Armando Rastelli[2], and Gregor Weihs[1] — [1]Institute for Experimental Physics, University of Innsbruck, Austria — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University of Linz, Austria

Semiconductor quantum dots are bright, on-demand single photon sources to realise quantum communication devices. We present our progress towards the deterministic generation of time-bin entangled photon states utilizing single GaAs/AlGaAs quantum dota as photon sources. Our scheme relies on the use of highly chirped picosecond laser pulses and an optically dark exciton state acting as a metastable state. The fidelity of the state preparation is supported by numerical simulations on the quantum dot dynamics. To demonstrate the effect of chirped excitation pulses on the quantum dot, we present an adiabatic-rapid-passage acting on a two-photon resonant transition to the neutral biexciton state. This scheme allows the implementation of a deterministic two-photon source insensitive to power fluctuations of the pump laser.

HL 18.4 Thu 14:30 H4

Quantum Efficiency and Oscillator Strength of InGaAs Quantum Dots for Single-Photon Sources emitting in the Telecommunication O-Band — •Jan Grosse[1], Paweł Mrowiński[1,2], Nicole Srocka[1], and Stephan Reitzenstein[1] — [1]Technische Universität Berlin, Institute for Solid State Physics, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Laboratory for Optical Spectroscopy of Nanostructures, Wrocław University of Technology, Wybrzeze Wyspiańskiego 27, Wrocław, Poland

We demonstrate experimental results based on time-resolved photoluminescence spectroscopy to determine the oscillator strength and the internal quantum efficiency (IQE) of InGaAs quantum dots (QDs) capped by a strain-reducing layer [1] which have been used in single-photon sources (SPS) emitting in the telecom O-Band [2]. The oscillator strength and IQE are evaluated by determining the radiative and non-radiative decay rate under variation of the optical density of states at the position of the QD [3]. We measure a QD sample with different thicknesses of the capping layer realized by a controlled wet-chemical etching process. From numeric modelling the radiative and nonradiative decay rates dependence on the capping layer thickness, we determine an oscillator strength of 24.6 * 3.2 and a high IQE of about (85 * 10)% for the long-wavelength InGaAs QDs [4].

[1] J. Bloch et al., Appl. Phys. Lett. 75, 2199 (1999).
[2] A. Musiał et al., Adv. Quantum Technol. 3, 2000018 (2020).
[3] J. Johansen et al., Phys. Rev. B 77, 073303 (2008).
[4] J. Große et al, arXiv:2106.05351 (2021).

HL 18.5 Thu 14:45 H4

Resonance fluorescence of single In(Ga)As quantum dots emitting in the telecom C-band — •Julius Fischer, Cornelius Nawrath, Hüseyin Vural, Richard Schaber, Simone Luca Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Quantum dots represent a rapidly developing platform as sources of non-classical states of light for tackling quantum communication and computation tasks. Especially quantum dots emitting in the telecom C-band (1530nm-1565nm) are promising candidates due to the low absorption losses in the existent telecommunication fiber network.

In this study, we investigate In(Ga)As quantum dots emitting in the telecom C-band under resonant excitation to examine coherence properties and to investigate their single-photon purity as well as photon indistinguishability. Under strong resonant cw excitation, high-resolution fluorescence spectra, namely the Mollow triplet, of a single quantum dot are investigated. These spectra, in combination with a comprehensive fitting procedure, are used as a method to quantitatively attribute decoherence processes and thus presenting an excellent method to provide important insights for future sample optimizations. In addition, under pulsed resonant excitation, the capability of emitting highly pure single photons ($g^{(2)}(0) = 0.023 \pm 0.019$) with a non-postselected indistinguishability of subsequently emitted photons of $V_{\text{TPI}} = 0.144 \pm 0.015$ is demonstrated.

15 min. break

HL 18.6 Thu 15:15 H4

Evaluating a Plug&Play Telecom-Wavelength Single-Photon Source for Quantum Key Distribution — Timm Gao[1], •Lucas Rickert[1], Felix Urban[1], Jan Grosse[1], Nicole Srocka[1], Sven Rodt[1], Anna Musiał[2], Kinga Zołnacz[3], Paweł Mergo[4], Kamil Dybka[5], Wacław Urbańczyk[3], Grzegorz Sek[2], Sven Burger[6], Stephan Reitzenstein[1], and Tobias Heindel[1] — [1]Institute of Solid State Physics, Technical University Berlin, 10623 Berlin, Germany — [2]Department of Experimental Physics, Wrocław University of Science and Technology, 50-370 Wroclaw, Poland — [3]Department of Optics and Photonics, Wroclaw University of Science and Technology, 50-370 Wrocław, Poland — [4]Institute of Chemical Sciences, Maria Curie Sklodowska University, 20-031 Lublin, Poland — [5]Fibrain Sp. z o.o., 36-062 Zaczernie, Poland — [6]Zuse Institute Berlin, 14195 Berlin, Germany

We report on quantum key distribution (QKD) tests using a 19-inch benchtop single-photon source at 1321 nm based on a fiber-pigtailed quantum dot (QD) integrated into a Stirling cryocooler. Emulating the polarization-encoded BB84 protocol, we achieve an antibunching of $g^{(2)}(0) = 0.10 \pm 0.01$, a raw key rate of up to 4.72 ± 0.13 kHz, and a maximum tolerable loss of 23.19 dB exploiting optimized temporal filters in the asymptotic limit [1]. Our study represents an important step forward in the development of fiber-based quantum-secured communication networks exploiting sub-Poissonian quantum light sources. [1] T. Kupko et al., arXiv.2105.03473 (2021)

HL 18.7 Thu 15:30 H4

Emission and absorption of a radiative Auger transition — •Clemens Spinnler[1], Liang Zhai[1], Giang N. Nguyen[1], Julian Ritzmann[2], Andreas D. Wieck[2], Arne Ludwig[2], Alisa Javadi[1], Doris E. Reiter[4], Paweł Machnikowski[3], Richard J. Warburton[1], and Matthias C. Löbl[1] — [1]Department of Physics, University of Basel, Switzerland — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany — [3]Department of Theoretical Physics, Wrocław University of Science and Technology, Poland — [4]Institut für Festkörpertheorie, Universität Münster, Germany

In multi-electron systems, such as charged semiconductor quantum dots (QD), several electron-hole recombination processes can take place. Besides the well-known resonance fluorescence, Coulomb interactions can lead to radiative Auger processes (shake-up) where part of the recombination energy is transferred to another electron. This Auger electron is left in an excited state and the emitted photon is correspondingly red-shifted.

We report the observation of emission and absorption of a radiative Auger transition from a negatively charged QD. By applying quantum optics techniques to the Auger emission we get insight into single-electron dynamics. We show photon absorption via the radiative Auger transition by driving the QD in a Λ-configuration: while monitoring the resonance fluorescence a second laser is tuned in resonance with the radiative Auger transition. A fluorescence reduction of up to 70% is observed - proving optical driving of the radiative Auger transition.

HL 18.8 Thu 15:45 H4

Interfacing colloidal quantum dots with nanophotonic circuits for integrated single photon sources — •Tobias Spiekermann, Alexander Eich, Helge Gehring, Lisa Sommer, Julian Bankwitz, Wolfram Pernice, and Carsten Schuck — Institute of Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Single photon sources are a key element for the realization of quantum communication, sensing and computing. While there exist several promising quantum emitter candidate systems, integration with nanophotonic networks in large numbers for wafer-scale quantum technologies has remained elusive. Here we show a lithographic technique that allows for interfacing nanophotonic waveguides with individual Colloidal Quantum Dots (CQD) from a solution applied across an entire chip [1]. We record the second order autocorrelation function to confirm single photon emission from CQDs into tantalum pentoxide (Ta_2O_5) waveguides that feature low intrinsic material fluorescence. Moreover, we demonstrate how iterative processing can be used to increase the yield of single CQDs with our technique. We further improve the photostability of CQDs positioned on a chip by subsequent site-passivation via atomic layer deposition of alumina (Al_2O_3). Our work paves the way for scalable integration of colloidal quantum dot single photon sources with photonic integrated circuits.

[1] Cherie R. Kagan, et al., Colloidal Quantum Dots as Platforms for Quantum Information Science, Chemical Reviews 121 (5), 3186-3233 (2021)

HL 18.9 Thu 16:00 H4

Electrical Characterisation of Te-doped InAs Nanowires grown by VS Molecular Beam Epitaxy — •Anton Faustmann, Pujitha Perla, Detlev Grützmacher, Mihail Lepsa und Thomas Schäpers — Peter-Grünberg-Institut PGI-9, FZ-Jülich, Jülich, Deutschland

InAs features high electron mobility and absence of a Schottky barrier at metal interfaces enabling ohmic contacts. In combination with large g-factor and high Rashba spin-orbit coupling this makes InAs nanowires a promising candidate for research of quantum effects. InAs nanowires with Te doping grown by molecular beam epitaxy were investigated in terms of their electrical transport properties at both room and cryogenic temperatures. The nanowires were grown in a catalyst-free vapour-solid process without using Au droplets. In contrast to Si, which shows amphoteric behaviour, Te acts as n-type dopant. It furthermore offers the possibility of an increased overall doping level. The Te doping concentration was found to affect both the morphology of the nanowires as well as electrical properties. The shape of the nanowires depends on Te uptake. Their intrinsic as well as contact resistances decrease considerably at increased doping level. Field-effect measurements using a global back gate show effect on the conductance, depending on the doping concentration. For higher doping no complete pinch-off was observable with conductance saturating at high negative gate voltages. Resistances were found to be only slightly increased at cryogenic temperatures.

HL 18.10 Thu 16:15 H4

Emission Time Statistics of a driven Single-Electron Transistor — •Johannes C. Bayer[1], Fredrik Brange[2], Adrian Schmidt[1], Timo Wagner[1], Christian Flindt[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Department of Applied Physics, Aalto University, Finland

Precisely controllable single particle sources are an essential part of different quantum technologies operating at fixed clock cycles. A high level of accuracy in the time domain thereby requires detailed understanding of the interplay between an external drive and the response of the single particle source [1,2]. We here present the influence of periodically modulated tunneling rates on the emission time statistics of electrons emitted from a single-electron transistor (SET) [3]. A highly sensitive charge detector allows to detect tunneling events in real-time. By ramping up the driving frequency from slower to faster than the electron tunneling rate, the response of the SET undergoes a transition from adiabatic to non-adiabatic dynamics. This transition is accompanied by significant changes in the emission time statistics, which can be visualized in the waiting time distribution and is well described by our detailed theory.

[1] T. Wagner, et. al., Nat. Phys. 15, 330-334 (2019).
[2] R. Hussein, et. al., Phys. Rev. Lett. 125, 206801 (2020).
[3] F. Brange, et. al., Sci. Adv. 7, eabe0793 (2021).

HL 19: Poster Session IV

Topics:
- Semiconductor lasers
- Semiconductors for quantum technologies
- Ultra-fast phenomena
- Oxide semiconductors
- Tailored Nonlinear Photonics

Time: Thursday 13:30–16:30 Location: P

HL 19.1 Thu 13:30 P

Bandgap and Secondary Phase Analysis of (A)CIGS Solar Cell Absorber and Buffer Layers Using Electroreflectance Spectroscopy — •Michael Dao[1], Jonas Grutke[1], Wolfram Witte[2], Dimitrios Hariskos[2], Heinz Kalt[1], and Michael Hetterich[1,3] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70563 Stuttgart, Germany — [3]Light Technology Institute, KIT, 76131 Karlsruhe, Germany

Thin-film solar cells based on Cu(In,Ga)Se_2 (CIGS) absorbers have established themselves as highly efficient photovoltaic devices. To further optimize their properties, the incorporation of silver (Ag) into the absorber layer (ACIGS) is currently investigated by many groups. In this contribution, the effect of Ag on the absorber bandgap energy as well as the corresponding inhomogeneous broadening is investigated by electroreflectance spectroscopy (ER) which allows a destruction-free analysis of full device structures. Additionally, angle-resolved ER (ARER) is applied to study the impact of Ag on the formation of secondary phases as well as possible interdiffusion effects at the absorber-buffer interface. Using this technique, the bandgap energies of both the buffer layer as well as secondary phases can be determined despite interference effects in the multi-layered device structure and the small thickness < 60 nm of the buffer layer.

HL 19.2 Thu 13:30 P

Electroreflectance as a Powerful Tool to Investigate Internal Device Parameters in CIGS Solar Cells — •Lennart Meyer[1], Jonas Grutke[1], Wolfram Witte[2], Dimitrios Hariskos[2], Heinz Kalt[1], and Michael Hetterich[1,3] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70563 Stuttgart, Germany — [3]Light Technology Institute, KIT, 76131 Karlsruhe, Germany

Recently, our group has developed and successfully utilized various advanced electroreflectance (ER) spectroscopy techniques for the destruction-free analysis of Cu(In,Ga)Se_2 (CIGS) solar cell absorber and buffer layers in full devices, including investigations into interdiffusion phenomena and secondary phase formation. In this contribution, we present first steps towards a novel ER approach that shall enable the determination of internal device parameters such as the built-in potential drop at the absorber-buffer interface, the carrier concentration in the absorber, or the width of the space charge region. To this end, the variation of the CIGS bandgap resonance amplitude in the ER spectra is analysed as a function of the simultaneously applied AC and DC reverse biases, respectively. The cell parameters can then be obtained via theoretical modelling of the experimental data. First examples and applications of this method will be discussed.

HL 19.3 Thu 13:30 P

Atomic and electronic structure of the GaP/Si(001) heterointerface studied by HAXPES — •Agnieszka Paszuk[1], Oleksandr Romanyuk[2], Igor Bartoš[2], Regan G. Wilks[3], Manali Nandy[1], Jakob Bombsch[3], Claudia Hartmann[3], Raül Garcia-Diez[3], Shigenori Ueda[4], Ivan Gordeev[2], Jana Houdkova[2], Peter Kleinschmidt[1], Marcus Bär[3], Peter Jiříček[2], and Thomas Hannappel[1] — [1]Institute of Physics, University of Technology, Ilmenau, German — [2]Institute of Physics, Prague, Czech Republic — [3]Department Interface Design, Helmholtz-Zentrum Berlin, Germany — [4]SPring-8, National Institute for Materials Science, Japan

For highly efficient III-V-on-Si optoelectronic devices it is crucial to prepare defect-free heterointerfaces with defined electronic properties. Commonly a thin, pseudomorphic GaP epilayer is deposited on Si prior to further III-V buffer growth, due to its close lattice matching to Si. Here, the atomic and electronic structures of buried GaP/Si(001) heterointerfaces prepared by MOCVD were investigated by hard X-ray photoelectron spectroscopy combined with theoretical modelling. 4 - 50 nm thick GaP films with a different density of antiphase domain boundaries were grown on Si(001) H-terminated surfaces, as controlled by optical *in situ* spectroscopy. We found that the core-level positions and width change with GaP film thickness and Si substrate type. These observations were related to charge replacement and band bending effects at the interface. In consequence, an inter-diffused layer interface structure model based on the formation of Si-P bonds at the heterointerface and P-doping of the Si substrate is suggested.

HL 19.4 Thu 13:30 P

Electric-field-driven evolution of anti-Frenkel defects in ErMnO3 — •Jiali He[1], Ursula Ludacka[1], Donald Evans[1], Theodor Holstad[1], Erik Roede[1], Kasper Hunnestad[1], Konstantin Shapovalov[2], Zewu Yan[3,4], Edith Bourret[4], Antonius Van Helvoort[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology(NTNU), Trondheim, Norway. — [2]Institute of Materials Science of Barcelona, Bellaterra, Spain — [3]ETH Zurich, Zürich, Switzerland. — [4]Lawrence Berkeley National Laboratory, Berkeley, USA.

The electronic properties of complex oxides can readily be tuned via oxygen defects, offering intriguing opportunities for precisely controlling the conductivity of materials. Recently, anti-Frenkel defects moved into focus for minimally invasive property engineering. Anti-Frenkel defects are charge-neutral interstitial-vacancy pairs, and their injection makes it possible to adjust the transport behavior in oxides without causing long-range ionic migration or changes in stoichiometry. Here, we present a detailed analysis of the electric-field-driven formation and response of anti-Frenkel defects in hexagonal ErMnO3. The defects are generated via an electrically biased nano-sized probe tip and imaged by cAFM and SEM. We investigate the spatio-temporal evolution of the written defects for different drive voltages, complemented by numerical simulations, which reveal a non-trivial evolution, allowing to separate the initially paired vacancies and interstitials. The results provide new insight into the local electronic properties of ErMnO3 and the nanoscale defect physics of functional oxides in in general.

HL 19.5 Thu 13:30 P

Modification of epitaxial La0.6Sr0.3CoO3-δ thin films by ion irradiation — •Yunxia Zhou[1,2], Lei Cao[1], Andreas Herklotz[3], Diana Rata[3], Suqin He[4], Felix Gunkel[4], Ulrich Kentsch[1], Manfred Helm[1], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum-Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany — [2]University of Electronic Science and Technology of China, State Key Laboratory of Electronic Thin Films and Integrated Device, Xiyuan Ave 2006, 611731 Chengdu, China — [3]Institute of Physics, Martin Luther University Halle-Wittenberg, Halle, 06120, Germany — [4]Peter Grünberg Institut (PGI-7), JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, 52425, Germany

Perovskite oxides exhibits rich physics related to ionic defects. In particular, defect concentration and distribution alter the lattice parameters and affect the competitive interplay between strongly correlated electrons, enabling numerous applications, including sensors, catalysts, and memristive devices. In this work, helium-implantation is demonstrated as a fast, low temperature tool to modulate the vacancy profiles in epitaxial La0.6Sr0.4CoO3-δ thin films. Not only a significant lattice expansion solely along the out-of-plane direction is observed, but also a distinct change in physical properties is evidenced. By proper tuning of the implantation parameters, an enhanced resistivity up to several orders of magnitude is achieved at room temperature. These results offer a new playground for the optimization of oxide-based spintronic and electronic devices.

HL 19.6 Thu 13:30 P

Electric-field-driven evolution of anti-Frenkel defects in ErMnO3 — •Jiali He[1], Ursula Ludacka[1], Donald Evans[1], Theodor Holstad[1], Erik Roede[1], Kasper Hunnestad[1], Konstantin Shapovalov[2], Zewu Yan[3,4], Edith Bourret[4], Antonius Van Helvoort[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology(NTNU), Trondheim, Norway. — [2]Institute of Materials Science of Barcelona, Bellaterra, Spain — [3]ETH Zurich, Zürich, Switzerland. — [4]Lawrence Berkeley National Laboratory, Berkeley, USA.

The electronic properties of complex oxides can readily be tuned via oxygen defects, offering intriguing opportunities for precisely controlling the conductivity of the materials. Recently, anti-Frenkel defects moved into focus for minimally invasive property engineering. Anti-Frenkel defects are charge-neutral interstitial-vacancy pairs, and their injection makes it possible to adjust the transport behavior in oxides without causing long-range ionic migration or changes in stoichiometry. Here, we present a detailed analysis of the electric-field-driven formation and response of anti-Frenkel defects in hexagonal ErMnO3. The defects are generated via an electrically biased nano-sized probe tip and imaged by cAFM and SEM. We investigate the spatio-temporal evolution of the written defects for different drive voltages, complemented by numerical simulations, which reveal a non-trivial evolution, allowing to separate the initially paired vacancies and interstitials. The results provide new insight into the local electronic properties of ErMnO3 and the nanoscale defect physics of functional oxides in general.

HL 19.7 Thu 13:30 P

Ammonia and Acetone Gas Sensor Based on Nanocomposites of Indium Oxide and Multiwalled Carbon Nanotubes — •Nipin Kohli — Technical University Berlin

This work reports the effect of introducing carbon nanotubes in indium oxide on structural, morphological, optical and ammonia sensing properties. Various characterization techniques such as X-ray diffraction, transmission electron microscopy, BET, Fourier transform infra-red, UV-visible and Raman spectroscopy were employed to understand the structural, morphological and optical properties of the synthesized samples. The gas sensors were fabricated out of the synthesized samples to test their response towards ammonia and acetone at different operating temperatures and at different concentrations. The nanocomposite exhibits enhanced sensing performance and is capable of detecting concentration of acetone and ammonia as low as 10 ppm at optimum operable temperature of 300°C and 200°C, respectively.

HL 19.8 Thu 13:30 P

Förster-Type Energy Transfer Between Molecules and Atomically Thin Semiconductors — •Manuel Katzer[1], Malte Selig[1], Sviatoslav Kovalchuk[2], Kyrylo Greben[2], Kirill Bolotin[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Department of Physics, Quantum Nanoelectronics of 2D Materials, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Interfaces of dye molecules and two-dimensional transition metal dichalcogenides (TMDCs) are promising candidates for optoelectronic applications since they combine the large molecular optical amplitudes and spectral range with high carrier mobilities in the semiconductor [1]. In such interfaces, Förster energy transfer is a key mechanism due to the large dipole moments, and has many intriguing technical applications [2].

In a joint theory-experiment study, we report microscopic calculations of the Förster induced transition rate from dye molecules to a TMDC layer and provide the corresponding optical signatures, with excellent agreement to the experimental data. The theoretic approach is based on microscopic Bloch equations which are solved self-consistently together with Maxwells equations [3], incorporating the sample geometry within the Rytova-Keldysh framework.

[1] Jariwala et al. Nat. Mater. **16**, 170 (2017)
[2] Dagher et al. Nat. Nanotech. **13**, 925-932 (2018)
[3] Selig et al. Phys. Rev. B **99**, 035420 (2019)

HL 19.9 Thu 13:30 P

Atomic Structure of Antiphase Domains on GaP/Si(100):As — Dominik Bratek[1], •Peter Kleinschmidt[1], Manali Nandy[1], Oliver Supplie[1,2], Agnieszka Paszuk[1], and Thomas Hannappel[1] — [1]Institut für Physik, Grundlagen von Energiematerialien, Technische Universität Ilmenau, 98693 Ilmenau, Deutschland — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Deutschland

We have investigated the atomic structure of antiphase domains on GaP(100) on As-terminated Si(100) by scanning tunneling microscopy (STM). Thin GaP layers of 5 nm and 10 nm thickness were deposited on predominately double atomic layer stepped, As-terminated Si(100)-substrates by metalorganic vapor phase epitaxy. Small residuals of the intermediate steps on the substrate lead to the formation of minority antiphase domains in the epitaxial GaP. We show that these antiphase domains extend parallel to the step edges of the substrate. In numerous locations, small residual antiphase domains are embedded in trenches parallel to these step edges, and in other locations only the trenches remain, suggesting that these trenches are residuals of overgrown antiphase domains. Our STM measurements reveal the atomic structure of the antiphase boundaries, which varies substantially: some of these boundaries are just characterized by a half bi-layer step, whereas deep trenches are also frequently observed.

HL 19.10 Thu 13:30 P

Ultrafast energy transfer triggers ionization energy offset dependent quantum yields in low-bandgap NFA solar cells — •Julien F. Gorenflot[1], Safakath Karuthedath[1], Yuliar Firdaus[1], Catherine S. De Castro[1], George Harrison[1], Anastasia Markina[2], Neha Chaturvedi[1], Jafar Khan[1], Ahmed H. Balawi[1], Sri H. K. Paleti[1], Thomas Anthopoulos[1], Derya Baran[1], Denis Andrienko[2], and Frédéric Laquai[1] — [1]KAUST Solar Center (KSC), Material Science and Engineering program (MSE), Physical Science and Engineering division (PSE), King Abdullah University of Science and Technology, Thuwal, Saudi Arabia. — [2]Max Planck Institute for Polymer Research, Mainz, Germany.

Organic solar cells associate an electron donor and an electron acceptor to drive exciton-to-charge conversion where the strong EA acceptor attracts electrons from donor excitons, and the low IE donor attracts holes from acceptor excitons. Recent studies however, claim efficient photocurrent generation in recent non-fullerene acceptor (NFA) based systems with close-to-zero IE or EA offsets. Here, we confirm that sizeable IE offsets are required to drive hole transfer from acceptor exciton. Further charge separation from the interface is however barrierless. Due to fast, Förster Resonant Energy Transfer to the low bandgap acceptor, charge transfer always occurs from the acceptor, making the EA offset unimportant. We model the IE offset dependence of hole transfer and find that two physical parameters are sufficient to describe it. Our model also explains barrierless charge separation and the high charge transfer states energies reported in NFA-based systems.

HL 19.11 Thu 13:30 P

Electronic properties of MoS_2 monolayer doped by donor, acceptor, and aromatic molecules — •Juan Pablo Guerrero[1,2], Ana M. Valencia[2,3], Jannis Krumland[2], and Caterina Cocchi[2,3] — [1]Department of Physics, Freie Universität Berlin (Germany) — [2]Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin (Germany) — [3]Institute of Physics, Carl von Ossietzky Universität Oldenburg (Germany)

The electronic properties of hybrid inorganic-organic interfaces are critically influenced by the level alignment across the heterostructure and by possible hybridization effects that occur therein. In turn, these properties are determined by the nature of the molecular dopants and by their arrangements. In the framework of (hybrid) density functional theory, we investigate the electronic structure of a single sheet of MoS_2 covered by monolayers of planar molecules such as pyrene, tetrathiafulvalene, and bithiophene, which are known to act as donors, as well as with the acceptors 7,7,8,8-tetracyanoquinodimethane and its tetrafluorinated counterpart. Our results show that all considered heterostructures exhibit a type II level alignment with negligible charge transfer at the interface. However, in the electronic structure of the systems, the signatures of electron or hole doping to the MoS_2 can be identified.

HL 19.12 Thu 13:30 P

Coulomb Blockade at room temperature of self-assembled GaN quantum dot ensembles, measured via Capacitance-Voltage spectroscopy — •Carlo Alberto Sgroi[1], Julien Brault[2], Jean-Yves Duboz[2], Philippe Vennéguès[2], Sébastien Chenot[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]CNRS - CRHEA, Rue Bernard Grégory, 06560 Valbonne, France

We present capacitance voltage (C(V)) measurements at room temperature of charge-tunable self-assembled wurtzite GaN quantum dots (QDs) in an $Al_xGa_{1-x}N$ matrix grown by MBE. GaN and its alloys have excellent properties such as their thermal stability, high thermal conductivity and wide bandgap energies which make them an ideal candidate for next-generation GaN-based power devices at elevated temperatures. Single-photon sources operating at up to 350 K are already possible1. Due to polarization and strain effects in wurtzite $GaN/Al_xGa_{1-x}N$ heterostructure layers, the band structure is different for the cross section with the GaN QDs and the GaN Wetting Layer (WL) on which the QDs are formed. Large electric fields and defect-assisted electron hopping promote charge transfer through the WL. Performing C(V) spectroscopy at 300 K on an AlGaN-Schottky diode structure with embedded GaN QDs, single-electron discharging in the C(V) spectrum and a Coulomb blockade energy of about 70 meV are measured.

[1] Holmes, M. J., et al. ACS Photonics **3**, 543-546 (2016).

HL 19.13 Thu 13:30 P

Exploration of the electrochemical Interface of InP under applied potentials with Reflection Anisotropy Spectroscopy — •Margot Guidat, Mario Löw, Vibhav Yadav, Jongmin Kim, and Matthias M. May — Universität Ulm, Institute of Theoretical Chemistry, Ulm, Germany

A possible way to achieve a low-carbon energy leads through hydrogen, which can be produced via photoelectrochemical water splitting, in which III-V semiconductors play an important role [1]. However, surface corrosion results in limited performance of photoelectrochemical solar cells.

Some studies have reported that surface functionalization is a way to protect the surface, achieved by etching processes. However, this faces fundamental challenges, especially in electrochemical environments [2]. In this work, we investigate photoelectrochemical etching of Indium Phosphide (100) in contact with hydrochloric acid controlled by Reflection Anisotropy Spectroscopy: an in situ optical probe of electrochemical interfaces with very high interface sensitivity.

The RA spectra show a reversible build-up of an optical anisotropy in cathodic potential ranges, which might account for the reduction of InP into phosphine and metallic In. The latter would further react with HCl to form InCl interfacial film.

[1] Wang, T. and Gong, J. Angew. Chem. Int. Ed. 54, 10718-10732 (2015).
[2] B. L. Pearce, S. J. Wilkins, T. Paskova, A. Ivanisevic. Journal of Materials Research 2015, 30, 2859-2870.

HL 19.14 Thu 13:30 P

Carrier effective masses in 2D halide perovskites from a first-principles approach — •Xiangzhou Zhu[1], Mateusz Dyksik[2,3], Jonas D. Ziegler[5], Matan Menahem[4], Jonas Zipfel[5], Barbara Meisinger[5], Michal Baranowski[3], Omer Yaffe[4], Alexey Chernikov[5,6], Paulina Plochocka[2,3], and David A. Egger[1] — [1]Technical University of Munich, Germany — [2]LNCMI CNRS, France — [3]Wroclaw University of Science and Technology, Poland — [4]Weizmann Institute of Science, Israel — [5]University of Regensburg, Germany — [6]Dresden University of Technology, Germany

Two-dimensional halide perovskites (2D HaPs) are attracting significant attention as promising optoelectronic materials. Effective masses of charge carriers are crucial parameters for device performance and exciton behavior. Here, we report first-principles calculations based on density functional theory (DFT) to investigate magnitudes, microscopic origins and consequences of carrier effective masses in 2D HaPs. We demonstrate that distortions due to organic spacers as well as orbital hybridization effects due to metal cations lead to a wide tunability of effectives mass in 2D HaPs[1]. Furthermore, it is shown that the knowledge of the DFT-computed electron and hole masses is key to capture efficient exciton diffusion, as measured by spatially-resolved optical spectroscopy[2].

[1] Dyksik, M, et al. ACS Energy Lett. 5, 3609 (2020)
[2] Ziegler, J. D., et al. Nano Lett. 20, 6674 (2020)

HL 19.15 Thu 13:30 P

The interfacial (electronic) structure of InP(001) in contact with electrolytes from computational spectroscopy — Vibhav Yadav, Margot Guidat, Mario Löw, •Jongmin Kim, and Matthias M. May — Institute of Theoretical Chemistry, Universität Ulm, Ulm, Germany

The relevance of controlling the electrochemical interface of InP derived materials for energy-conversion has already been established [1]. A tandem structure with the ternary compound, AlInP, in contact with the electrolyte showed 19%, solar-to-hydrogen efficiency [2]. In practical applications under operating conditions, a surface in contact with water oxidizes by insertion or substitution. This leads to surface polymerisation: formation of PO_x and In_2O_3. These species improve the stability of the surface and reduce surface charge-carrier recombination. Therefore, an investigation of the interfacial properties is crucial. In this computational work, we model the electrochemical interface, using first-principles calculations, in accordance with previous experimental studies. Using this model, we will probe the electrochemical double layer region to take into account the electric field fluctuations during a molecular dynamics simulation: simulating open circuit conditions. We develop a methodology, enabling the understanding of surface processes, by means of computational reflection anisotropy spectroscopy (RAS) results. Finally, we compare our results with experiments to derive a comprehensive understanding.

[1] O. Khaselev, et al. Science **280**, 425 (1998).
[2] M. M. May, et al. Nat. Commun. **6**, 8286 (2015).

HL 19.16 Thu 13:30 P

Reduction of crystal defects in GaP buffer layers grown on Si(100) by MOCVD — •Manali Nandy[1], Agnieszka Paszuk[1], Markus Feifel[2], Christian Koppka[1], Peter Kleinschmidt[1], Frank Dimroth[2], and Thomas Hannappel[1] — [1]TU Ilmenau, Gustav-Kirchhoff-Straße 5, 98693, Ilmenau — [2]Fraunhofer Institute for Solar Energy Systems ISE, Freiburg 79110, Germany

The performance of III-V-on-Si multijunction solar cells is still limited by a high density of defects at the GaP/Si heterointerface and in the III-V buffer layers. Here, in order to improve the crystal quality of the GaP(100) buffer layer, we modified the GaP pulse nucleation by substituting the first five TEGa pulses with TMAl. The influence of Al on the defect density in the GaP buffer layers is investigated by electron channeling contrast imaging. 60 nm thick GaP(100) buffer layers grown on GaP nucleation exhibit short misfit dislocations (MDs) and therefore, a high density of threading dislocations (TDs). In contrast, GaP(100) buffer layers grown on GaP/AlP nucleation exhibit less, but longer MDs, which result in a lower density of TDs. In addition, the density of stacking faults and stacking faults pyramids in the GaP layer grown on the AlGaP nucleation is significantly reduced. The surface morphology at the initial growth stage of GaP buffer layers grown on AlGaP nucleation, is smoother compared to buffer layer grown on the GaP nucleation. The application of Al in the GaP nucleation process provides a two-dimensional, smooth layer on which subsequent, high-quality GaP films could be grown, and therefore, shows a promising pathway for improving the performance of III-V-on-Si devices.

HL 19.17 Thu 13:30 P

Understanding surface properties of CsK_2Sb from first principles — •Richard Schier[1], Holger-Dietrich Sassnick[2], and Caterina Cocchi[2] — [1]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin — [2]Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg

Among the most promising compounds for next-generation photocathodes in particle accelerators, CsK_2Sb is regarded with particular interest. While first-principles calculations have recently contributed to gain insight into the bulk characteristics of this system [1], for most physical processes related to photoemission, surface properties are essential. To fill this gap, we use density functional theory to simulate and analyze the stability and the electronic properties of the low-Miller-index surfaces of CsK_2Sb. After assessing the formation energies, we calculate ionization potential (IP), band structure, and projected density of states (PDOS). Depending on the surface, we find IPs ranging from 2.2 eV to 3.4 eV. The computed band structures reveal that CsK_2Sb surfaces can exhibit either direct and indirect bandgaps, and in some specific cases they can even become metallic. The calculated PDOS offers insight into the atomic contributions to the bands around the Fermi energy.

[1] C. Cocchi et al., J. Phys: Condens. Matter 31, 014002 (2019)

HL 19.18 Thu 13:30 P

Copper iodide thin films: Multistack AFM studies of local electrical properties — •Tillmann Stralka, Holger von Wenckstern, and Marius Grundmann — Solid State Physics, Leipzig, Germany

The search for high-performance p-type transparent conductive materials has been a major challenge for decades [1]. Copper iodide (CuI) or alloys based on CuI [2] could offer a solution, since CuI does outperform all other known p-type TCMs, concerning transmittance in the visible spectrum as well as electrical conductivity at room temperature [3]. In this contribution polycrystalline CuI thin films grown by sputtering, are investigated. Hereby we strive to understand and differentiate the contribution of grains and grain boundaries (GBs) to transport mechanisms. Topographic features as GBs lead to a depletion of majority charge carriers and even a localised inversion (two dimensional electron gas) within GBs [4]. To acquire morphological and electrical properties with a high spatial resolution we employ atomic force microscopy, which additionally offers current probe mode to characterise electrical properties. These measurements will be conducted and evaluated with a novel approach that offers voltage spectroscopy and localisation of nm sized objects at the same time furthermore correlate topographic features with electrical properties.

[1] M. Grundmann et al., J.Phys.D.Apps.Phys.,49(213001), 2016 [2] T.Jun et al., Adv. Mater. 30(1706573) [3] C.Yang et al., PNAS 113(412929) [4] M. Kneiß et al., Adv. Mater. Interfaces, 5(6), 2018

HL 19.19 Thu 13:30 P

Pump-probe measurements to detect ultra-fast carrier dynamics and carrier density saturation in GaN-based quantum wells — •Malte Schrader, Philipp Henning, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik & Laboratory for Emerging Nanometrology, Technische Universität Braunschweig, 38106 Braunschweig, Germany

The aim of our study is to understand the carrier dynamics in GaN-based quantum wells at high carrier densities. An accurate estimation of the excited charge carrier density in pulsed laser experiments by indirect fluence-to-charge-density conversion is flawed, because the available states for the excited electrons in the conduction band might already be completely filled by the high fluence laser pulse. We therefore show in this contribution a direct approach by using two pulsed laser beams in quick succession in a pump-probe setup: a pump beam excites the carriers and a probe beam measures the transmission shortly thereafter, and therefore the occupation of the states above the band edge. A laser pulse duration of 35 fs at 5 kHz repetition rate is used in a degenerate setup, meaning pump and probe beam have the same wavelength. The decay of the excited carrier states is encoded in the transmitted probe beam as a function of the delay between pump and probe beam. To detect a saturation limit the fluence of the pump beam is increased. Besides two distinct decay times of around 10 ps and several 100 ps respectively, the ultra-fast intraband relaxation in the fs domain is of special interest.

HL 19.20 Thu 13:30 P

Tuning the electrochemical properties of multifunctional catalyst layers by plasma-enhanced atomic layer deposition — •Matthias Kuhl, Alex Henning, Lukas Haller, Laura Wagner, Chang-Ming Jiang, Verena Streibel, Ian D. Sharp, and Johanna Eichhorn — Walter Schottky Institut, Technische Universität München

Major challenges in photoelectrochemical (PEC) energy conversion systems are the poor efficiency and material instability of semiconductor photoelectrodes under the harsh operating conditions. Recently, it was demonstrated that plasma-enhanced atomic layer deposition (PE-ALD) can be used to fabricate conformal, biphasic Co_3O_4/$Co(OH)_2$ catalyst layers on semiconductor photoelectrodes, which are simultaneously robust and electrochemically active. The nanocrystalline Co_3O_4 layer forms a durable interface to the substrate and the disordered $Co(OH)_2$ surface layer significantly improves the electrocatalytic oxygen evolution reaction (OER) activity.

Here, we leverage the precise control of PE-ALD to further tailor the thickness ratio of the surface and interface layers of the Co_3O_4/$Co(OH)_2$ bilayer by tuning the plasma exposure time during growth. Short pulses lead to the formation of porous, unstable, catalytically active $Co(OH)_2$ layers due to an incomplete precursor decomposition, while long pulses result in denser films and form stable, inactive Co_3O_4 layers. More generally, this work highlights the power of PE-ALD for engineering catalyst/semiconductor interfaces simultaneously exhibiting multiple functionalities.

HL 19.21 Thu 13:30 P

Effect of hydrogen in low temperature GaN underlayer on the effective carrier lifetime in GaInN/GaN single quantum wells — •Rodrigo De Vasconcellos Lourenço[1,2], Philipp Henning[1,2], Samar Hagag[1,2], Uwe Rossow[1], Heiko Bremers[1,2], and Andreas Hangleiter[1,2] — [1]Institute of Applied Physics, Technische Universität Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Braunschweig, Germany

The luminescence efficiency of GaInN single quantum well (SQW) structures is affected by the growth conditions of all the layers grown before it and especially those ones directly before the quantum well - the so-called underlayer (UL). Usually, nitrogen is used as carrier gas during low temperature UL growth in low-pressure MOVPE. In this work, molecular hydrogen was added to the carrier gas during pure GaN UL growth and its supply was closed well before the QW is grown. Time-resolved photoluminescence measurements of SQWs with UL containing hydrogen and intentional Si doping suggest that they have better internal quantum efficiency at low temperature compared to the reference sample. Additionally, those showed longer radiative lifetime and longer emission wavelengths at low temperature compared to SQWs with doped UL and without hydrogen. This may indicate that hydrogen reduces the free carriers density by partly compensating the Si doping. Comparing SQWs with UL not intentionally doped, the one containing hydrogen showed shorter effective lifetime at low temperature, which could suggest that hydrogen acts as a donor or that hydrogen induces non-radiative centers.

HL 19.22 Thu 13:30 P

Transient Dielectric Function of Ge, Si, and InP from Femtosecond Pump-Probe Ellipsometry — •Carola Emminger[1,2], Shirly Espinoza[3], Steffen Richter[3,4], Oliver Herrfurth[5,6], Mateusz Rebarz[3], Martin Zahradník[3], Rüdiger Schmidt-Grund[6,7], Jakob Andreasson[3], and Stefan Zollner[1] — [1]New Mexico State University — [2]Masaryk University — [3]ELI Beamlines — [4]Linköpings universitet — [5]Active Fiber Systems — [6]Universität Leipzig — [7]Technische Universität Ilmenau

Structures in the dielectric function (DF), known as critical points (CPs), depend on temperature, strain, composition, and doping. We investigate CPs in the transient DF of Ge, Si, and InP measured with femtosecond pump-probe spectroscopic ellipsometry by calculating the second derivatives of the DF with respect to energy using a linear filter technique, which combines interpolation, noise reduction, scale change, and differentiation. From fitting an n-dimensional CP lineshape to the second derivatives, we find the amplitude, excitonic phase angle, threshold energy, and broadening as functions of delay time. A distinctive change of the CP parameters occurs within the first couple of picoseconds after the pump pulse. In the case of Ge, the CP energies red-shift due to band gap renormalization and an increase in temperature due to laser heating. After about 4 ps, the DF and CP parameters start to recover. Up to about 30 ps, coherent acoustic phonon oscillations are observed in the temporal evolution of the CP parameters. The period of these oscillations is approximately 11 ps, which is in good agreement with theory.

HL 19.23 Thu 13:30 P

X-ray absorption fingerprints in $LiCoO_2$ and CoO_2 — •Daniel Duarte Ruiz and Caterina Cocchi — Carl von Ossietzky Universität Oldenburg, Institut für Physik, Oldenburg, Deutschland

$LiCoO_2$ is a popular cathode material for Li-ion batteries, whereby X-ray absorption near-edge structure (XANES) is typically used to characterize electrodes in operando conditions. Identifying the spectral fingerprints of this compound and of its delithiated counterpart is therefore essential to provide references for the interpretation of the experimental spectra. In an *ab initio* work based on all-electron density functional theory and many-body perturbation theory (Bethe-Salpeter equation)[1], the XANES spectra of LiCoO2 and CoO2 are computed and analized for the O K-edge as well as for the Co K- and $L_{2,3}$-edges. With the adopted approach, we are able to assess that in all spectra, excitonic effects manifest themselves only via a red-shift on the absorption peaks. Clear signatures distinguishing binary and ternary compounds in the O K-edge and Co $L_{2,3}$-edges spectra can be identified.

[1] C. Vorwerk et al. *Electron. Struc.* 1, 037001 (2019).

HL 19.24 Thu 13:30 P

RF beat note analysis of a semiconductor optical frequency comb — •Duc Nam Nguyen[1], Dominik Auth[1], Quentin Gaimard[2], Abderrahim Ramdane[2], and Stefan Breuer[1,3] — [1]Institute of Applied Physics, TU Darmstadt, Darmstadt, Germany — [2]Centre de Nanosciences et Nanotechnologies, Palaiseau, France — [3]John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, USA

We experimentally study the RF beat note and optical spectra evolution of a frequency-modulated near-infrared semiconductor comb laser. We show and explain a transition towards stable optical frequency comb generation in dependence on the electrical biasing conditions.

HL 19.25 Thu 13:30 P

Contactless Measurement of the Sheet Resistance of two-dimensional Electron Gases — •Timo A. Kurschat, Arne Ludwig, and Andreas D. Wieck — Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum

The aim of this work is to measure the sheet resistance of two-dimensional electron gases in GaAs without the need for built-in contacts. Thus a characterization is possible without destroying the wafer. This method can be used to create spatially resolved maps of whole wafers to evaluate quality and homogeneity prior to further processing.

The sheet resistance is measured by placing two electrodes (round metal plates) close to the sample. These electrodes form capacitances C with the conductive layer. With a high-frequency alternating voltage applied to one electrode, the transmitted power can be measured at the other one. The measured amplitude depends on the sample resistance and the impedance of the capacitances, which are proportional to $1/\omega C$.

The electrodes have a diameter of 3 mm and 6 mm center-to-center distance. The measurement range starts at about 300 Ω/□ and goes up to 50 kΩ/□. The sheet resistance is determined by sweeping the frequency between 1 MHz and 400 MHz and then applying a fit.

Besides the measurements of samples with known sheet resistance, maps of complete wafers are shown. The lateral resolution of about 5 mm depends on the size of the electrodes and was estimated by etching a structure on a wafer.

HL 19.26 Thu 13:30 P

Thermal Conductivity Measurements in β-Ga_2O_3 Thin Films — •Robin Ahrling[1], Olivio Chiatti[1], Rüdiger Mitdank[1], Zbigniew Galazka[2], Andreas Popp[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

As a wide-band gap semiconductor with a high breakthrough field, gallium oxide (Ga_2O_3) has shown to be a promising material for applications in high power electronics. However, due to the materials low thermal conductivity [1,2] heat dissipation is a challenge for future device applications. Therefore, it is crucial to investigate the thermal transport in Ga_2O_3 films. Electrical measurements have shown that in very thin films the scattering processes change drastically with decreasing film thickness [3]. In this work, we investigate the thermal conductivity in these thin films, using the 3-ω and 2-ω method.

A variation of the 3-ω method with sub μm heater widths, with heaters thinner than the thickness of the examined films, is used. The heaters are realized by electron beam lithography. We investigate the thermal conductivity in dependence of the temperature and the thickness of the Ga_2O_3 films, with a special interest in changes in the the phonon transport mechanisms in a quasi-ballistic phonon transport regime.

[1] M. Handwerg *et al.*, Semicond. Sci. Technol. **30**, (2015) 024006
[2] M. Handwerg *et al.*, Semicond. Sci. Technol. **31**, (2016) 125006
[3] R. Ahrling *et al.*, Sci. Rep. **9**, 13149 (2019).

HL 19.27 Thu 13:30 P

Contact Preparation and Thermoelectric Properties of Bismuth Nanowires — •Mahni Müller[1], Rüdiger Mitdank[1], Hoda Moosavi[2], Michael Kröner[2], Peter Woias[2], Jeongmin Kim[3], Wooyoung Lee[3], Adnan Hammoud[4], Thomas Lunkenbein[4], and Saskia Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Laboratory of Design of Microsystems, University of Freiburg, IMTEK, 79110 Freiburg, Germany — [3]Department of Material Science and Engineering, Yonsei University, 03722 Seoul, Repuplic of Korea — [4]Fritz Haber Institute of the Max Planck Society, 14195 Berlin, Germany

Bismuth-based thermoelectric materials have always been promising for improving the thermoelectric figure of merit [1]. Those properties can strongly be modified through nanostructuring and additionally a high surface-to-volume-ratio is obtained with nanowires [2].

However, due to air exposure, a native oxide shell forms around the bismuth core, which leads to non-ohmic contact resistances. To achieve ohmic contacts for low temperature measurements, we present a preparation method with focused-ion-beam-induced deposition (fibid). Measurements of the electrical and thermal conductivity and of the Seebeck coefficient of bismuth nanowires with fibid-contacts between 10 K and 300 K were performed and compared to bulk. We discuss the change in properties and the possible influence of the contacting method.

[1] M. S. Dresselhaus *et al.*, Phys. Solid State **41**, 679-682 (1999).
[2] T. E. Huber *et al.*, Phys. Rev. B **83**, 2354414 (2011).

HL 19.28 Thu 13:30 P

Nonlinear down-conversion in a single quantum dot — •Björn Jonas, Dirk Heinze, Eva Schöll, Patricia Kallert, Timo Langer, Sebastian Krehs, Alex Widhalm, Klaus D. Jöns, Dirk Reuter, Stefan Schumacher, and Artur Zrenner — Paderborn University, Physics Department, Warburger Straße 100, 33098 Paderborn, Germany

In our work we study an all optical approach based on nonlinear principles, to tune the emission of the biexciton state in a single quantum dot[1]. After preparation of the biexciton state via phonon-assisted two-photon excitation, we introduce a control-laser which enables a nonlinear down-conversion via a virtual state. Previous theoretical work suggests that the spectral and polarization properties of this stimulated emission can be fully controled by adjusting the respetive properties of the control-laser[2]. In this work we show the first experimental demonstration of this process. The stimulated down-conversion works best if the virtual state is tuned close to the exciton energy and we can achieve a tuning range of about 0.5 meV around the exciton and biexciton emission. We furthermore make use of the spin conservation in the system to demonstrate control of the polarization of the emitted photon.

[1] http://arxiv.org/abs/2105.12393
[2] D. Heinze et al., Nature Communications **6**, 8473 (2015)

HL 19.29 Thu 13:30 P

Spin lasing in bimodal quantum dot micropillar cavities — •Niels Heermeier[1], Tobias Heuser[1], Jan Grosse[1], Natalie Jung[2], Markus Lindemann[2], Nils Gerhard[2], Martin Hofmann[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Tech- nische Universiät Berlin, D-10623 Berlin, Germany — [2]Lehrstuhl für Photonik und Terahertztechnologie, Fakulktät für Elektrotechik und Informationstechnik, Ruhr-Universität Bochum, D-44780 Bochum

Spin-controlled lasers are highly interesting photonic devices and have been shown to provide ultra-fast polarization dynamics in excess of 200 GHz. In contrast to conventional semiconductor lasers their tem- poral properties are not limited by the intensity dynamics, but are governed primarily by the birefringent mode splitting that determines the polarization oscillation frequency. Another class of modern semi- conductor lasers are high-beta emitters which benefit from enhanced light-matter interaction due to strong mode confinement in low-mode- volume microcavities. In such structures, the emission properties can be tailored by the resonator geometry to realize for instance bimodal emission behavior in slightly elliptical micropillar cavities. We utilize this attractive feature to demonstrate and explore spin-lasing effects in bimodal high-beta quantum dot micropillar lasers. The studied micro- lasers show spin laser effects with polarization oscillation frequencies up to 15 GHz which is controlled by the ellipticity of the resonator. Our results reveal appealing prospects for very compact and energy- efficient spin lasers and can pave the way for future purely electrically injected spin lasers enabled by short injection path lengths.

HL 19.30 Thu 13:30 P

Non-integer high-harmonic generation in a topological insulator — Christoph P. Schmid[1], Leonard Weigl[1], Patrick Grössing[2], Vanessa Junk[2], Cosimo Gorini[2], Stefan Schlauderer[1], Suguru Ito[3], •Manuel Meierhofer[1], Niklas Hofmann[1], Dmytro Afanasiev[1], Jack Crewse[2], Konstantin A. Kokh[4,5], Oleg E. Tereshchenko[5,6], Jens Güdde[3], Ferdinand Evers[2], Jan Wilhelm[2], Klaus Richter[2], Ulrich Höfer[3], and Rupert Huber[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Institute of Theoretical Physics, University of Regensburg, Germany — [3]Department of Physics, Philipps-University of Marburg, Germany — [4]V.S. Sobolev Institute of Geology and Mineralogy SB RAS, Novosibirsk, Russia — [5]Novosibirsk State University, Russia — [6]A.V. Rzhanov Institute of Semiconductor Physics SB RAS, Novosibirsk, Russia

We demonstrate multi-THz high-harmonic generation (HHG) in the topological insulator bismuth telluride. The frequency of the driving field discriminates between HHG from the bulk and the topological surface, where long scattering times and the quasi-relativistic dispersion enable unusually efficient HHG. All observed orders, generated in the surface state, can be continuously shifted to arbitrary non-integer multiples of the driving frequency by varying the carrier-envelope phase of the driving field. The anomalous Berry curvature enforces meandering ballistic trajectories of the Dirac fermions, causing a hallmark HH polarization pattern. Our study provides a fascinating new platform to explore topology and relativistic strong-field quantum physics.

HL 19.31 Thu 13:30 P

Exciton-phonon coupling in transition metal dichalcogenides revealed by ultrafast electron diffraction. — •Ahmed Hassanien, Arne Ungeheuer, Mashood Tarek Mir, Lukas Nöding, Arne Senftleben, and Thomas Baumert — Institute of Physics and CINSaT, University of Kassel, Heinrich-Plett-Strasse 40, D-34132 Kassel, Germany

Exciton-phonon coupling (EXPC) is responsible in principle for the temperature-dependence of optoelectronic and transport properties of transition metal dichalcogenides (TMDCs). The signatures of EXPC are usually observed in resonance Raman scattering [1], time-resolved transmission measurements [2], in optical absorption [3] or recently in two-dimensional electronic spectroscopy (2DES) [4]. Using a highly compact femtosecond electron diffractometer developed in our group [5], we were able to probe a polarization-dependent lattice dynamics in mechanically exfoliated few-layers ReS2. These anisotropic structural dynamics followed the photoexcitation by femtosecond laser pulses spectrally in resonance with the lowest excitonic transitions in ReS2 [6].

[1] Yang, Jinho, et al. FlatChem 3 (2017): 64-70.
[2] Jeong, Tae Young, et al. Acs Nano 10.5 (2016): 5560-5566.
[3] Christiansen, Dominik, et al. Physical review letters 119.18 (2017): 187402.
[4] Li, Donghai, et al. Nature communications 12.1 (2021): 1-9.
[5] Gerbig, C., et al. New J. Phys. 17.4 (2015):043050.
[6] Sim, Sangwan, et al. Nature communications 7 (2016): 13569.

HL 20: Annual General Meeting of the Semiconductor Physics Division

Time: Thursday 18:00–19:00 Location: MVHL

Duration 60 min.

HL 21: Focus Session: Highlights of Materials Science and Applied Physics II (joint session DS/HL)

Jointly organized on the occasion of the 60th anniversary of the *physica status solidi* journals (*pss*, http://www.pss-journals.com), this Focus Session features several invited presentations, talks and posters from key contributors on core condensed matter and applied physics topics. Highlights comprise the latest results on diamond, nitride semiconductors, organic materials, two-dimensional and quantum systems, oxides, magnetic materials, solar cells, thermoelectrics and more.

physica status solidi was launched by Akademie-Verlag Berlin in July 1961 and is published by Wiley-VCH Berlin and Weinheim today, supported by Wiley colleagues in China and the US. While in its first three decades it served as an East-West forum for solid state physics, since 1990 it has evolved into a family of journals with international author- and readership in a globalized scientific world. Its professional editorial services include topical curation, peer review organization, technical editing, special issue and hybrid open access publication.

The Focus session celebrates the numerous close collaborations and the steady support which the journals receive from their Advisory Board members, authors, reviewers and guest editors, including many members of the DPG and the condensed matter physics community in Germany.

(More information on '60 years of *pss*' is available at http://bit.ly/60_years_pss)

Organizers: Stefan Hildebrandt (Editor-in-Chief, pss), Norbert Esser (TU Berlin, ISAS) and Stephan Reitzenstein (TU Berlin)

Time: Friday 10:00–11:00 Location: H1

See DS 9 for details of this session.

HL 22: Focus Session: Emerging Semiconductor Laser Concepts

The fabrication and study of semiconductor lasers lie at the heart of the field of solid-state photonic devices. Current research efforts are driven by the incorporation of emerging emitter materials such as organic dyes, quantum dots or 2D materials on the one side, and by harnessing novel and complex photonic mode engineering concepts like in the case of topological lasers or coupled laser arrays. Combining these two directions opens a rich research direction and paves the way to new fundamental phenomena as well as engineering perspectives for ultra-compact laser devices with additional features and functionalities.

Organizers: Christian Schneider (Universität Oldenburg), Sebastian Klembt (Universität Würzburg)

Time: Friday 10:00–12:45 Location: H4

Invited Talk HL 22.1 Fri 10:00 H4
Two-dimensional gain materials for new nanolaser concepts — •Christopher Gies — Institut für Theoretische Physik, Universität Bremen
The talk will give an overview of the many-facetted physics of nanolasers. A particular focus will be on the gain properties when using TMD (transition metal dichalcogenide) monolayers and heterostuctures inside optical microresonators to design a new class of nanolasers [C. Gies and A. Steinhoff, Laser&Photonics Review 2021, 2000482]. Operating close to the ideal limit, high-β lasers require extra effort in unambiguously identifying laser operation. For this, quantum-optical studies have become the state of the art. Atomically thin TMD semiconductors hold much promise for optoelectronics, but have yet to demonstrate their application potential in new technologies. We will discuss possible gain mechanisms in TMD based nanolasers and identify signatures of lasing operation in these devices. For this, the interplay of excitonic effects caused by strong Coulomb interaction, and plasma effects in the high-excitation-density regime, need to be taken into consideration.

Invited Talk HL 22.2 Fri 10:30 H4
Room-temperature polariton lattices for quantum simulation — •Stephane Kena-Cohen — Polytechnique Montreal, Montreal, Canada
Polaritons are quasiparticles that form in semiconductor microcavities when the light-matter interaction rate is faster than the dissipation rate. At high densities, these quasiparticles can condense into a single macroscopic state that behaves qualitatively like a conventional laser. In addition to possessing intrinsically low lasing thresholds, the strong nonlinearities and tunability of polaritons is currently being exploited to realize efficient nonlinear devices and for quantum information.

In this talk, we will describe 2 platforms that allow for the formation of room-temperature polariton lasers: organic semiconductors and halide perovskites. We will describe the basic physics behind such devices and recent experiments where lattices were used to realize analog quantum simulators (e.g. XY Hamiltonian) under ambient conditions.

Invited Talk HL 22.3 Fri 11:00 H4
Topological nanocavity lasers and topological high-power lasers — •Yasutomo Ota[1,2], Yasuhiko Arakawa[2], and Satoshi Iwamoto[2,3,4] — [1]Keio University — [2]Nanoquine, The University of Tokyo — [3]RCAST, The University of Tokyo — [4]IIS, The University of Tokyo
Topological photonics offers ways to advance optical resonator design. In particular, resonators based on topological edge states emerging at the exteriors of bulk optical structures have been intensively studied because they behave robustly against certain disorders. Combinations of such topological cavities with gain materials also gather enormous interest as a straightforward route to topological lasers. In this contribution, we discuss our recent efforts on topological lasers based on 0D edge states supported in 1D photonic topological structures. We realized single-mode topological nanocavities by interfacing two topologically-distinct photonic crystal nanobeams. Combined with quantum dot gain, we demonstrated the first topological nanocavity laser. Furthermore, we theoretically extended the concept of the 0D topological cavity design to high-power lasers. We considered sizable arrays of coupled resonators that form topological optical bands. In a similar manner to the topological nanocavity, by interfacing two topologically-different cavity arrays, we designed topological interface modes broadly-distributed among the whole systems. Properly supplying gain to the system, we numerically uncovered the possibility of robust single mode lasing from the broad-area mode, paving the way to high-power and high-beam-quality topological lasers.

15 min. break.

Invited Talk HL 22.4 Fri 11:45 H4
Topological Insulator Lasers — •Miguel A. Bandres[1], Steffen Wittek[1], Gal Harari[2], Mordechai Segev[2], Demetrios N. Christodoulides[1], and Mercedeh Khajavikhan[3] — [1]CREOL, University of Central Florida — [2]Technion, Haifa, Israel — [3]University of Southern California
Topological insulators are a new phase of matter with insulating bulk but robust edge conductance. These topological edge states are extremely robust, propagate in a unidirectional manner immune to imperfections, defects, or disorder, and as such they are promising unprecedented advantages in technological applications. In recent years, research in topological photonics has flourished with numerous photonic platforms. Until recently research on topological systems in all fields of science was carried out in entirely passive and linear settings. However, the idea of introducing gain and nonlinearity to topological systems has raised many challenges and fundamental questions.

Recently, we demonstrated that topological protection can be combined with gain and loss to give rise to a new kind of laser whose lasing mode is a topologically protected edge mode, a topological insulator laser. The topological insulator laser displays slope efficiency that is considerably higher than in the corresponding trivial realizations even in the presence of defects and disorder, and operates at a single lasing mode even considerably above threshold. These results paved the way towards the new era of active topological photonics, in which topological protection, nonlinearity, and gain, combined in nontrivial ways, to give rise to new active photonic devises.

Invited Talk HL 22.5 Fri 12:15 H4
When polariton condensates have dissipations or have no excitons — •Hui Deng — University of Michigan, Ann Arbor, MI USA
Microcavity exciton-polaritons are formed in a semiconductor with strong exciton-photon coupling and low carrier density. They have been widely studied as a weakly interacting boson gas that can form a Bose-Einstein condensation (BEC) like many-body state in a solid. However, the cavity dissipation and fermionic nature of the electrons can lead to phenomena outside the well established framework for quasi-equilibrium polariton condensation. We discuss two such examples. We first discuss the formation of limit cycles with two coupled condensates, as a result of dissipative coupling and polariton nonlinearity. We then look "inside" the polaritons and reveal an electron-hole-photon condensate that share similar spectral properties as a polariton BEC but with a microscopic origin similar to a BCS-state.

HL 23: Focus Session: Highlights of Materials Science and Applied Physics III (joint session DS/HL)

Time: Friday 11:15–13:00 Location: H1

See DS 10 for details of this session.

HL 24: Quo Vadis Quantum Technologies? About Promises, Prospects, and Challenges

In 2016 the quantum satellite 'Micius' started its successful mission in space, and about a year ago, Google announced the achievement of reaching a quantum advantage with a quantum computer based on superconducting qubits. Both stories impressively illustrate the transition from basic research in quantum physics to applications of quantum technologies. In this light we will have a panel discussion on "Quo Vadis Quantum Technologies? About Promises, Prospects, and Challenges"

Time: Friday 13:30–15:00 Location: Audimax 2

Discussion HL 24.1 Fri 13:30 Audimax 2

Panel Discussion on Quantum Technologies — •Tobias Heindel[1] and Doris Reiter[2] — [1]Technische Universität Berlin — [2]Universität Münster

The panel discussion brings together experts and young scientists of different communities to jointly discuss viewpoints on the second quantum revolution and quantum technologies. We will exchange our ideas and perspectives of the different fields and how they might develop. Beyond identifying urgent scientific questions, we also aim to discuss the potential impact on industry, politics, and society in general, and to which extend we believe that these promises are realistic. The discussions will be moderated by the spokespersons of AGyouLeaP, Doris Reiter and Tobias Heindel. We invite in particular students and young researchers to join in and learn what to expect when they enter the field.

We are excited to welcome to the discussion panel: Jens Eisert (Freie Universität Berlin), Brian Geradot (Heriot-Watt University), Tracy Northup (Universität Innsbruck), Simone Portalupi (Universität Stuttgart), Rupert Ursin (TBC, IQOQI Wien), Jian-Wei Pan (TBC, University of Science and Technology of China, Hefei)

HL 25: 2D semiconductors and van der Waals heterostructures II (joint session HL/DS)

Time: Friday 13:30–14:45 Location: H4

HL 25.1 Fri 13:30 H4

Femtosecond contact-free nanoscopy of ultrafast interlayer transport in 2D heterostructures — •Felix Schiegl[1], Markus Plankl[1], Paulo Eduardo Faria Junior[1], Fabian Mooshammer[1], Tom Siday[1], Martin Zizlsperger[1], Fabian Sandner[1], Simon Maier[1], Markus Andreas Huber[1], Martin Gmitra[1,4], Jaroslav Fabian[1], Jessica Louise Boland[1,2], Tyler Liam Cocker[1,3], and Rupert Huber[1] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Regensburg, Germany — [2]Photon Science Institute, Department of Electrical and Electronic Engineering, University of Manchester, Manchester, UK — [3]Department of Physics and Astronomy, Michigan State University, East Lansing, MI, USA — [4]Institute of Physics, Pavol Jozef Šafárik University in Košice, Košice, Slovakia

Tunneling is one of the most direct results of quantum mechanics, and a hallmark of interlayer exciton formation in semiconducting van der Waals heterostructures. Here, we introduce a new contact-free terahertz nanoscopy technique to trace ultrafast charge dynamics in both conducting and non-conducting materials. We demonstrate < 50 nm spatial and subcycle temporal resolution and probe the interlayer tunneling across an atomically sharp WSe_2/WS_2 interface. Pronounced variations of the formation and annihilation of excitons emerge as a direct result of nanoscale strain and changes in atomic registry. Our results show the potential of this technique for revealing how ultrafast tunneling shapes the functionalities of a broad range of condensed matter systems.

HL 25.2 Fri 13:45 H4

Moiré phonons in twisted $MoSe_2$-WSe_2 heterobilayers and their correlation with interlayer excitons — •Philipp Parzefall[1], Johannes Holler[1], Marten Scheuck[1], Andreas Beer[1], Kai-Qiang Lin[1], Bo Peng[2], Bartomeu Monserrat[2,3], Philipp Nagler[1], Michael Kempf[4], Tobias Korn[4], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Deutschland — [2]Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge, UK — [3]Department of Materials Science and Metallurgy, University of Cambridge, UK — [4]Institut für Physik, Universität Rostock, Deutschland

We report about the investigation of twisted $MoSe_2$-WSe_2 heterobilayers by means of low-frequency Raman spectroscopy (LFRS) and low-temperature micro photoluminescence (μPL). We identify moiré phonons of both constituting materials in heterobilayers, which enables us to determine the relative twist angles of the heterobilayers on a local scale with high precision. Atomically reconstructed regions, which are identified by the observation of an interlayer shear mode in LFRS experiments, exhibit in μPL a strong, momentum-allowed interlayer-exciton signal.

HL 25.3 Fri 14:00 H4

Transport Properties of Bulk Black Phosphorus Below and Above the Quantum Limit — •Davide Pizzirani[1], Jasper Linnartz[1], Claudius Müller[1], Brian Kiraly[2], Alexander Khajetoorians[2], and Steffen Wiedmann[1] — [1]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Nijmegen, Netherlands — [2]Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands

Black phosphorus (bPh) has emerged as a promising and novel platform for nano-electronic applications due to its in-plane anisotropy and direct band gap that depends on the sample thickness. We present low-temperature magneto-transport experiments on bulk bPh up to 30 T with thicknesses ranging from 40 to 100 μm. A negative magneto-resistance (MR) that turns into a positive linear one is found by increasing the magnetic field. This MR remains quasi-isotropic upon changing the tilt angle from out-of-plane to in-plane with respect to the applied magnetic field. Using samples with different carrier concentrations, we are able to determine the transport properties below and above the quantum limit, and in the regime of variable range hopping.

HL 25.4 Fri 14:15 H4

Excitation-induced optical nonlinearities and charge carrier localization in atomically thin TMD semiconductors — •Daniel Erben, Alexander Steinhoff, Michael Lorke, Christian Carmesin, Matthias Florian, and Frank Jahnke — Institute for Theoretical Physics, University of Bremen

To interpret the nonlinear optical properties of atomically thin transition metal dichalcogenides (TMD), the density of photoexcited carriers is of central importance. However, in experiments the excited carrier density is practically not accessible. For above band-gap optical pumping of TMD monolayers, we utilize the semiconductor Bloch equations to determine the excitation density as function of the optical pump fluence. Our theory includes Pauli-blocking, band-gap renormalization, dephasing and screening of the Coulomb interaction due to excited carriers. The excitation density strongly depends on the wavelength of the exciting laser pulse. For pumping at the band gap, Pauli blocking of available phase space and renormalizations of the single particle energies are the dominant sources of a nonlinear density dependence, even at small pump fluence. In another study, we investigate the charge-carrier confinement in TMD nanobubbles. These are formed during stacking processes and exhibit quantum light emission upon optical excitation. We demonstrate that the emission originates from strong carrier localization, caused by the interplay of surface wrinkling, strain-induced confinement, and local changes of the dielectric environment. These effects combine to a specific localization signature that is found in recent spatially resolved photoluminescence experiments.

HL 25.5 Fri 14:30 H4

Spatio-temporal dynamics of phonon sidebands in 2D materials — •Roberto Rosati[1], Koloman Wagner[2], Samuel Brem[1], Raül Perea-Causín[3], Jonas D. Ziegler[2], Jonas Zipfel[2], Takashi Taniguchi[4], Kenji Watanabe[4], Alexey Chernikov[2,5], and Ermin Malic[1,3] — [1]Philipps University of Marburg — [2]University of Regensburg — [3]Chalmers University of Technology — [4]National Institute for Materials Science — [5]Dresden University of Technology

The semiconducting monolayers of transition metal dichalcogenides (TMDs) display a complex manifold of bright and dark exciton states, the latter giving rise to sharp phonon sidebands (PSB) in low-temperature photoluminescence. In this joint theory-experiment study we theoretically predict and experimentally demonstrate time-resolved low-temperature PSB, thus gaining direct access to the evolution of dark excitons in time, energy and space [1,2]. In an excellent theory-experiment agreement we reveal a spectral red-shift of phonon sidebands on a time scale of tens of picoseconds due to phonon-driven thermalization of initially-formed hot momentum-dark excitons [1]. After confined optical excitation, such hot-exciton distribution gives rise to a transient exciton diffusion one order of magnitude faster than the conventional diffusion observed at later times [2]. The obtained insights are applicable to other 2D materials with multiple exciton valleys.

[1] Rosati, R. et al. ACS Photonics 7, 2756 (2020).
[2] Rosati, R. et al. arXiv:2105.10232 (2021).

Crystalline Solids and their Microstructure Division
Fachverband Kristalline Festkörper und deren Mikrostruktur (KFM)

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Overview of Invited Talks and Sessions

(Lecture hall H1, H2, and H5; Poster P)

Invited Talks

KFM 1.1	Tue	10:00–10:30	H2	**Effect of humidity on the ferroelectric domain wall dynamics in BaTiO3 thin films** — Irena Spasojevic, Albert Verdaguer, Gustau Catalan, •Neus Domingo
KFM 1.5	Tue	11:30–12:00	H2	**Magnetic avalanche of non-oxide conductive domain walls** — •Somnath Ghara, Korbinian Geirhos, Lukas Kuerten, Peter Lunkenheimer, Vladimir Tsurkan, Manfred Fiebig, István Kézsmárki
KFM 4.1	Tue	14:15–14:45	H2	**Single crystal diamond growth by chemical vapor deposition for high-end applications: Recent trends and state of the art** — •Matthias Schreck, Theodor Grünwald
KFM 4.2	Tue	14:45–15:15	H2	**Development of diamond based kinetic inductance detectors** — •Francesco Mazzocchi, Dirk Strauss, Theo Scherer

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium Novel phases and dynamical properties of magnetic skyrmions (SYMS)

See SYMS for the full program of the symposium.

SYMS 1.1	Tue	10:00–10:30	Audimax 2	**Imaging skyrmions in synthetic antiferromagnets by single spin relaxometry** — •Aurore Finco
SYMS 1.2	Tue	10:30–11:00	Audimax 2	**Microwave spectroscopy of the skyrmionic states in a chiral magnetic insulator** — •Aisha Aqeel, Jan Sahliger, Takuya Taniguchi, Stefan Maendl, Denis Mettus, Helmuth Berger, Andreas Bauer, Markus Garst, Christian Pfleiderer, Christian H. Back
SYMS 1.3	Tue	11:15–11:45	Audimax 2	**Archimedean Screw in Driven Chiral Magnets** — •Nina del Ser
SYMS 1.4	Tue	11:45–12:15	Audimax 2	**Frustration-driven magnetic fluctuations as the origin of the low-temperature skyrmion phase in $Co_7Zn_7Mn_6$** — •Jonathan White, Victor Ukleev, Kosuke Karube, Peter Derlet, Chennan Wang, Hubertus Luetkens, Daisuke Morikawa, Akiko Kikkawa, Lucile Mangin-Thro, Andrew Wildes, Yuichi Yamasaki, Yuichi Yokoyama, Le Yu, Cinthia Piamonteze, Nicolas Jaouen, Yusuke Tokunaga, Henrik Rønnow, Taka-hisa Arima, Yoshinori Tokura, Jonathan White
SYMS 1.5	Tue	12:15–12:45	Audimax 2	**Magnetic Skyrmions as Topological Multi-Media Influencers** — •Sebastián A. Díaz

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Diversity on the Device Scale (SYHN)

See SYHN for the full program of the symposium.

SYHN 1.1	Thu	10:00–10:30	Audimax 1	**Scaling behavior of stiffness and strength of hierarchical network nanomaterials** — •Shan Shi
SYHN 1.2	Thu	10:30–11:00	Audimax 1	**Functional and programmable DNA nanotechnology** — •Laura Na Liu
SYHN 1.3	Thu	11:15–11:45	Audimax 1	**Multivalent nanoparticles for targeted binding** — •Stefano Angioletti-Uberti
SYHN 1.4	Thu	11:45–12:15	Audimax 1	**Programming Nanoscale Self-Assembly** — •Oleg Gang
SYHN 1.5	Thu	12:15–12:45	Audimax 1	**Achieving Global Tunability via Local Programming of a Structure's Composition** — •Jochen Mueller

Sessions

KFM 1.1–1.8	Tue	10:00–12:45	H2	**Focus Session I: Ferroics - Domains and Domain Walls**
KFM 2.1–2.2	Tue	11:15–11:45	H5	**Materials for Energy Storage**
KFM 3.1–3.2	Tue	13:30–14:00	H2	**Focus Session II: Ferroics - Domains and Domain Walls**
KFM 4.1–4.5	Tue	14:15–16:15	H2	**Focus Session III: Diamond**
KFM 5.1–5.24	Tue	16:00–17:00	P	**Poster Session KFM**
KFM 6.1–6.12	Wed	10:00–13:15	H5	**Skyrmions I (joint session MA/KFM)**
KFM 7.1–7.3	Wed	10:00–10:45	H1	**Dielectric, Elastic and Electromechanical Properties**
KFM 8.1–8.4	Wed	10:45–11:45	H1	**Crystal Structure / Real Structure / Microstructure**
KFM 9.1–9.3	Wed	12:00–12:45	H1	**Instrumentation and Methods**
KFM 10	Wed	13:00–13:30	MVKFM	**Annual General Meeting of the KFM division**
KFM 11.1–11.9	Thu	13:30–16:15	H3	**Organic Electronics and Photovoltaics, Electrical and Optical Properties (joint session CPP/KFM)**
KFM 12.1–12.12	Fri	10:00–13:15	H5	**Skyrmions II (joint session MA/KFM)**
KFM 13.1–13.10	Fri	10:00–12:45	H7	**Topological Insulators and Semimetals (joint session TT/KFM)**

Annual General Meeting of the Crystalline Solids and their Microstructure Division

Mittwoch 13:00–13:30 MVKFM

- Bericht
- Verschiedenes

Sessions

– Invited Talks, Contributed Talks, and Posters –

KFM 1: Focus Session I: Ferroics - Domains and Domain Walls

The Focus Sessions: Ferroics - Domains and Domain Walls is dedicated to the detection of multiferroic and ferroelectric domain pattern, their manipulation as well as the modeling of domains. These domains and domain walls are fascinating building blocks for novel (nanoscale) electronics ranging from switches, memristive elements towards diodes and reconfigurable wires.

Chairman: Stephan Krohns (University of Augsburg)

Time: Tuesday 10:00–12:45 Location: H2

Invited Talk KFM 1.1 Tue 10:00 H2

Effect of humidity on the ferroelectric domain wall dynamics in BaTiO3 thin films — Irena Spasojevic[1], Albert Verdaguer[2], Gustau Catalan[1], and •Neus Domingo[1] — [1]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain — [2]Institut de Ciència de Materials de Barcelona (ICMAB), CSIC, Campus UAB, Bellaterra, 08193 Barcelona, Spain

The switching dynamics of ferroelectric polarization under electric fields depends on the availability of screening charges in order to stabilize the switched polarization. In ferroelectrics thin films with exposed surfaces investigated by piezoresponse force microscopy (PFM), the main source of external screening charges is the atmosphere and the water neck, and therefore relative humidity (RH) plays a major role. In this context dynamic writing of linear domains in BaTiO3 thin films changes by varying scanning speeds in the range of RH between 2.5% and 60% reveal that the critical speed for domain writing increases non-monotonically with RH. Additionally, the width of line domains shows a power law dependence on the writing speed, with a growth rate coefficient decreasing with RH. The size of the written domains at a constant speed as well as the creep-factor describing the domain wall kinetics follow the behavior of water adsorption represented by the adsorption isotherm, indicating that the screening mechanism dominating the switching dynamics is the thickness and the structure of adsorbed water structure and its associated dielectric constant and ionic mobility.

KFM 1.2 Tue 10:30 H2

Charged ferroelectric domain walls for a.c. signal control — •Jan Schultheiss[1], Erik Lysne[1], Lukas Puntigam[2], Zewu Yan[3,4], Edith Bourret[4], Stephan Krohns[2], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, 7034, Trondheim, Norway — [2]University of Augsburg, 86159, Augsburg, Germany — [3]ETH Zurich, 8093, Zurich, Switzerland — [4]Lawrence Berkeley National Laboratory, 94720, Berkeley, CA, USA

Ferroelectric domain walls are natural interfaces separating volumes with different orientation of the spontaneous polarization. Depending on the local charge state, the domain walls exhibit unusual direct current (d.c.) conduction ranging from insulating to metallic-like behavior. Because of their unique electronic properties, they bear great potential as nanoelectronic components, serving, e.g., as switches and synaptic devices. In contrast to the functional d.c. behavior at charged walls, their response to alternating currents (a.c.) falls into an uncharted territory. Here, we explore the a.c. characteristics of charged ferroelectric walls in $ErMnO_3$ in the adiabatic regime (kHz-MHz), using a combination of atomic force microscopy and macroscopic dielectric spectroscopy. We demonstrate a pronounced non-linear response at the electrode-domain wall junction, which correlates with the charge state of the wall. The dependence on the a.c. drive voltage and frequency enables us to reversibly switch between uni- and bipolar output signal, providing conceptually new opportunities for the application of charged domain walls as functional nano-elements in a.c. circuitry.

KFM 1.3 Tue 10:45 H2

Conductivity control via minimally invasive anti-Frenkel defects in a functional oxide — •D. M. Evans[1,2], T. S. Holstad[2], A. B. Mosberg[2], D. R. Småbråten[2], P. E. Vullum[3], A. L. Dadlani[1], K. Shapovalov[4], Z. Yan[5,6], E. Bourret[6], D. Gao[2,7], J. Akola[2,8], J. Torgersen[2], A. T. J. van Helvoort[2], S. M. Selbach[2], and D. Meier[2] — [1]University of Augsburg, Germany — [2]NTNU, Norway — [3]SINTEF, Norway — [4]ICMAB-CSIC, Spain — [5]ETH Zurich, Switzerland — [6]LBNL, USA — [7]Nanolayers Research Computing LTD, London, — [8]Tampere University, Finland

The control of conductivity is critical to any electronic device. In this context, oxide materials are particularly interesting as their conductivity can be continuously tuned via an electric field. In addition, they have a plethora of inherent functionalities arising from the electronic degrees of freedom, such as, superconductivity, magnetism, and ferroelectricity. However, utilizing both these changes in conductivity and electronic degrees of freedom simultaneously requires the ability to change one without affecting the other. Usually this is a problem, as the net redox reaction that gives the change in conductivity also affects the electronic degrees of freedom. In this talk, I demonstrate how stable, nanoscale, enhancement of conductivity can be achieved in ferroelectrics without net mass transfer, net change in stoichiometry, or the build-up of spurious electric and chemical gradients. This approach permits both the multiple orders of magnitude change in conductivity and the inherent functionality of oxides to be utilized independently and in parallel to each other.

KFM 1.4 Tue 11:00 H2

Atomic-scale analysis of individual dopants in a functional oxide — •Kasper Hunnestad[1], Constantinos Hatzoglou[1], Antonius van Helvoort[2], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), 7491 Trondheim, Norway — [2]Department of Physics, Norwegian University of Science and Technology (NTNU), 7491 Trondheim, Norway

Oxide materials exhibit unique electronic and ionic properties that can readily be tuned via compositional variations and local defect chemistry. Intriguing examples are point-defect driven insulator-metal transitions, interfacial magnetism and superconductivity. However, 3D imaging of the individual point defects that are responsible for the emergent phenomena remains a challenge.

Here, we apply atom probe tomography (APT) to overcome this challenge, gaining first experimental insight into the 3D distribution of dopants in the multiferroic oxide $ErMn_{0.998}Ti_{0.002}O_3$. We resolve the position of individual Ti atoms within the crystal lattice, and study local characteristics such as density fluctuations, gradient effects and clustering.

Our results establish a pathway for resolving individual dopants in functional oxides, bringing us an important step closer to understanding the complex atomic-scale physics and ultimately control lattice, charge and spin degrees of freedom at the local scale.

15min. break.

Invited Talk KFM 1.5 Tue 11:30 H2

Magnetic avalanche of non-oxide conductive domain walls — •Somnath Ghara[1], Korbinian Geirhos[1], Lukas Kuerten[2], Peter Lunkenheimer[1], Vladimir Tsurkan[1], Manfred Fiebig[2], and István Kézsmárki[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — [2]Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Conductive domain walls have been exclusively observed in oxides, where off-stoichiometry and defects often hamper the domain wall conductivity and render the walls immobile and thus curtail their usefulness and flexibility. In this talk, we will show the giant conductivity of domain walls in the non-oxide multiferroic GaV_4S_8, investigated by macroscopic transport as well as microscopic PFM and c-AFM measurements. We observe a fascinating architectures of ribbon- and folded sheet-like conductive domain walls emerging in the polar rhombohedral state below its Jahn-Teller transition T_{JT} = 45 K. Besides the giant negative magnetoresistance (~80%) inherent to these conductive domain walls, their high conductivity is exploited to trigger unprecedentedly large changes of the bulk resistance via on-demand magnetic or electric conversions between multi- and mono-domain states. Such a transformation to the insulating mono-domain state through an avalanche-like domain-wall expulsion process leads to an abrupt conductance changes as large as eight orders of magnitude.

Reference: S. Ghara, K. Geirhos et al., Nature Communications 12, 3975 (2021).

KFM 1.6 Tue 12:00 H2

Conductivity of ferroelectric domain walls in the lacunar spinel GaV_4S_8 — •Lukas Puntigam, Donald Evans, Markus Altthaler, Somnath Ghara, Lilian Prodan, Vladimir Tsurkan, Stephan Krohns, and Istvan Kézsmárki — University of Augsburg, 86159, Augsburg, Germany

Ferroelectric domain walls, which can be written, tuned or erased at will, are being considered as functional building blocks for nano devices. Especially, the case of conductive domain walls, where their spatially confined electronic responses, that differ from the bulk of the host material, caused the idea of domain wall for nanoengineering.

To date, the origin for such increased conductivity in ferroelectrics domain walls has been attributed to the formation of screening charges driven by polar discontinuities.

Here, we discuss how other phenomena, such as strain, could induce enhanced conductivity of domain walls, using the lacunar spinel GaV_4S_8 as a template system. This system exhibits ferroelectric domain pattern below the Jahn-Teller transition at 42 K. Temperature dependent conductive and piezoresponse force microscopy, as well as local I(V)-spectroscopy, are employed to understand the local conductivity. We reveal at low temperatures that the conductivity is non-trivial consistent with the conventional polar-discontinuity approach, but rather - at secondary domain walls - is consistent with a strain-based mechanism. This provides a new mechanism on generating conductivity at domain walls, which is not limited by polar discontinuity requirements.

KFM 1.7 Tue 12:15 H2

Understanding the Electronic Structure of Lacunar Spinels GaM_4X_8 by *ab initio* Multi-Configurational Calculations — •Thorben Petersen, Liviu Hozoi, and Ulrich Rössler — Institute for Theoretical Solid State Physics, Leibniz IFW Dresden, Germany

Generally, transition-metal based compounds show a large manifold of structural motifs that are based on molecular-like lattices which often lead to strong correlations due to the sharing of the valence electrons between multiple transition metal centers [1]. In particular, lacunar spinels of the formula GaM_4X_8 (A = Ga; M = V, Nb, Ta; X = S, Se) are a representative class of such materials and have shown to exhibit various electronic and magnetic properties [2]. In this study, we apply *ab initio* multi-reference methods in the framework of CASSCF to understand the underlying electronic configuration of these materials. This will allow for the calculation of excited states that can be compared to experimentally available RIXS data of $GaTa_4Se_8$ [3]. In addition, a thorough analysis of the electronic structure will path the way towards modeling inter-site couplings and associated magnetic properties of this material class.

[1] R. L. Dally *et al.*, Phys. Rev. B **102**, 014410 (2020). [2] I. Kézsmárki *et al.*, Nat. Mater. **14**, 11, 1116 (2015). [3] M. Y. Jeong *et al.*, Nat. Commun. **8**, 782 (2017).

KFM 1.8 Tue 12:30 H2

Defeating depolarizing fields with artificial flux closure inultrathin ferroelectrics — •Elzbieta Gradauskaite[1], Natascha Gray[1], Quintin N. Meier[2], Marco Campanini[3], Thomas Moran[4], Bryan D. Huey[4], Marta D. Rossell[3], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]CEA Grenoble, LITEN, Grenoble, France — [3]Electron Microscopy Center, Empa, Switzerland — [4]Department of Materials Science and Engineering, University of Connecticut, Storrs, USA

Material surfaces encompass structural and chemical discontinuities that often lead to the loss of the property of interest in the so-called "dead layers". It is notably problematic in nanoscale oxide electronics, where the integration of ferroic materials into devices is obstructed by the thickness threshold required for the emergence of their functionality. Here, we report the stabilization of ultrathin out-of-plane ferroelectricity in oxide heterostructures through the design of an artificial flux-closure-like architecture. Inserting an in-plane polarized Aurivillius epitaxial buffer provides continuity of polarization at the interface, and despite its insulating nature we observe the emergence of polarization in our out-of-plane-polarized model ferroelectric $BaTiO_3$ from the very first unit cell. Our model heterostructure futher enables the stabilization of charged domain walls with pronounced chiral textures in multiferroic $BiFeO_3$ films. Thus, we show that the smart integration of insulating materials can surpass standard metals in the design of the next generation ferroelectric-based oxide electronics.

KFM 2: Materials for Energy Storage

Chairman: Theo Scherer (KIT Karlsruhe)

Time: Tuesday 11:15–11:45 Location: H5

KFM 2.1 Tue 11:15 H5

Self-assembled monolayers of *para*-aminobenzoic acid on V_2O_5 - a theoretical and experimental study — •Fabian Dietrich[1], Juan Fernandez[2], Eduardo Cisternas[1], and Marcos Flores[2] — [1]Universidad de La Frontera, Temuco, Chile — [2]Universidad de Chile, Santiago, Chile

Lithium ion batteries (LIB) can contribute to environment-friendly energy supply due to the storage for renewable energies. As important part of their characteristics, the number of charge/discharge cycles and the capacity after several cycling processes strongly depend on the electro-chemical reactions taking place on the surface of the electrodes, *e.g.* building the so called solid-electrolyte interface (SEI). To control the formation of the SEI, the surface can be functionalized with organic molecules, building a self-assembled monolayer (SAM).

We investigated the assembling of para-aminobenzoic acid (pABA) on V_2O_5, a potential cathode material for LIB, in a collaborative experimental (XPS) and theoretical study. The simulations using Density Functional Theory with dispersion corrections include several configurations letting different sides of the pABA interact with the V2O5 surface. We found out that for low concentrations, the molecules prefer a lying-down configuration, while for higher concentrations they are in an up-standing configuration building a more organized SAM. From the comparison with the experimental data, a high coverage of the surface with pABA can be concluded. Hence, we infer the existence of the up-standing configuration and also the building of a well-ordered SAM.

KFM 2.2 Tue 11:30 H5

Thermoelectric properties of novel semimetals: A case study of YbMnSb2 — •Yu Pan[1], Feng-Ren Fan[1], Xiaochen Hong[2], Bin He[1], Congcong Le[1], Walter Schnelle[1], Yangkun He[1], Kazuki Imasato[3], Horst Borrmann[1], Christian Hess[2], Bernd Büchner[2], Yan Sun[1], Chenguang Fu[1], Jeffrey Snyder[3], and Claudia Felser[1] — [1]Department of Solid State Chemistry, Max Planck Institute for Chemical Physics of Solids, Dresden 01187, Germany — [2]Leibniz-Institute for Solid State and Materials Research (IFW-Dresden), Helmholtzstraße 20, Dresden 01069, Germany — [3]Materials Science & Engineering (MSE), Northwestern University, Evanston, IL 60208, USA

The emerging class of topological materials provides a platform to engineer exotic electronic structures for a variety of applications. As complex band structures and Fermi surfaces can directly benefit thermoelectric perfor-mance it is important to identify the role of featured topological bands in thermoelectrics particularly when there are coexisting classic regular bands. In this work, the contribution of Dirac bands to thermoelectric performance and their ability to concurrently achieve large thermopower and low resistivity in novel semimetals is investigated. By examining the YbMnSb2 nodal line semimetal as an example, the Dirac bands appear to provide a low resistivity along the direction in which they are highly dispersive. Moreover, because of the regular-band-provided density of states, a large Seebeck coefficient is achieved. The present work highlights the potential of such novel semimetals for high thermo-electric performance.

KFM 3: Focus Session II: Ferroics - Domains and Domain Walls

The Focus Sessions: Ferroics - Domains and Domain Walls is dedicated to the detection of multiferroic and ferroelectric domain pattern, their manipulation as well as the modeling of domains. These domains and domain walls are fascinating building blocks for novel (nanoscale) electronics ranging from switches, memristive elements towards diodes and reconfigurable wires.

Chairman: Donald M. Evans (University of Augsburg)

Time: Tuesday 13:30–14:00 Location: H2

KFM 3.1 Tue 13:30 H2

Tunable conductive domain wall switches in 200- μm-thick lithium niobate single crystals — •Henrik Beccard[1], Benjamin Kirbus[1], Ekta Singh[1], Zeeshan Amber[1], Michael Rüsing[1], Elke Beyreuther[1], and Lukas M. Eng[1,2] — [1]Institut für Angewandte Physik, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany ct.qmat — [2]ct.qmat Dresden-Würzburg Cluster of Excellence EXC 2147, TU Dresden, 01062 Dresden, Germany

In the ferroelectric model material lithium niobate (LNO), state-of-the- art techniques allow the targeted poling of ferroelectric domains, as well as the enhancement of domain wall (DW) conductivity over several orders of magnitude [1]. Imaging and analyzing these properties can be performed with piezoresponse force microscopy (PFM) and confocal 3D second harmonic generation (SHG) microscopy [2]. The correlation between DW geometry and electrical DW conductivity is well established. Moreover, it can be simulated e.g. using a resistor network model [3]. Hence, an increasing focus in the ferroelectrics community is set on the realization of DW-based nanoelectronic devices. Recently, tunable DW switches have been reported for LNO thin films [4]. On the contrary, we report on tunable DW switches inside of 200- μm-thick LNO single crystals, relying purely on solid electrodes [5].

[1] C. Godau et al. ACS Nano 11, 4816 (2017)
[2] T. Kämpfe et al. Phys. Rev. B 8, 035314 (2014)
[3] B. Wolba et al. Adv. Electron. Mater. 4, 1700242 (2018)
[4] H. Lu et al. Adv. Mater. 1902890 (2019)
[5] B. Kirbus et al. ACS Appl. Nano Mater. 2, 5787 (2019)

KFM 3.2 Tue 13:45 H2

Lithium Niobate(LiNbO3) under uniaxial Stress — •Ekta Singh[1], Michael Lange[1], Sven Reitzig[1], Henrik Beccard[1], Michael Rüsing[1], Clifford Hicks[2], and Lukas M. Eng[1,3] — [1]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]ct.qmat: Dresden-Würzburg Cluster of ExcellenceEXC 2147

Ferroelectric properties can be tuned by external fields such as light, dc electric fields, or mechanical strain. Amongst these, strain engineering plays an important role, where a correlation between strain and polarization has been a subject of study in recent years [1, 2]. Conventionally, strain is applied by lattice-mismatched epitaxial growth of thin films on selected substrates, which limits the method to certain materials.

Here, we present a prospective alternative based on piezoelectric actuators that is suitable to apply both compressive and tensile strain to single crystals in a controlled manner, while simultaneously performing dedicated optical or AFM experiments in-situ. To demonstrate the functionality of this device, we present shifts in phonon frequencies with applied strain on stoichiometric Lithium Niobate, measured by Raman spectroscopy. Such control of strain will provide valuable new insights into ferroelectric domain walls and their properties such as electrical conductivity.

[1] V. Stepkova et.al.; J. Phys.: Condens. Matter 24, 212201 (2012) [2] A. Alsubaie et.al.; Nanotechnology 28, 075709 (2017)

KFM 4: Focus Session III: Diamond

This focus session is dedicated to the growth of single and polycrystalline diamond. Applications for the use of diamond in nuclear fusion reactors as microwave transmission system for high power mm-waves will be discussed. New Diamond-based kinetic inductance detectors are described as well. Defects in diamond and their influence to microwave properties are described.

Chair: Theo Scherer (KIT Karlsruhe)

Time: Tuesday 14:15–16:15 Location: H2

Invited Talk KFM 4.1 Tue 14:15 H2

Single crystal diamond growth by chemical vapor deposition for high-end applications: Recent trends and state of the art — •Matthias Schreck and Theodor Grünwald — Institut für Physik, Universität Augsburg, 86135 Augsburg, GERMANY

In order to profit from diamond´s unique material properties for demanding device applications, wafer size single crystals are needed. Currently, two alternative concepts based on chemical vapor deposition (CVD) are being explored. Crystals grown by homoepitaxy on seeds from the high pressure method excel in structural quality but suffer from severe size limitations. In contrast, heteroepitaxy on iridium using the multilayer substrate Ir/YSZ/Si(001) has recently provided the first real wafer with a diameter of 92 mm (155 carat). While dislocation densities of 7 $\times 10^6$ cm^{-2} and mosaic spread values of 0.03° (polar) and 0.05° (azimuthal) document significant progress, the defect structure is still inferior to homoepitaxial diamond. After reviewing the current state of the art, recent and new attempts for further reduction of the dislocation densities are described. These comprise different variants of epitaxial lateral overgrowth (ELO) and metal assisted termination (MAT). Next, the electronic properties of threading dislocations in heteroepitaxial diamond have been investigated. Experimentally derived lifetime values enable estimations of capture cross sections for electrons and holes. In the final part, a new smart-cut technique is presented that facilitates a duplication of large area diamond wafers removing the need for new nucleation and elaborate dislocation density reduction procedures to be applied for every new wafer.

Invited Talk KFM 4.2 Tue 14:45 H2

Development of diamond based kinetic inductance detectors — •Francesco Mazzocchi, Dirk Strauss, and Theo Scherer — KIT IAM-AWP

Kinetic Inductance Detectors (KIDs) have proven themselves as a very versatile cryogenic detector technology capable of applications in various fields due to their flexibility of design, sensibility and ease of production. We have recently proposed a polarization sensitive Lumped Elements KID as sensor for an innovative polarimetric diagnostics based on quantum cascade lasers (QCL) for application in the nuclear fusion. Each detector unit is composed by 4 pixels arranged at the vertices of a square, each pixels being sensible to only one polarization direction. The current system is based on niobium nitride (NbN) superconductor over High Resistivity Silicon (HRSi) substrate. Such material delivers good performances but its relatively high dielectric constant and loss tangent lead to increased substrate losses. Using a transparent substrate may improve this aspect and also the radiation resistance of such devices. Diamond is the substrate of choice, being a material already widely studied and used in the fusion environment as high power microwave window, due to its outstanding optical and mechanical performances. In this work we present the preliminary design study for a diamond based Kinetic Inductance Detector and subsequent characterization measurements of the first prototypes.

KFM 4.3 Tue 15:15 H2

MPA CVD diamond in nuclear fusion: dielectric characterization and influence of defects — •Gaetano Aiello, Theo Scherer, Andreas Meier, Sabine Schreck, and Dirk Strauss — Karlsruhe Institute of Technology, Institute for Applied Materials, D-76021 Karlsruhe, Germany

Microwave Plasma Assisted (MPA) Chemical Vapour Deposition (CVD) diamond is used as window material in the shape of a disk in the heating and diagnostic systems for fusion reactors due to its combination of extraordinary thermal, mechanical and optical properties. CVD diamond polycrystalline disks with central loss tangent lower than 2E-05 allow for transmission of high power microwave beams (1-2 MW). However, the effect on the dielectric losses in diamond of defects like dislocations and nitrogen-vacancy centers introduced by the growing process and/or by subsequent neutrons and gammas irradiation has not fully investigated and understood so far. Investigations by several spectroscopic methods on non-irradiated and irradiated diamond samples are thus planned. In particular, first Elastic Recoil Detection Analysis (ERDA) measurements of small diamond samples have been carried out at the Tandem Laboratory in Uppsala, Sweden, aiming to calculate the sample composition with major focus on nitrogen content. The nitrogen plays an important role in the CVD process as it allows faster growth rates, but it causes greater dielectric losses in diamond.

KFM 4.4 Tue 15:35 H2

Defect structures related to dielectric properties in diamond — •Theo Scherer, Gaetano Aiello, Sabine Schreck, Andreas Meier, and Dirk Strauss — KIT Karlsruhe (IAM-AWP)

State of the art windows used in high power electron cyclotron heating and current drive systems for large fusion devices such as ITER consist of a disk which is aligned perpendicular to the millimetre wave beam propagation. As reflection have to be kept on a minimal level, the window thickness restricts the allowed frequencies to a limited set defined by multiples of half wavelengths in the dielectric matter. Actual loss tangent values are several 1E-6 for the best polycrystalline materials. For frequency tunable systems in fusion reactors, corresponding to the gyrotron development, BREWSTER windows must be realized, where the elliptic cut diamond disk is inclined under the BREWSTER angle in the waveguide structure.

KFM 4.5 Tue 15:55 H2

Photoconductive gain in single crystal diamond detectors used for dosimetry — •Theodor Grünwald, Christina Bestele, and Matthias Schreck — Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

Diamond crystals equipped with metal electrodes can be used for the detection of energetic radiation, i.e., x-rays, γ-rays and ionizing particles. Operated as solid state ionization chamber, single α-particles are completely stopped generating e-h pairs which can be collected with a maximum efficiency of ∼ 100%. When the same device is used as dosimeter in high intensity beams of energetic photons or particles, photoconductive gain G with values from < 1 to > 10^6 have been observed by various groups. This contribution analyzes first theoretically the irradiation induced conductivity of perfect diamond single crystals containing nitrogen and boron as electronically active defects. A system of coupled rate equations is formulated for the charging states of N and B, the concentration of electrons in the conduction band plus the neutrality condition. Analytical solutions are obtained for the gain as a function of the impurity concentrations, the detector thickness and the excitation density. The theoretical predictions cover the full range of experimentally derived values in literature. Photocurrent measurements on three series of heteroepitaxial samples grown under nearly identical conditions yielded G values ranging from < 1 to > 10^4. All the data are interpreted in terms of the measured absolute boron concentrations N_B and the potential concentrations N_N of nitrogen. In addition, the role of the dislocations as charge carrier traps is discussed.

KFM 5: Poster Session KFM

Time: Tuesday 16:00–17:00 Location: P

KFM 5.1 Tue 16:00 P

Integration of physics instruments of the ITER EC Upper Launcher — •Peter Späh, Gaetano Aiello, Andreas Meier, Theo Scherer, Sabine Schreck und Dirk Strauss — Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Hermann-von-Helmholtz-Platz 1

Physics instruments installation often causes challenging mechanical design requirements and components must be protected properly from harsh environmental conditions. This is particularly the case for fusion plants like ITER, where sensitive applications shall operate under severe conditions in terms of heat, mechanical loads and radiation.

For ITER an EC Heating and Current Drive System has been designed where delicate components like microwave reflectors (mirrors), corrugated waveguides, mirror actuators, dielectric transmission devices (CVD Diamond windows) and shutter valves were precisely integrated into heavy system components, designed to sustain substantial mechanical loads and equipped with powerful cooling systems and radiation shielding.

This poster presents the mechanical integration of physics instruments of the ITER EC Upper Launcher and their connection to appropriate cooling systems.

KFM 5.2 Tue 16:00 P

Application of CVD Diamond disks for ECRH systems of fusion reactors — •Sabine Schreck, Gaetano Aiello, Andreas Meier, Theo Scherer, and Dirk Strauss — Karlsruhe Institute of Technology, Institute for Applied Materials, D-76021 Karlsruhe, Germany

In fusion reactors, Electron Cyclotron Heating and Current Drive (EC H&CD) systems are used for plasma heating and stabilization. Key components of these systems are diamond windows, which consist of a chemical vapor deposition (CVD) diamond disk (p.c.) joined into a metallic housing. Such windows, employed as gyrotron- or torus windows, allow transmission of high power microwave beams and serve as vacuum boundaries. A very low dielectric loss and a sufficient mechanical stability is thus required.

The ITER EC torus window consists of a diamond disk with a diameter of 70mm and a thickness of 1.11mm (resonance thickness for 170GHz). The window serves also as confinement barrier for tritium and is classified as "Protection Important Component". A specific test program is required for its qualification, including prototypical activities. For future fusion machines like DEMO, most likely broadband window solutions as the double disk window or the Brewster window will come into operations. This implies also new requirements for the disks, e.g. large diameters of minimum 180mm for the inclined Brewster-angle disk for a typical aperture of 63.5mm.

KFM 5.3 Tue 16:00 P

Time-Resolved Nonlinear Diffuse Femtosecond-Pulse Reflectometry Using Lithium Niobate Nanoparticles with Two Pulses of Different Colors — •Jan Klenen[1,2], Christian Kijatkin[1,2], Björn Bourdon[1,2], Laura Vittadello[1,2], and Mirco Imlau[1,2] — [1]Department of Physics, Osnabrück University, Germany — [2]Center for Cellular Nanoanalytics, Osnabrück University, Germany

In the context of biophotonics and material science, harmonic nanoparticles (HNPs) attract elevated interest owing to their versatile nonlinear optical (NLO) properties, such as their broad spectral tunability [C. Kijatkin, *Photonics* **2017**, *4*, 11]. However, the characterization of the time-evolution of light-matter interaction in such nanoscale media is yet to be completed. In this study we are using femtosecond-pulse diffuse reflectometry to investigate the time-resolved sum-frequency generation (SFG) of two differently colored, infrared femtosecond laser pulses in lithium niobate nanoparticle pellets [C. Kijatkin, *Adv. Photonics Res.* **2020**, DOI: 10.1002/adpr.202000019]. The pulse shape of the remitted SFG shows an asymmetry in the temporal domain. This finding can be explained within the framework of light propagation in random media and is generalized on the basis of numerical simulations. As a consequence, ultrashort pulse shapes can now be comprehensively predicted in nanoscale, densely packed media with a NLO response. In this respect we discuss the potential of HNPs as a flexible alternative to crystalline media for the determination of a pulses chirp. Funded by the DFG (IM37/12-1, FOR 5044, INST 190/165-1 FUGG).

KFM 5.4 Tue 16:00 P

Ferroelektrischer Phasenübergang in Mg dotiertem $LiNbO_3$ — •Leonard Verhoff und Simone Sanna — Justus-Liebig-Universität, Gießen, Deutschlnd

Lithiumniobat ($LiNbO_3$) ist besonders in der Optoelektronik ein beliebtes Material und nimmt dort den Stellenwert von Silizium in der Elektronik ein.

Eine Dotierung mit Magnesium kann eine Verminderung von Eigendefekten im Material bewirken, was zu einer geringeren Photorefraktivität führen kann.

$LiNbO_3$ besitzt bei tiefen Temperaturen eine ferroelektrische Phase, allerdings ist der Phasenübergang in die paraelektrische Phase nicht besonders gut bekannt. Wir haben *ab initio* Moleküldynamik im Rahmen der Dichtefunktionaltheorie verwendet, um einen Einblick in die Dynamik des Phasenübergangs von reinem und Mg dotiertem $LiNbO_3$ zu erhalten.

Dabei ergibt sich in beiden Fällen ein Phasenübergang 2. Ordnung. Zudem erhalten wir durch die Dotierung eine Steigerung der Curie- Temperatur und des Absolutwerts der spontanen Polarisation bei 0 K.

KFM 5.5 Tue 16:00 P

Theoretische Bestimmung der minimalen Energiepfade und Energiebarrieren für die Diffusion von Lithium und Sauerstoff in Lithium-Niobat und Lithium-Tantalat — •Brendan Muscutt und Simone Sanna — Justus-Liebig-Universität, Gießen, Deutschland

Lithium-Niobat (LN) und Lithium-Tantalat (LT) sind von herausragender Bedeutung für aktuelle Forschung und Technik, denn sie besitzen u.a. einzigartige ferroelektrische und elektro-optische Eigenschaften.

Um die Kristalle auf verschiedenste technische Anwendungen optimal anpassen zu können, müssen auch die Stabilität bzw. die Dynamik von Defekten und möglichen Defektstrukturen im Detail verstanden werden.

In unserer Arbeit wurden LN- und LT-Kristalle mit Lithium- und Sauerstoff-Leerstellen simuliert. Auf Basis der Dichtefunktionaltheorie und mit Hilfe der *climbing image nudged elastic band method* wurden dann die Energiebarrieren und minimalen Energiepfade für die Lithium- und Sauerstoff-Leerstellendiffusion *ab initio* berechnet.

Die Ergebnisse lassen in beiden Stoffen auf eine hohe Dynamik der Lithium-Leerstellen bei Temperaturen ab etwa 200 Grad Celsius schließen. Die Sauerstoff-Diffusion findet laut Berechnungen dagegen bereits bei Raumtemperatur statt.

Die Erkenntnisse können bei der Modellierung von Defektstrukturen in LN und LT sowie zur Deutung von entsprechenden Transport-Messungen genutzt werden.

KFM 5.6 Tue 16:00 P

Defect physics in $LiTaO_3$ — •Mike Nico Pionteck, Jonas Fey, and Simone Sanna — Institut für Theoretische Physik und Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

While the defect physics of $LiNbO_3$ has been object of many investigations, the nature of point defects in the isomorphic and isoelectronic $LiTaO_3$ is much less known. Although the existence of small bound polarons [1,2] in $LiTaO_3$ might be expected due to the high lattice polarizability, the verification of this assumption is still missing. In this work we provide the atomistic description of small bound polarons $Ta_{Li}^{5+/4+}$ in $LiTaO_3$ and of many other point defects such as Ta and Li vacancies. The calculations performed within density functional theory with Hubbard corrections predict the large lattice relaxation of the oxygen ligands associated to the electronic capture at the antisite center, which can be interpreted as due to the polaron formation. The relative formation energies of the investigated defects closely mirror those of corresponding defects in $LiNbO_3$ [3], suggesting a rather similar defect physics in the two materials. [1] O. F. Schirmer et al., J. Phys.: Condens. Matter **21**, 123201 (2009). [2] F. Freytag et al., Nature Scientific Reports **6**, 36929 (2016). [3] Y. Li, W. G. Schmidt, S, Sanna, Phys. Rev. B **89**, 094111 (2014).

KFM 5.7 Tue 16:00 P

Vibrational properties of strained $LiNbO_3$ and $LiTaO_3$ crystals — •Mike Nico Pionteck and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

The investigation of Raman frequencies is a widely used non-destructive way to characterize crystalline solids and nanostructures. X-ray diffraction measurements have shown that domain walls in $LiNbO_3$ and $LiTaO_3$ behave like compressed bulk material [1]. Hence, knowledge of the dependence of Raman frequencies on uniaxial strain can help, i.a., to characterize domain walls in $LiNbO_3$ and $LiTaO_3$ crystals.

In our work, we model the vibrational properties of $LiNbO_3$ and $LiTaO_3$ crystals from first principles as a function of compressive and tensile strain in *x*-, *y*- and *z*-direction. The calculations show a roughly linear dependence of the phonon frequencies on the applied strain, which is similar for $LiNbO_3$ and $LiTaO_3$ crystals. The frequencies increase linearly under compressive strain. On the other hand, they decrease linearly under tensile strain. In particular, we observe a strong dependence on strain in *x*- and *y*-direction for the E TO_5 and TO_6 modes which can be thus exploited as markers of the strain. While E modes of unstrained $LiNbO_3$ and $LiTaO_3$ crystals are degenerate [2], we predict non-degenerate E modes under strain, due to the breaking of rotational symmetry by strain in *x*- and *y*-direction. [1] M. Rüsing et al., Phys. Rev. Mat. **2**, 103801 (2018). [2] S. Sanna et al., Phys. Rev. B **91**, 224302 (2015).

KFM 5.8 Tue 16:00 P

Light-induced transient absorption of lithium niobate as a function of temperature and composition — •Mira Hesselink, Simon Messerschmidt, Laura Vittadello, and Mirco Imlau — Department of Physics, Osnabrueck University, Germany

Small polaron hopping in lithium niobate, $LiNbO_3$ (LN), takes a crucial role in optical process. Its behavior is investigated with a systematic study as a function of temperature, composition and doping. [Messerschmidt, S. *et al. Crystals* **2020**, 10, 109.; Vittadello, L. *et al. Crystals* **2018**, 8, 294.] The number and type of hopping processes are measured by means of light-induced transient absorption spectroscopy. All measurements are performed in a cryostat using a setup with ns-pump and cw-probe. Different sample compositions and dopings (Fe- or Mg-doped LN) go along with different polaron traps inside the crystal. At room temperature, the absorption signals decay in the range of milliseconds, while at lower T the processes are slowed down extensively. The decay rate of the light-induced absorption in Mg:LN appears Arrhenius temperature dependent in range 200K - 120K but this dependence weakens and becomes non-Arrhenius as T is lowered. For the Fe:LN, it is observed that different temperatures lead to different hopping processes by measuring the activation energy. Moreover, the experimental results are in good coincidence with numerical and analytical models based on the Holstein theory. At elevated T ionic diffusion is expected to play a big role and the influence on polaronic charge transport is to be investigated in a next step. Financial support by the DFG (IM3/12-1, FOR 5044) is gratefully acknowledged.

KFM 5.9 Tue 16:00 P

In-vivo tracking of potassium niobate nanoparticles by means of the TIGER microscope — •Laura Vittadello[1], Jan Klenen[1], Karsten Koempe[2], and Mirco Imlau[1] — [1]Department of Physics, Osnabrueck University, Germany — [2]Department of Biology/Chemistry, Osnabrueck University

In recent year, remarkable progress in the area of in-vivo harmonic nanoparticle (HNPs)-based nonlinear optical (NLO) microscopy has been reported. From one side the NLO microscopy has emerged as a successful tool within the biomedical research field enabling the imaging of intact living organisms. From the other side, polar ferroelectric HNPs have been identified as a good marker candidate in such type of technique for their high nonlinear optical coefficients. Despite of this success, realtime in-vivo tracking based on HNPs has not been exploited so far, mainly because of a lack of an appropriate microscopy tool, i.e. a nonlinear optical widefield microscope. We realised this by means of a regeneratively amplified fs-laser coupled to an inverted microscope creating an easy alignable and reproducible Tunable hIGh Energy (TIGER) widefield microscope [Vittadello *et al.* Opt. Mater. Express 11, 1953-1969 (2021)]. This new approach is successfully applied for HNPs tracking in a area up to $1.5 \, x \, 1.5 \, mm^2$ in the blood flow of the heart system of a *Drosophila* larvae, a powerful platform to study social relevant diseases, such as congenital heart defects in human beings. The goal is to access the blood circulation in the heart of a larve, a quantity directly linked to the presence of cardiac disease. Financial support (DFG INST 190/165-1) is gratefully acknowledged.

KFM 5.10 Tue 16:00 P

Einsichten in den Phasenübergang von LiNbO3 und LiTaO3 — •Nils André Schäfer und Simone Sanna — Justus-Liebig-Universität, Gießen, Deutschland

Lithiumniobat (LiNbO3, LN) sowie Lithiumtantalat (LiTaO3, LT) sind ferroelektrische Kristalle, die unter anderem in der integrierten Optik oft eingesetzt werden.

Niob und Tantal kommen in der gleichen Nebengruppe vor und sind chemisch sehr ähnlich. Dementsprechend kristallisieren LN und LT in derselben Struktur, sowohl in der ferroelektrischen Phase (mit Raumgruppe R3c) als auch in der paraelektrischen Phase (mit Raumgruppe R-3c). Dennoch weisen diese Stoffe eine um 500 K voneinander abweichende Curie-Temperatur auf.

Der Phasenübergang von der ferroelektrischen in die paraelektrische Phase beider Stoffe ist bisher noch nicht gut verstanden und daher ist der Ursprung dieser überraschend großen Diskrepanz nicht geklärt. Um Ähnlichkeiten und Unterschiede beider Phasenübergänge zu untersuchen, haben wir *ab initio* Molekulardynamik Simulationen im Rahmen der Dichtefunktionaltheorie durchgeführt. Unsere Rechnungen zeigen, dass, obwohl die Mechanismen der Phasenübergänge ähnlich sind, die Temperaturbereiche in denen sie stattfinden sehr voneinander abweichen.

KFM 5.11 Tue 16:00 P

Comparative evaluation of polar oxide $LiTaO_3$ and $LiNbO_3$ by means of ultrafast transient absorption and luminescence spectroscopy — •Anton Pfannstiel, Andreas Krampf, and Mirco Imlau — Univ. of Osnabrück, School of Physics, Germany

The two model systems $LiNbO_3$ (LN) and $LiTaO_3$ (LT) are commonly assumed to show equivalent (nonlinear) optical and electrical response and that the possibility to generate self-localized quasiparticles, such as polarons and self-trapped excitons exists in both systems. The latter are thoroughly studied in LN however, for LT there is nearly no information available in literature so far. We have adressed this topic by a systematic study on pulse induced transient absorption and luminescence of LN and LT [A Krampf *et al* 2021 *New J. Phys.* 23 033016].

As a result, a qualitatively similar behavior is found that can be attributed to the presence of Nb_{Li}^{4+} and Ta_{Li}^{4+} polarons as-well-as to the formation of excitonic states localized at Nb-O-octahedra. But, a more closer inspection of the data set reveals significant differences in the temporal behavior. In particular, specific time constants are found for short- and long term relaxation.

Discussion of the results is based on the individual crystallographic characteristics, defects, optical features, but also in conjuncture with *ab-initio* modeling results for carrier self-localization in both systems. A conclusion for the ultrafast optical response in $LiNb_xTa_{1-x}O_3$ mixed crystals is deduced. Financial support by the DFG (IM 37/12-1, FOR5044, INST FUGG) is gratefully acknowledged.

KFM 5.12 Tue 16:00 P

High pressure and temperature X-ray emission and diffraction studies of iron containing minerals at the European XFEL — •Johannes Kaa[1,2], Christian Sternemann[2], Christian Albers[2], Karen Appel[1], Valerio Cerantola[1], Mirko Elbers[2], Lélia Libon[3], Mikako Makita[1], Thomas Preston[1], Sylvain Petitgirard[4], Christoph Sahle[5], Georg Spiekermann[3,4], Christian Plückthun[1], Vladimir Roddatis[6], Metin Tolan[2], Max Wilke[3], Ulf Zastrau[1], and Zuzana Konopkova[1] — [1]European X-ray Free-Electron Laser Facility GmbH, Holzkoppel 4, 22869 Schenefeld, Germany — [2]TU Dortmund Fakultät Physik DELTA, Maria-Goeppert-Mayer-Straße 2, 44227 Dortmund, Germany — [3]University of Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany — [4]ETH Zürich, Rämistrasse 101, 8092 Zürich, Switzerland — [5]European Synchrotron Radiation Facility ESRF, 71 Avenue des Martyrs, 38000 Grenoble, France — [6]Geoforschungszentrum Telegrafenberg, 14473 Potsdam, Potsdam, Germany

Data on the spin state of iron bearing minerals are scarce at high temperatures and pressures found in the deep Earth's interior, due to limitations of the commonly used techniques to heat and probe the spin state in situ. To overcome these limitations, we conducted an experiment with a different approach. We used the unique properties of a pulsed and highly brilliant XFEL beam that allowed us to heat samples contained in a DAC via X-ray heating, while measuring X-ray emission and X-ray diffraction on $FeCO_3$ pressurized within a diamond anvil cell at the HED instrument at the Eu-XFEL.

KFM 5.13 Tue 16:00 P

X-ray emission scanning imaging setup to study electronic structure of iron bearing compounds in-situ at conditions of the Earth's mantle — •Christian Albers[1], Georg Spiekermann[2], Lélia Libon[3], Robin Sakrowski[1], Max Wilke[3], Johannes Kaa[4], Nicola Thiering[1], Hlynur Gretarrson[5], Martin Sundermann[5], Metin Tolan[1], and Christian Sternemann[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, Dortmund, Germany — [2]Institut für Geochemie und Petrologie, ETH Zürich — [3]Institut für Geowissenschaften, Universität Potsdam, Potsdam, Germany — [4]HED Group, European XFEL GmbH, Hamburg, Germany — [5]Deutschen-Elektronen-Synchrotron DESY, Hamburg, Germany

The determination of the electronic structure in iron-bearing compounds under high pressure and high temperature (HPHT) conditions is of crucial importance for the understanding of the Earth's interior and planetary matter.

We present a setup to investigate the electronic structure of iron-bearing compounds *in-situ* at HPHT conditions using X-ray emission spectroscopy (XES) and show first results for tetracarbonate phases emerged from laser heated siderite ($FeCO_3$) at about 80 GPa and 3000 K. Information on the spin state are obtained by *in-situ* XES of the iron's Kβ-emission. A dedicated sample preparation together with highly intense synchrotron radiation shortens the duration of the measurements to an extend that *in-situ* XES, including valence-to-core XES, as well as *in-situ* spin state imaging becomes feasible.

KFM 5.14 Tue 16:00 P

Investigation of the Electronic Structure of Iron in Bridgmanite at Deep Mantle Pressure Conditions by (Resonant) X-ray Emission Spectroscopy — •Robin Sakrowski[1], Georg Spiekermann[2], Christian Albers[1], Nicola Thiering[1], Lélia Libon[3], Hlynur Gretarsson[4], Martin Sundermann[4], Jean-Pascal Rueff[5], James Ablett[5], Metin Tolan[1], Max Wilke[3], and Christian Sternemann[1] — [1]Faculty of Physics/DELTA, TU Dortmund University — [2]Institute of Geochemistry and Petrology, ETH Zurich — [3]Institute of Geosciences, University of Potsdam — [4]Deutsches-Elektronen-Synchrotron DESY — [5]Synchrotron SOLEIL

We study the controversially discussed iron spin state in pressurized ferrous (Fe^{2+}) and ferric (Fe^{3+}) bridgmanite, as well as coordination state and oxidation state. For that, we use a combination of novel approaches like in situ resonant X-ray emission (RXES) at the iron K-pre-edge region, iron Kβ- and valence-to-core (vtc) X-ray emission spectroscopy (XES). We evaluate the Fe K pre-edge feature position and intensity from Kα HERFD XANES. Consequently, these methods help to further constrain the observed gradual (ferrous) or sharp (ferric) change in spin state, local coordination and oxidation state of iron in ferrous- (up to 140 GPa) and ferric- (up to 75 GPa) bridgmanite, aiming to solve the controversy on the iron's spin state in bridgmanite.

KFM 5.15 Tue 16:00 P

Spatially-resolved lithium and electrolyte distribution in cylindrical 18650-type lithium-ion batteries — •Dominik Petz[1,2], Anatoliy Senyshyn[2], and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, Garching, Deutschland — [2]Heinz Maier-Leibnitz Zentrum, Garching, Deutschland

Extensive cycling of lithium-ion batteries leads to a partial loss of their capacity due to various side effects like formation of the solid-electrolyte-interphase (SEI), loss of active lithium etc. Typical profiles of side reactions, instantaneous temperature and current density display non-uniform distributions throughout the volume, which leads to a stabilization of intrinsic heterogeneous state in the Li-ion battery. The loss of active lithium is typically correlated with the formation of SEI during cycling, whereas the quantitative role of electrolyte in the cell operation and cell fatigue remains not fully quantified yet.

In the current study we report an attempt of non-destructive quantification of lithium and electrolyte, their spatial distribution throughout the cell and concentration changes vs. cell fatigue. Combined experimental studies including electrochemistry, X-ray computed tomography, and neutron diffraction are applied for 18650-type cylinder cell with NCA|C chemistry. High-resolution neutron diffraction independently reveals a direct volume-averaged correlation between losses of active lithium in the graphite anode and these of the liquid electrolyte. The 3D lithium distribution is mapped by spatially resolved neutron powder diffraction, displaying the non-trivial character of active lithium and electrolyte losses.

KFM 5.16 Tue 16:00 P

Polar oxides: Electrical conductivity of LiNb1-xTaxO3 solid solutions from 400 to 800 °C in air — •Ahsanul Kabir, Vanik Sargsyan, Yuriy Suhak, Stepan Hurskyy, and Holger Fritze — Institute of Energy Research and Physical Technologies, Clausthal University of Technology, Am Stollen 19 B, 38640 Goslar, Germany

The electrical conductivity of lithium niobate-lithium tantalate (LNT, LiNb0.5Ta0.5O3) solid solutions is studied in air at temperatures ranging from 400 to 800 °C. The results were compared with lithium niobate (LN) and lithium tantalate (LT) reference samples grown by the Czochralski method, received from the Institute of Microelectronics Technology and High Purity Materials (IMT), Russia, and Precision Micro-Optics (PMO), USA, respectively. Electrical conductivity was measured by impedance spectroscopy in the frequency range of 1 MHz-1 Hz. Over the studied temperature range, LNT sample displays similar electrical conductivity to LN/LT (IMT), e.g. with a value of 2.9*10-4 S/m at 600 °C. In contrast, LN/LT (PMO) compounds illustrate conductivity that is nearly 2 times higher than that of their counterparts. As noticed, the conductivity follows an Arrhenius relation, uncovering a single thermally activated process. The activation energy ranges from 1.20-1.25 eV which is a typical value for the ionic migration in the lithium niobate family and is governed by mobile lithium (Li) vacancies. This result is consistent with theoretical modeling, which predicts the spontaneous formation of Li vacancies in the band gap for a wide range of Fermi energy values. The research is funded by the German Research Foundation and done within the research unit 5044.

KFM 5.17 Tue 16:00 P

Tracking ferroelectric domain formation during epitaxial growth of $PbTiO_3$ films — •Martin F. Sarott, Manfred Fiebig, and Morgan Trassin — Department of Materials, ETH Zurich, Switzerland

The pronounced impact of growth conditions on the formation of domains in ferroelectric thin films obstructs the effective design of devices based on ferroelectrics that require controlled polarization states. Here, we overcome this notorious difficulty by tracking in-situ, during growth, the ferroelectric domain formation in ultrathin films of the tetragonal ferroelectric model system $PbTiO_3$. By combining in-situ optical second harmonic generation (ISHG) with post-growth piezoresponse force microscopy and ex-situ SHG imaging, we identify the thickness threshold for the epitaxial strain-driven partial conversion of out-of-plane polarized c-domains into in-plane oriented a-domains during the deposition. Furthermore, we find that in the strongly compressive regime the formation of a-domains is triggered during the early stages of growth, which favors a remarkable randomization in the distribution of a- and c-domains upon further deposition. This extraordinary heterogeneity is reminiscent of the domain distribution at the morphotropic phase boundary in technologically relevant PZT and thus highlights the significance of control over the c-to-a domain interconversion for applications.

KFM 5.18 Tue 16:00 P

Impact of domain walls on ferroelectric switching: an ab initio based MD study on orthorhombic $BaTiO_3$ — •Yijing Yang, Ruben Khachaturyan, and Anna Grünebohm — ICAMS, RUB, Bochum, Germany

Ferroelectric switching by domain walls motion is very important for many applications. In this work, we explore the coupling between the external electric field and domain walls in the so far rarely explored orthorhombic phase of $BaTiO_3$. Therefore, we employ molecular dynamics simulations using the effective Hamiltonian approach [1, 2] to study the electric field induced domain wall motion and the local polarization on the walls. In particular, we find polarization vortices on 180° nonelastic domain wall which can minimize the charge density.

[1] A. Grünebohm and M. Madhura, Phys. Rev. Mater. 4, 114417 (2020)
[2] T. Nishimatsu et al. Phys. Rev. B 82.13, 134106 (2010)

KFM 5.19 Tue 16:00 P

Second-harmonic microscopy in optically confining nanostructures — •Zeeshan Hussain Amber[1], Benjamin Kirbus[1], Michael Rüsing[1], and Lukas M Eng[1,2] — [1]Technische Universität Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence EXC 2147, TU Dresden, 01062, Dresden, Germany

Second-harmonic (SH) microscopy is a very power tool for investigating material properties and noninvasively visualising domains and domain walls in ferroelectic materials [1,2]. Contrary to the conventional assumption when working with a confining structure such as a thin film, the co-propagating phase matched SH signal may also be detected in back-reflection. Interference effects further affect the SH response. Therefore understanding the effects of geometrical confinement is necessary.

We performed SH experiments on wedge-shaped samples of 5% Mg-doped congruent Lithium tantalate, un-polled & Periodically polled Lithium niobate and compared them with full-vectorial numerical calculations of the SH process [1,3]. We found that the coherent interaction length obtained from the back-reflected SH signal is that of co-propagating phase matched signal. The excellent agreement between the simulated and experimental data confirms that co-propagating signal is detected in back-reflection geometry.

[1] M. Ruesing et al., J. Appl. Phys. 126,114105 (2019).
[2] S. Cherifi-Hertel et al., Nat. commun 8,15768 (2017).
[3] D. Sandkuijl et al., J. Opt. Soc. Amer. B 30, 382 (2013)

KFM 5.20 Tue 16:00 P

Colossal dielectric constant in h-$ErMnO_3$ — •Lima Zhou[1], Lukas Puntigam[1], Markus Altthaler[1], Dennis Meier[2], István Kézsmárki[1], Donald M. Evans[1], and Stephan Krohns[1] — [1]University of Augsburg, 86159, Augsburg, Germany — [2]NTNU Norwegian University of Science and Technology, 7034, Trondheim, Norway

Ferroelectric domain walls can be in some specific cases created, erased and rewritten making them interesting as functional nanoscale object in electronics. In the improper ferroelectric system h-$ErMnO_3$ memristive switching and rectification of charged domain walls has been shown. Here, we explore if also the more insulating domain walls provide functionality in terms of an internal barrier layer capacitance leading to colossal dielectric constants. A recent work [1] already demonstrated via bulk dielectric spectroscopy that insulating domain walls are responsible for a dielectric relaxation-like feature. Our approach is to reveal the dielectric properties for a h-$ErMnO_3$ single crystal before and after a distinct heat treatment leading to an increase in domain size by a factor of 10. Interestingly, the dielectric constant most likely ascribed to the internal barrier layers increases also by a factor of 10 according to the decrease of the volume fraction of the insulating domain walls (overall decrease in insulating barrier thickness giving rise to higher capacitance). With this work we provide a strategy of designing colossal dielectric constant based on internal insulating domain wall barriers. [1] Puntigam et al., *Journal of Applied Physics* **129**, 074101 (Feb. 2021)

KFM 5.21 Tue 16:00 P

Quantitative mapping of nanotwin variants and elastic energy in the bulk — •Jan Schultheiss[1], Lukas Porz[2], Lalitha Kodumudi Venkataraman[2], Marion Höfling[2], Can Yildirim[3], Phil Cook[3], Carsten Detlefs[3], Semen Gorfman[4], Jürgen Rödel[2], and Hugh Simons[5] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Technical University of Darmstadt, Darmstadt, Germany — [3]European Synchrotron Radiation Facility, Grenoble, France — [4]Tel Aviv University, Tel Aviv, Israel — [5]Technical University of Denmark, Lyngby, Denmark

Most state-of-the-art high-resolution imaging techniques are limited to probing the sample surface. This is a particular drawback for the characterization of twinned materials as the strain state changes from biaxial at the surface to triaxial in the bulk, dramatically influencing the functional properties. Here, we demonstrate mapping of nanotwin variants highly localized in the bulk utilizing the full reciprocal space intensity distributions obtained from Dark-Field X-Ray micorscopy. We demonstrate our method for a high-performance polycrystalline ferroelectric/ferroelastic (Ba,Ca)(Zr,Ti)O_3 model system whose excellent piezoelectric properties originate from domain sizes of 10-100 nm. We find that the density of twin variants inside the grain is 30% smaller compared to the density in the vicinity of the grain boundary, following the trend of the elastic energy. The obtained elasto-morphological correlations are crucial for many twinned materials, ranging from complex oxides to martensitic materials or high entropy alloys.

KFM 5.22 Tue 16:00 P

X-ray emission spectroscopy setup at beamline BL9 of DELTA — •Nicola Thiering[1], Eric Schneider[1], Kevin Lehninger[1], Christian Albers[1], Florian Otte[1,2], Johannes Kaa[1,2], Michael Paulus[1], Christian Sternemann[1], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund, Germany — [2]European XFEL, Holzkoppel 4, D-22869 Schenefeld, Germany

Beamline BL9 is a multi-purpose X-ray scattering and spectroscopy beamline at the synchrotron radiation facility DELTA located at the TU Dortmund, Dortmund, Germany. The beamline is served by a new superconducting wiggler which provides X-rays in the energy range between 5 and 30 keV. Recently, a setup for X-ray emission spectroscopy was implemented exploiting a von Hamos type spectrometer by combination of cylindrically bent analyzers with a Pilatus 100k area detector. This setup allows to study electronic valence and core hole excitations of low Z elements as well as transition metals. The current experimental setup will be presented along with selected samples of typical applications and the first experimental results.

KFM 5.23 Tue 16:00 P

Nested mirror systems for neutron extraction, transport and focusing — •Christoph Herb[1], Oliver Zimmer[2], Robert Georgii[1,3], and Peter Böni[1] — [1]Physics Department E21, Technical University Munich, 85748 Garching, Germany — [2]Institute Laue-Langevin, F-38042 Grenoble, France — [3]Heinz Maier-Leibnitz Zentrum, Technical University Munich, 85748 Garching, Germnay

The investigation of small samples by neutron scattering is usually very time consuming due to the low neutron flux of contemporary sources and small signals from the sample. Elliptic neutron guides are used to transport neutrons over large distances to make room for additional beamlines and for improving the signal-to-noise ratio by focusing the available neutrons onto the sample. However, elliptic guides do not image objects properly due to coma aberrations. We propose using nested arrays of short elliptic mirrors to reduce the coma aberrations.

We report on the investigation of a nested mirror optic at the MIRA beamline. The key properties of the optic are a large brilliance transfer of approximately 72% and the possibility of adjusting the beam size and the divergence of the neutron beam at the sample position by apertures placed before the nested mirror optic. Therefore, no beam shaping devices are required close to the sample position, thus reducing the background.

Nested mirrors will also be particularly useful for the efficient extraction of neutrons from small, highly brilliant moderators such as at the ESS, since common illumination losses associated with using neutron guides are mitigated.

KFM 5.24 Tue 16:00 P

Intrinsic electronic structure of TiCoSb half-heusler single crystals by ARPES — •Federico Serrano-Sanchez[1], Mengyu Yao[1], Suchitra Prasad[1], Andrei Gloskovskii[2], Alexander Fedorov[3], Gudrun Auffermann[1], Ulrich Burkhardt[1], Gerhard Fecher[1], Claudia Felser[1], Yu Pan[1], and Chenguang Fu[1] — [1]MPI-CPfS, Dresden, Germany — [2]DESY, Hamburg, Germany — [3]HZB fur Materialien und Energie, Berlin, Germany

In half-Heulser thermoelectric TiCoSb, defects yield elusive intrinsic properties and a wide range of properties reported in the literature[1-3]. To tackle these inconsistencies, single crystals of TiCoSb have been grown and their crystallographic and electronic properties characterized. The crystals display an almost perfect stoichiometry, while XRD display the half-Heusler $F\bar{4}3m$ structure only. Electrical resistivity shows a metallic behaviour due to the intrinsic p-type nature of the crystals, while the temperature evolution of the conductivity indicates the presence of point defects. Nevertheless, no in-gaps states in the valence band top are detected by HAXPES, suggesting the absence of interstitial defects. ARPES displays a diffusive surface state above the VBM and the band convergence at the L and Γ band maxima points, which is compared to previous theoretical calculations and gives a further hint on the excellent electronic performance of this family of materials.

[1] S. Ouardi *et al.*, Phys. Rev. B - Condens. Matter Mater. Phys., 2012, 86, 045116. [2] E. Rausch *et al.*, Acta Mater., 2016, 115, 308-313. [3] P. Dey and B. Dutta, Phys. Rev. Mater., 2021, 5, 35407.

KFM 6: Skyrmions I (joint session MA/KFM)

Time: Wednesday 10:00–13:15 Location: H5

See MA 7 for details of this session.

KFM 7: Dielectric, Elastic and Electromechanical Properties

Chairman: Stephan Krohns (University of Augsburg)

Time: Wednesday 10:00–10:45 Location: H1

KFM 7.1 Wed 10:00 H1

Tunable Graphene Phononic Crystal — •Jan Niklas Kirchhof[1], Kristina Weinel[1,2], Sebastian Heeg[1], Victor Deinhart[2,3], Sviatoslav Kovalchuk[1], Katja Höflich[2,3], and Kirill I. Bolotin[1] — [1]Department of Physics, Freie Universität Berlin, Germany — [2]Ferdinand-Braun-Institut, Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

In the field of phononics, periodic patterning controls vibrations and thereby the flow of heat and sound in matter. Bandgaps arising in such phononic crystals (PnCs) realize low-dissipation vibrational modes and enable applications towards mechanical qubits, efficient waveguides, and state-of-the-art sensing. Here, we combine phononics and two-dimensional materials and explore tuning of PnCs via applied mechanical pressure. To this end, we fabricate the thinnest possible PnC from monolayer graphene and simulate its vibrational properties.

We find a bandgap in the MHz regime, within which we localize a defect mode with a small effective mass of 0.72 ag = 0.002 $m_{physical}$. We exploit graphene's flexibility and simulate mechanical tuning of a finite size PnC. Under electrostatic pressure up to 30 kPa, we observe an upshift in frequency of the entire phononic system by ~ 350%. At the same time, the defect mode stays within the bandgap and remains localized, suggesting a high-quality, dynamically tunable mechanical system.

KFM 7.2 Wed 10:15 H1

Multi-step stochastic polarization reversal in orthorhombic ferroelectrics — Yuri Genenko[1], Maohua Zhang[1], •Ivan Vorotiahin[1], Ruben Khachaturyan[2], Yi-Xuan Liu[3], Ke Wang[3], and Jurij Koruza[1] — [1]Institute für Materialwissenschaft, Technische Universität Darmstadt, Darmstadt, Germany — [2]Interdisciplinary Center for Advanced Materials Simulation, Ruhr-Universität Bochum, Bochum, Germany — [3]State Key Laboratory of New Ceramics and Fine Processing, School of Materials Science and Engineering, Tsinghua University, Beijing, China

Polarization switching under applied electric fields is an important property of ferroelectrics, being crucial for the operation of the data storage FeRAM-devices and for setting up properties of piezoelectric films. Mathematical models such as KAI, NLS and IFM help understand underlying mechanisms and parameters of switching processes. Moving to structures with lower symmetries, there is a need for more complex models to describe the switching events.

A stochastic model has been developed to describe the multistep switching behaviour of a potassium sodium niobate (KNN)-based orthorhombic ceramic sample. The polarization and strain changes were measured over a large time scale and a wide range of applied electric fields. The switching paths for one-, two- and three-step processes were isolated, and the existence of coherent switching events over the multidomain structures was confirmed. The predicted and detected parameters of the processes give us a glimpse into the properties of the orthorhombic KNN materials family.

KFM 7.3 Wed 10:30 H1

Symmetry breaking by 4f-electron ordering in $NdGaO_3$ — •Lea Forster[1], Katrin Fürsich[2], Eva Benckiser[2], Thomas Lottermoser[1], Manfred Fiebig[1], and Mads C. Weber[1] — [1]ETH Zurich, Switzerland — [2]MPI Stuttgart, Germany

Despite intense investigations, the low temperature behavior of 4f electrons in neodymium gallate, $NdGaO_3$, is not fully understood. Several studies suggest that the 4f electrons affect the physical properties of $NdGaO_3$ at low temperature, and even a potential structural phase transition has been discussed in light of Raman measurements [1]. In this study, we shed light on these anomalies. We applied optical second harmonic generation (SHG), a highly symmetry-sensitive technique. Furthermore, SHG spectroscopy also gives us an insight into the physical origin of the anomalies. We reveal a strong SHG signal of $NdGaO_3$ characterized by many spectrally sharp features with increasing intensity toward low temperatures. While the spectral signature identifies the features as 4f transitions, our symmetry analysis reveals a lower symmetry with respect to the expected *Pbnm* phase of $NdGaO_3$. We therefore conclude that an orbital ordering of the 4f electrons gives rise to a symmetry breaking in $NdGaO_3$. This result raises the question whether a similar effect could also appear in other rare-earth compounds.

[1] B. K. De *et al.*, PRB **103**, 054106 (2021).

KFM 8: Crystal Structure / Real Structure / Microstructure

Chairman: Jan Schultheiß (NTNU Trondheim)

Time: Wednesday 10:45–11:45 Location: H1

KFM 8.1 Wed 10:45 H1

Hyperfine Structure of Transition Metal Defects in SiC — •Benedikt Tissot and Guido Burkard — Universität Konstanz

Transition metal (TM) defects in silicon carbide (SiC) are a promising platform in quantum technology, especially because some TM defects emit in the telecom band. We develop a theory for the interaction of an active electron in the *D*-shell of a TM defect in SiC with the TM nuclear spin and derive the effective hyperfine tensor within the Kramers doublets formed by the spin-orbit coupling. Based on our theory we discuss the possibility to exchange the nuclear and electron states with potential applications for nuclear spin manipulation and long-lived nunclear-spin based quantum memories.

KFM 8.2 Wed 11:00 H1

Exploring Binary Cesium-based Photocathode Materials via High-Throughput Density Functional Theory Calculations — •Holger-Dietrich Sassnick[1] and Caterina Cocchi[1,2] — [1]Carl von Ossietzky Universität Oldenburg - Physics Department, Oldenburg, Germany — [2]Humboldt-Universität zu Berlin - Physics Department and IRIS Adlershof, Berlin, Germany

Cesium-based photocathodes are commonly used as electron sources in particle accelerators; one relevant issue hindering the control over these systems and hence their photoemission performance is their polycrystalline structure which often includes non-stoichiometric compositions. To predict which compounds are more likely to form and to control their properties, we apply an efficient high-throughput workflow based on density functional theory calculations and explore the compositional phase space of cesium-based materials. First, we calculate the formation energies as well as the electronic properties of crystalline phases obtained from computational databases employing the meta-GGA functional SCAN, which is known to provide accurate results for these systems [1]. Then, we include additional crystal structures based on chemical similarity as a preliminary step towards crystal structure prediction combined with machine learning approaches. Our results indicate that a larger number of different crystal structures may be formed and thus contribute to the macroscopic material properties.

[1] Saßnick & Cocchi, *Electron. Struct.* **3** 027001 (2021)

KFM 8.3 Wed 11:15 H1

Mobility functions for [001] CSL grain boundaries in Nickel from Molecular Dynamics — •Etienne Ngenzi, Zakaria El Omari, Charlie Kalhoun, Brigitte Bacroix, and Sylvain Queyreau — LSPM UPR 3407 CNRS, Université Sorbonne Paris Nord, 93430, Villetaneuse, France

Multiscale simulations constitute a possible path to improve our understanding of the evolution of microstructures. In this work, we have systematically studied the migration of [001] CSL Grain Boundaries (GB) by Molecular Dynamics to provide input data for a mesoscale Phase Field model. We have systematically studied GB in nickel over a wide range of driving forces and temperature. To identify common features between very different GB and to sample different migration processes, we explored a large number of Σ5, Σ13, and Σ25, covering symmetric pure tilt, pure twist, and mixed characters ranging from low to high misorientation angle GB. Since we systematically probed both driving force and temperature, the temperature dependence of migration was unambiguous. The response of grain boundary mobility to temperature is highly dependent on the structure of the grain boundary. Most of the studied GB show successive distinct behaviours, with an initially thermally activated regime at low driving force and temperature. When increasing the driving force, the GB velocity may transition to a linear regime. A correlation is made with the elementary migration mechanisms that are observed. A phenomenological velocity law covering the entire parameter space for each GB is proposed.

KFM 8.4 Wed 11:30 H1

Electronically driven anharmonicity in charge-density-wave materials — •Arne Schobert[1], Jan Berges[1], Erik van Loon[1,2], Michael Sentef[3], and Tim Wehling[1] — [1]Institut für Theoretische Physik, Bremen Center for Computational Materials Science, and MAPEX Center for Materials and Processes, Otto-Hahn-Allee 1, Universität Bremen, D-28359 Bremen, Germany — [2]Department of Physics, Lund University, Lund, Sweden — [3]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany

Charge-density waves (CDWs) occupy an important position in the phase diagram of low- dimensional systems such as the transition metal dichalcogenide monolayers. Although a CDW can often be identified already from the undistorted structure in linear response, anharmonic effects are eventually responsible for the stabilization of the distorted phase and its precise properties. To study the mechanisms responsible for the anharmonicity, we calculate Born-Oppenheimer potential energy surfaces for lattice distortions in 1T-TaS2, 1T-VS2, and 2H-NbSe2, and we establish a connection to the electronic structure of these materials.

Financial support by the Deutsche Forschungsgemeinschaft (DFG) through GRK 2247, EXC 2077 and the Emmy Noether program (SE 2558/2), the European Graphene Flagship, and the Zentrale Forschungsförderung of the Universität Bremen is gratefully acknowledged.

KFM 9: Instrumentation and Methods

Chairman: Jan Schultheiß (NTNU Trondheim)

Time: Wednesday 12:00–12:45 Location: H1

KFM 9.1 Wed 12:00 H1

Broadband Coherent Anti-Stokes Raman Scattering (B-CARS) on Solid State Systems — •Franz Hempel[1], Sven Reitzig[1], Michael Rüsing[1], and Lukas M. Eng[1,2] — [1]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]ct.qmat Dresden-Würzburg Cluster of Excellence*EXC 2147, TU Dresden, 01062 Dresden, Germany

Broadband coherent anti-Stokes Raman scattering (B-CARS) combines the vibrational sensitivity of spontaneous Raman scattering (SR) with the gigantic signal amplification of coherent scattering techniques. B-CARS sees widespread applications in the biomedical fields for chemically-sensitive imaging, but has rarely been adapted to solid-state systems. In this work, we apply polarization-sensitive B-CARS to ferroelectric lithium niobate, and systematically investigate how the CARS signal depends on selection rules, power dependence and phase matching. In contrast to SR, B-CARS spectra are distorted in their spectral shape and position due to signal mixing with the non-resonant background (NRB). Here, we successfully apply Kramers-Kronig transformations, that originally were developed for biological samples but have been adapted here to crystalline-sample spectra. As a result, SR and B-CARS spectra become directly comparable, hence providing a brilliant basis for future inspections of nanoscale objects such as domain walls and defects in ferroelectrics.

KFM 9.2 Wed 12:15 H1

Silicon Highly Enriched in 28Si: Probing Artificial Crystals for the Dissemination of the Mole and Kilogram — •Axel Pramann and Olaf Rienitz — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

The revision of the SI units mole and kilogram has been enabled by the redetermination of the Avogadro constant with the lowest uncertainty by the the X-ray-crystal-density (XRCD) method *counting* silicon atoms in single-crystalline silicon spheres (1) and the complementary realization of the Planck constant using a Kibble balance (2). For the XRCD method applied by PTB, a few unique silicon single crystals highly enriched in 28Si has been produced and characterized. Using a high-resolution MC-ICP mass spectrometer and a tailored analytical methodology in a key experiment, the isotopic composition (the molar mass M) of these crystals has been determined with associated uncertainties of urel(M) < 1 x 10-9, which is unique in chemistry up to now. After developing and improving this method during the last decade, the uncertainties u(M) were reduced by almost three orders of magnitude. The way how to disseminate the amount of substance and mass after the revision of the SI is outlined (1, 3).

(1) K. Fujii et al., Metrologia, 53, A19 (2016). (2) I. A. Robinson, S. Schlamminger, Metrologia, 53, A46 (2016). (3) B. Guettler, O. Rienitz, A. Pramann, Annalen der Physik, 1800292 (2018).

KFM 9.3 Wed 12:30 H1

High-Q microresonators facilitate efficient electron-photon interaction — Jan-Wilke Henke[1,2], Arslan Sajid Raja[3], Armin Feist[1,2], Guanhao Huang[3], •Germaine Arend[1,2], Yujia Yang[3], F. Jasmin Kappert[1,2], Rui Ning Wang[3], Marcel Möller[1], Jiahe Pan[3], Junqiu Liu[3], Ofer Kfir[1,2,4], Claus Ropers[1,2], and Tobias J. Kippenberg[3] — [1]Georg-August Universität, Göttingen, Germany — [2]Max Planck Institute for Biophysical Chemistry, Göttingen, Germany — [3]Swiss Federal Institute of Technology, Lausanne, Switzerland — [4]School of Electrical Engineering, Tel-Aviv University, Tel Aviv, Israel

High-Q Si_3N_4 microresonators are not only an ideal platform for studying nonlinear effects, such as Kerr solitons. Their flexible dispersion engineering capability also makes them an ideal candidate for phase-matched interactions between free electrons and confined light. This allows for nanoscale optical mode mapping and possibilities in free-electron quantum optics.

In this work, we demonstrate how velocity phase-matching can be used for highly efficient free-electron-photon coupling inside a transmission electron microscope [1]. The evanescent tail of optical near fields excited in an air-cladded Si_3N_4 microcavity via a continuous-wave laser beam interacts with passing electrons. We observe multiple orders of electron-photon scattering resulting in a strong broadening of the electron energy spectrum. This coupling enables various further studies such as electron-triggered single photon sources.

[1] J.-W. Henke, A. S. Raja, et al., preprint, arXiv:2105.03729 (2021)

KFM 10: Annual General Meeting of the KFM division

Time: Wednesday 13:00–13:30 Location: MVKFM

30 min. Meeting.

KFM 11: Organic Electronics and Photovoltaics, Electrical and Optical Properties (joint session CPP/KFM)

Time: Thursday 13:30–16:15 Location: H3

See CPP 10 for details of this session.

KFM 12: Skyrmions II (joint session MA/KFM)

Time: Friday 10:00–13:15 Location: H5

See MA 17 for details of this session.

KFM 13: Topological Insulators and Semimetals (joint session TT/KFM)

Time: Friday 10:00–12:45 Location: H7

See TT 27 for details of this session.

Magnetism Division
Fachverband Magnetismus (MA)

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Overview of Invited Talks and Sessions

(Lecture halls H2 and H5; Poster P)

Invited Talks

MA 1.1	Mon	10:00–10:30	H5	**Utilizing Vacuum States above Surfaces for Imaging and Manipulation of Atomic-Scale Magnetism** — •Anika Schlenhoff
MA 2.1	Mon	13:30–14:00	H5	**Magnon-polarons in magnetic insulators** — •Benedetta Flebus
MA 2.2	Mon	14:00–14:30	H5	**Spin-phonon coupling in non-local spin transport through magnetic insulators** — •Rembert Duine
MA 2.3	Mon	14:30–15:00	H5	**Double accumulation and anisotropic transport of magneto-elastic bosons in yttrium iron garnet films** — •Alexander A. Serga
MA 2.5	Mon	15:15–15:45	H5	**Magnon polarons and the low-temperature spin-Seebeck effect** — •Piet Brouwer, Rico Schmidt
MA 2.6	Mon	15:45–16:15	H5	**Magnon-Polarons in different flavors: (anti)ferromagnetic to topological** — •Akashdeep Kamra
MA 2.7	Mon	16:15–16:45	H5	**Magnon polarons in antiferromagnetic insulator Cr2O3** — •Jing Shi
MA 4.1	Tue	10:00–10:30	H5	**2D Magnetic materials** — •Alberto Morpurgo
MA 6.1	Tue	13:30–14:00	H5	**Spin-charge interconversion with oxide 2-dimensional electron gases** — •Manuel Bibes
MA 6.2	Tue	14:00–14:30	H5	**Spin-to-charge current conversion for logic devices** — •Felix Casanova
MA 6.3	Tue	14:30–15:00	H5	**Electrical and thermal generation of spin currents by magnetic graphene** — •B.J van Wees, T.S. Ghiasi, A.A. Kaverzin, D.K. de Wal, A.H. Dismukes, Bart Wees
MA 6.4	Tue	15:15–15:45	H5	**Ferroelectric switching of spin-to-charge conversion in GeTe** — •Christian Rinaldi
MA 6.5	Tue	15:45–16:15	H5	**Theory of spin and orbital Edelstein effects in a topological oxide two-dimensional electron gas** — •Annika Johansson, Börge Göbel, Jürgen Henk, Manuel Bibes, Ingrid Mertig
MA 6.6	Tue	16:15–16:45	H5	**Nonlinear magnetoresistance and Hall effect from spin-momentum locking** — •Giovanni Vignale
MA 7.1	Wed	10:00–10:30	H5	**Anatomy of skyrmion-defect interactions and their impact on detection protocols** — •Samir Lounis
MA 10.1	Wed	13:30–14:00	H5	**Topological spin crystals stabilized by itinerant frustration** — •Yukitoshi Motome
MA 10.2	Wed	14:00–14:30	H5	**Formation of spin-hedgehog lattices and giant topological transport properties in chiral magnets** — •Naoya Kanazawa
MA 10.3	Wed	14:30–15:00	H5	**Topological-chiral magnetic interactions driven by emergent orbital magnetism** — •Sergii Grytsiuk, Jan-Philipp Hanke, Markus Hoffmann, Juba Bouaziz, Olena Gomonay, Gustav Bihlmayer, Samir Lounis, Yuriy Mokrousov, Stefan Blügel
MA 10.4	Wed	15:15–15:45	H5	**Complex spin structures in thin transition metals films and their oxides** — •Matthias Bode
MA 13.1	Thu	10:00–10:30	H5	**Magnetism and superconductivity: new physics one atom at a time** — •Alexander Balatsky
MA 13.3	Thu	10:45–11:15	H5	**Magnetic adatom chains on superconducting $NbSe_2$** — Eva Liebhaber, Lisa M. Rütten, Gael Reecht, Jacob F. Steiner, Sebastian Rohlf, Kai Rossnagel, Felix von Oppen, •Katharina J. Franke
MA 13.5	Thu	11:30–12:00	H5	**Yu-Shiba-Rusinov states and ordering of magnetic Impurities near the boundary** — •Jelena Klinovaja
MA 13.7	Thu	12:15–12:45	H5	**Resonance from antiferromagnetic spin fluctuations for spin-triplet superconductivity in UTe2** — •Pengcheng Dai

MA 14.1	Thu	13:30–14:00	H5	**The role of itinerant electrons and higher order magnetic interactions among fluctuating local moments in metallic magnets** — •Julie Staunton
MA 17.1	Fri	10:00–10:30	H5	**Emergent electromagnetic response of nanometer-sized spin textures** — •Max Hirschberger, Takashi Kurumaji, Leonie Spitz
MA 19.1	Fri	13:30–14:00	H5	**"Neuromorphic Computing": A Productive Contradiction in Terms** — •Herbert Jaeger
MA 19.2	Fri	14:00–14:30	H5	**Neuromorphic computing with radiofrequency spintronic devices** — •Alice Mizrahi, Nathan Leroux, Danijela Markovic, Dedalo Sanz Hernandez, Juan Trastoy, Paolo Bortolotti, Leandro Martins, Alex Jenkins, Ricardo Ferreira, Julie Grollier
MA 19.3	Fri	14:40–15:10	H5	**Data Storage and Processing in the Cognitive Era** — •Giovanni Cherubini
MA 19.4	Fri	15:10–15:40	H5	**Brain-inspired approaches and ultrafast magnetism for Green ICT** — •Theo Rasing

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium Potentials for NVs sensing magnetic phases, textures and excitations (SYNV)

See SYNV for the full program of the symposium.

SYNV 1.1	Mon	13:30–14:00	Audimax 2	**Harnessing Nitrogen Vacancy Centers in Diamond for Next-Generation Quantum Science and Technology** — •Chunhui Du
SYNV 1.2	Mon	14:00–14:30	Audimax 2	**Nanoscale imaging of spin textures with single spins in diamond** — •Patrick Maletinsky
SYNV 1.3	Mon	14:30–15:00	Audimax 2	**Spin-based microscopy of 2D magnetic systems** — •Jörg Wrachtrup
SYNV 1.4	Mon	15:15–15:45	Audimax 2	**Exploring antiferromagnetic order at the nanoscale with a single spin microscope** — •Vincent Jacques
SYNV 1.5	Mon	15:45–16:15	Audimax 2	**Nanoscale magnetic resonance spectroscopy with NV-diamond quantum sensors** — •Dominik Bucher

Invited talks of the joint symposium Novel phases and dynamical properties of magnetic skyrmions (SYMS)

See SYMS for the full program of the symposium.

SYMS 1.1	Tue	10:00–10:30	Audimax 2	**Imaging skyrmions in synthetic antiferromagnets by single spin relaxometry** — •Aurore Finco
SYMS 1.2	Tue	10:30–11:00	Audimax 2	**Microwave spectroscopy of the skyrmionic states in a chiral magnetic insulator** — •Aisha Aqeel, Jan Sahliger, Takuya Taniguchi, Stefan Maendl, Denis Mettus, Helmuth Berger, Andreas Bauer, Markus Garst, Christian Pfleiderer, Christian H. Back
SYMS 1.3	Tue	11:15–11:45	Audimax 2	**Archimedean Screw in Driven Chiral Magnets** — •Nina del Ser
SYMS 1.4	Tue	11:45–12:15	Audimax 2	**Frustration-driven magnetic fluctuations as the origin of the low-temperature skyrmion phase in $Co_7Zn_7Mn_6$** — •Jonathan White, Victor Ukleev, Kosuke Karube, Peter Derlet, Chennan Wang, Hubertus Luetkens, Daisuke Morikawa, Akiko Kikkawa, Lucile Mangin-Thro, Andrew Wildes, Yuichi Yamasaki, Yuichi Yokoyama, Le Yu, Cinthia Piamonteze, Nicolas Jaouen, Yusuke Tokunaga, Henrik Rønnow, Taka-hisa Arima, Yoshinori Tokura, Jonathan White
SYMS 1.5	Tue	12:15–12:45	Audimax 2	**Magnetic Skyrmions as Topological Multi-Media Influencers** — •Sebastián A. Díaz

Invited talks of the joint symposium Facets of many-body quantum chaos (SYQC)

See SYQC for the full program of the symposium.

SYQC 1.1	Tue	13:30–14:00	Audimax 2	**Holographic interpretation of SYK quantum chaos** — •Alexander Altland
SYQC 1.2	Tue	14:00–14:30	Audimax 2	**Non-Fermi liquids and the lattice** — •Sean Hartnoll
SYQC 1.3	Tue	14:30–15:00	Audimax 2	**Dual-unitary circuits: non-equilibrium dynamics and spectral statistics** — •Bruno Bertini
SYQC 1.4	Tue	15:15–15:45	Audimax 2	**Post-Ehrenfest many-body quantum interferences in ultracold atoms** — •Steven Tomsovic
SYQC 1.5	Tue	15:45–16:15	Audimax 2	**Dynamics in unitary and non-unitary quantum circuits** — •Vedika Khemani

Invited talks of the joint symposium Curvilinear condensed matter (SYCL)

See SYCL for the full program of the symposium.

SYCL 1.1	Wed	10:00–10:30	Audimax 2	**Curvature Effects and Topological Defects in Chiral Condensed and Soft Matter** — •Avadh Saxena
SYCL 1.2	Wed	10:30–11:00	Audimax 2	**Topology and Transport in nanostructures with curved geometries** — •Carmine Ortix
SYCL 2.1	Wed	11:15–11:45	Audimax 2	**Superconductors and nanomagnets evolve into 3D** — •Oleksandr Dobrovolskiy
SYCL 2.2	Wed	11:45–12:15	Audimax 2	**Properties of domain walls and skyrmions in curved ferromagnets** — •Volodymyr Kravchuk
SYCL 2.3	Wed	12:15–12:45	Audimax 2	**X-ray three-dimensional magnetic imaging** — •Valerio Scagnoli

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Attosecond and coherent spins: New frontiers (SYAS)

See SYAS for the full program of the symposium.

SYAS 1.1	Thu	10:00–10:30	Audimax 2	**Ultrafast Coherent Spin-Lattice Interactions in Iron Films** — •Steven Johnson
SYAS 1.2	Thu	10:30–11:00	Audimax 2	**Ultrafast spin, charge and nuclear dynamics: ab-initio description** — •Sangeeta Sharma, John Kay Dewhurst

SYAS 1.3	Thu	11:15–11:45	Audimax 2	**Light-wave driven Spin Dynamics** — •Martin Schultze, Markus Münzenberg, Sangeeta Sharma
SYAS 1.4	Thu	11:45–12:15	Audimax 2	**All-coherent subcycle switching of spins by THz near fields** — •Christoph Lange, Stefan Schlauderer, Sebastian Baierl, Thomas Ebnet, Christoph Schmid, Darren Valovcin, Anatoly Zvezdin, Alexey Kimel, Rostislav Mikhaylovskiy, Rupert Huber
SYAS 1.5	Thu	12:15–12:45	Audimax 2	**Ultrafast optically-induced spin transfer in ferromagnetic alloys** — •Stefan Mathias

Invited talks of the joint symposium The Rise of Photonic Quantum Technologies – Practical and Fundamental Aspects (SYPQ)

See SYPQ for the full program of the symposium.

SYPQ 1.1	Fri	10:00–10:30	Audimax 2	**Quantum dots operating at telecom wavelengths for photonic quantum technology** — •Simone Luca Portalupi
SYPQ 1.2	Fri	10:30–11:00	Audimax 2	**Photonic graph states for quantum communication and quantum computing** — •Stefanie Barz
SYPQ 1.3	Fri	11:00–11:30	Audimax 2	**Rare-earth ion doped solids at sub-Kelvins: practical and fundamental aspects** — •Pavel Bushev
SYPQ 1.4	Fri	11:45–12:15	Audimax 2	**Quantum Light and Strongly Correlated Electronic States in a Moiré Heterostructure** — •Brian Gerardot
SYPQ 1.5	Fri	12:15–12:45	Audimax 2	**Quantum communication in fibers and free-space** — •Rupert Ursin

Sessions

MA 1.1–1.9	Mon	10:00–12:30	H5	**Surface Magnetism (joint session MA/O)**
MA 2.1–2.8	Mon	13:30–17:00	H5	**Focus Session: Magnon Polarons - Magnon-Phonon Coupling and Spin Transport (joint session MA/HL)**
MA 3.1–3.20	Mon	13:30–16:30	P	**Posters Magnetism I**
MA 4.1–4.4	Tue	10:00–11:15	H5	**Spin-Dependent 2D Phenomena**
MA 5.1–5.22	Tue	10:00–13:00	P	**Posters Magnetism II**
MA 6.1–6.6	Tue	13:30–16:45	H5	**Focus Session: Spin-Charge Interconversion (joint session MA/HL)**
MA 7.1–7.12	Wed	10:00–13:15	H5	**Skyrmions I (joint session MA/KFM)**
MA 8.1–8.4	Wed	10:00–12:10	H2	**INNOMAG e.V. Dissertationspreis / Ph.D. Thesis Prize (2020)**
MA 9.1–9.4	Wed	12:30–14:20	H2	**INNOMAG e.V. Diploma/Master Prize (2021)**
MA 10.1–10.7	Wed	13:30–16:30	H5	**Focus Session: Higher-Order Magnetic Interactions - Implications in 2D and 3D Magnetism I**
MA 11.1–11.34	Wed	13:30–16:30	P	**Posters Magnetism III**
MA 12.1–12.3	Wed	14:30–16:15	H2	**INNOMAG e.V. Dissertationspreis / Ph.D. Thesis Prize (2021)**
MA 13.1–13.7	Thu	10:00–12:45	H5	**PhD Focus Session: Symposium on Strange Bedfellows - Magnetism Meets Superconductivity" (joint session MA/AKjDPG) (joint session MA/TT)**
MA 14.1–14.6	Thu	13:30–15:15	H5	**Focus Session: Higher-Order Magnetic Interactions - Implications in 2D and 3D Magnetism II**
MA 15.1–15.47	Thu	13:30–16:30	P	**Posters Magnetism IV**
MA 16	Thu	17:30–18:30	MVMA	**General Assembly of the Division of Magnetism**
MA 17.1–17.12	Fri	10:00–13:15	H5	**Skyrmions II (joint session MA/KFM)**
MA 18.1–18.42	Fri	10:00–13:00	P	**Posters Magnetism V**
MA 19.1–19.5	Fri	13:30–16:30	H5	**PhD Focus Session: Symposium on "Magnetism - A Potential Platform for Big Data?" (joint session MA/O/AKjDPG)**

General Assembly of the Division of Magnetism

Thursday 17:30–18:30 MVMA

Sessions

– Invited Talks, Discussions, Contributed Talks, and Posters –

MA 1: Surface Magnetism (joint session MA/O)

Time: Monday 10:00–12:30 Location: H5

Invited Talk MA 1.1 Mon 10:00 H5

Utilizing Vacuum States above Surfaces for Imaging and Manipulation of Atomic-Scale Magnetism — •Anika Schlenhoff — Department of Physics, University of Hamburg, Germany

Non-collinear spin textures in ultra-thin films raise expectations for spintronic applications, demanding for atomic-scale, spin-sensitive, but yet robust probe techniques. Spin-polarized vacuum resonance states (sp-RS) are unoccupied electronic states in the vacuum gap between a probe tip and a magnetic sample. They exhibit the same local spin quantization axis as the surface, even when it rotates on the atomic scale [1]. In a spin-polarized scanning tunneling microscopy (SP-STM) setup, the sp-RS can be addressed by spin-polarized electrons tunneling resonantly from the magnetic tip via these states into the surface. As I will show, this technique allows for atomic-scale magnetic imaging at tip-sample distances of up to 8 nm, providing a loophole from the hitherto existing dilemma of losing spatial resolution when increasing the tip-sample distance in a scanning probe setup [2]. Experimental results will be discussed in terms of the sp-RS' spin-splitting and the magnetic contrast as a function of bias and tip-sample distance, and in terms of the atomic-scale nature of the resonant tunneling condition. In combination with thermally-assisted spin-transfer torque switching via sp-RS [3], our approach qualifies for a spin-sensitive read-write technique with ultimate lateral resolution in future spintronic applications. [1] A. Schlenhoff *et al.*, Phys. Rev. Lett. **123**, 087202 (2019). [2] A. Schlenhoff *et al.*, Appl. Phys. Lett. **116**, 122406 (2020). [3] A. Schlenhoff *et al.*, Phys. Rev. Lett. **109**, 097602 (2012).

MA 1.2 Mon 10:30 H5

The effect of trapped Helium atoms on spin polarized tunneling in an STM tunnel junction — •Christopher Trainer[1], Chi Ming Yim[1,2], Christoph Heil[3], Vladimir Tsurkan[4,5], Alois Loidl[4], Liam Farrar[1], and Peter Wahl[1] — [1]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, UK — [2]Tsung Dao Lee Institute & School of Physics and Astronomy,Shanghai Jiao Tong University, Shanghai, 200240, China — [3]Institute of Theoretical and Computational Physics, Graz University of Technology, NAWI Graz, 8010 Graz, Austria — [4]Center for Electronic Correlations and Magnetism, Experimental Physics V, University of Augsburg, D-86159 Augsburg, Germany — [5]Institute of Applied Physics, MD 2028 Chisinau, Republic of Moldova

I will present a study of the influence of a Helium probe particle on spin-polarized imaging with an STM. Helium was inserted into the junction between a magnetic Iron tip and an Iron Telluride sample. From tunneling spectra acquired at different tip-sample distances we have mapped out the binding energy of the Helium atom in the tunneling junction. We find that imaging with Helium trapped in the tunneling junction makes the STM sensitive to the magnetic exchange interaction between the tip and the sample. I will demonstrate that by changing the tip sample separation the intensity of the imaged magnetic order can be both enhanced and suppressed and that the overall spin polarization of the junction can be tuned by varying the bias voltage, effectively enabling voltage-control of the spin-polarization of the tunneling current across the junction.

MA 1.3 Mon 10:45 H5

Zero-point magnetic exchange interactions — •Juba Bouaziz[1,2], Julen Ibañez Azpiroz[3], Filipe S. M. Guimarães[1], and Samir Lounis[1,4] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich 52425, Germany — [2]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom — [3]Centro de Física de Materiales, Universidad del País Vasco/Euskal Herriko Unibertsitatea, 20018 Donostia, San Sebastián, Spain — [4]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany

Quantum fluctuations are ubiquitous in physics. Their emergence, magnitude and impact on various physical properties is a fascinating research topic of strong implications in nanotechnologies. They impact non-trivially the behaviour of nanostructures. Hinging on the fluctuation-dissipation theorem and the random phase approximation [1], we show that quantum fluctuations play an important role in determining the fundamental magnetic exchange interactions and account for the large overestimation of the magnetic interactions as obtained from conventional static first-principles frameworks, filling in an important gap between theory and experiment. Our analysis further reveals that quantum fluctuations tend to promote the noncollinearity and stability of chiral magnetic textures such as skyrmions. [1] J. Bouaziz et al. PRR 2, 043357 (2020).

This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (ERC-consolidator Grant No. 681405, DYNASORE)

MA 1.4 Mon 11:00 H5

Iron growth on Be(0001) studied by STM — •Hermann Osterhage, Karoline Oetker, Roland Wiesendanger, and Stefan Krause — Department of Physics, University of Hamburg, Germany

Under high pressure, bulk Fe undergoes a phase transition to the ϵ-phase in a hexagonal close-packed (hcp) structure [1]. To date, the need for anvil cells to create ϵ-Fe prohibits an experimental validation of the noncollinear or antiferromagentic ground states predicted theoretically [2]. In our approach, Be(0001) is used as a closely-spaced hcp substrate that may accommodate ϵ-Fe provided that pseudomorphic growth occurs.

The clean Be(0001) surface was characterized using scanning tunneling spectroscopy at low temperatures. It hosts a parabolically dispersing surface state that couples strongly to phonon modes as evidenced in inelastic tunneling spectroscopy [3].

Fe growth on this surface was studied in dependence of coverage and substrate temperature during deposition. The Fe grows in multilayer islands when deposited at room temperature. For elevated temperatures, a combination of high resolution scanning tunneling microscopy and Auger electron spectroscopy shows hints of the formation of a locally ordered alloy of Fe and Be. The morphology of the resulting films and scanning tunneling spectra acquired on this system will be presented and discussed.

[1] I. Leonov *et al.*, Phys. Rev. Lett. **106**, 106405 (2011).
[2] R. Lizárraga *et al.*, Phys. Rev. B **78**, 064410 (2008).
[3] H. Osterhage *et al.*, Phys. Rev. B **103**, 155428 (2021).

MA 1.5 Mon 11:15 H5

Spin-resolved Fermi Surface of Ultrathin Ferromagnetic FePd Alloy Monolayers — •Xin Liang Tan[1], Kenta Hagiwara[1], Ying-Jiun Chen[1,2], Vitaliy Feyer[1], Claus M. Schneider[1,2], and Christian Tusche[1,2] — [1]Forschungszentrum Jülich, Peter Grünberg Institut, Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen, Duisburg

Magnetism in reduced dimensions is one of the preconditions for the realization of nanoscale spintronics. Despite the recent discovery of ferromagnetism in monolayers of two-dimensional materials, tunability and engineering on such systems are challenging. Here we have studied the electronic structure of ultrathin ferromagnetic iron-palladium alloy films using spin-resolved momentum microscopy. Momentum microscopy enables the two-dimensional detection of photoelectrons with an in-plane crystal momentum over the full Brillouin zone. By employing an imaging spin filter, spin-resolved momentum maps of the iron-palladium alloy were acquired. Breaking of time reversal symmetry by the remanent magnetization of the film manifests in a pronounced anisotropy of the electron states in the Fermi surface. In particular, the competition between exchange interaction and strong spin-orbit coupling in the FePd alloy leads to the formation of wave-vector dependent local gaps in the Fermi surface. Moreover, the spin-resolved maps recorded by the momentum microscope give evidence for a non-collinear spin texture of the electron states at the Fermi surface, where the local spin polarization vector points orthogonal to the remanent magnetization of the sample.

MA 1.6 Mon 11:30 H5

On-surface synthesis of magnetic organometallic chains on the superconducting Ag/Nb(110) substrate — •Jung-Ching Liu[1], Philipp D'Astolfo[1], Carl Drechsel[1], Xunshan Liu[2], Silvio Decurtins[2], Shi-Xia Liu[2], Rémy Pawlak[1], Wulf Wulfhekel[3], and Ernst Meyer[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, Basel, CH 4056 — [2]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, Bern, CH 3012 — [3]Physikalisches Institut, Karlsruhe Institute of Technology, Wolfgang-Gaede-Str. 1, D-76131 Karlsruhe, Germany

With proximity to s-wave superconductivity, spin texture arises on a magnetic chain and Majorana bound states (MBSs) can be found at two ends[1-3]. To study MBSs with diverse magnetic structures, we propose to conjugate magnetic atoms with organic molecules via on-surface reaction. Choosing Fe and PTO, we fabricate magnetic chains on the superconducting Ag/Nb substrate[4,5]. With the investigation with STM and AFM at 4.7K, we confirm the proximity-induced superconductivity on Ag from Nb, as well as the success in growing magnetic organometallic chains. We believe our work demonstrates the feasibility of growing tunable magnetic lattices by changing organic molecules. Above all, the direct synthesis on a superconductor offers a convenient way to study the interaction between magnetic lattices and superconductivity. [1]S. Nadj-Perge et al. Science 2014, 346, 602-607 [2]M. Ruby et al. Nano Lett. 2017, 17, 4473-4477 [3]R. Pawlak et al. Npj Quantum Inf. 2016, 2, 16035 [4]A. D. Pia et al. Chem. Eur. J. 2016, 22, 8105-8112 [5]T. Tomanic et al. Phys. Rev. B 2016, 94, 220503

MA 1.7 Mon 11:45 H5

Interplay of magnetic states and hyperfine fields of iron dimers on MgO(001) — •SUFYAN SHEHADA[1,2], Manuel dos Santos Dias[1], Muayad Abusaa[3], and Samir Lounis[1,4] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Department of Physics, RWTH Aachen University, 52056 Aachen, Germany — [3]Department of Physics, Arab American University, Jenin, Palestine — [4]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany

Individual nuclear spin states can have very long lifetimes and could be useful as qubits. Progress in this direction was achieved on MgO/Ag(001) via detection of the hyperfine interaction (HFI) of Fe, Ti and Cu adatoms using scanning tunneling microscopy (STM) [1,2]. Previously, we systematically quantified from first-principles the HFI for the whole series of 3d transition adatoms (Sc*Cu) deposited on various ultra-thin insulators, establishing the trends of the computed HFI with respect to the filling of the magnetic s and d-orbitals of the adatoms and on the bonding with the substrate [3]. Here we take one step further by investigating the impact of the magnetic coupling between the dimer atoms on the HFI of Fe dimers on MgO(001) and its dependence on where the Fe atoms are located on the surface.

–Work funded by the Palestinian German Science Bridge (BMBF–01DH16027) and Horizon 2020–ERC (CoG 681405–DYNASORE).

[1] Willke *et al.*, Science **362**, 336 (2018); [2] Yang *et al.*, Nat. Nano. **13**, 1120 (2018); [3] Shehada *et al.*, Npj Comput. Mater. **7**, 87 (2021).

MA 1.8 Mon 12:00 H5

Pairwise magnetic exchange interaction tensor from tight-binding models of noncollinear magnetism — •Kseniia Vodenkova[1] and Pavel Bessarab[1,2] — [1]ITMO University, St. Petersburg, Russia — [2]University of Icelad, Reykjavik, Iceland

The microscopic origin of the exchange interactions for noncollinear ordering of atomic magnetic moments in itinerant-electron systems is a subject of ongoing scientific discussions. In this work, we derive by means of the multiple-scattering theory a general expression for pairwise magnetic exchange interaction parameters for an arbitrary noncollinear, nonstationary magnetic state. In contrast to previous approaches, our formalism takes into account the variation of the fast degrees of freedom such as charge density and magnetic moment length. Application of the formalism to a tight-binding model reveals a range of magnetic systems that can be described by a classical Heisenberg Hamiltonian reasonably well. For other systems, our approach makes it possible to systematically derive atomistic spin Hamiltonians beyond the Heisenberg model. Moreover, the expression for the pairwise interaction tensor describes a local curvature of the energy surface of the system as a function of the orientation of magnetic vectors. This can be used in various contexts including description of thermal stability of magnetic states within the harmonic transition state theory and efficient identification of stable magnetic configurations using the Newton-Raphson method.

MA 1.9 Mon 12:15 H5

The chiral Hall effect in canted ferromagnets and antiferromagnets — •Jonathan Kipp[1], Kartik Samanta[1], Fabian Lux[1,2,3], Maximilian Merte[1,2,3], Dongwook Go[1,3], Jan-Philip Hanke[1], Matthias Redies[1,2], Frank Freimuth[1,3], Stefan Blügel[1], Marjana Lezaic[1], and Yuriy Mokrousov[1,3] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum — [2]RWTH Aachen University, Aachen, Germany — [3]Institute of Physics, Johannes Gutenberg-University Mainz

There are numerous exciting classes of antiferromagnets, where the anomalous and recently discovered crystal Hall [1] effect as well as the topological Hall effect in non-coplanar antiferromagnets [2] have been studied in the past decades. In this work, we uncover a novel type of Hall effect emerging in generic canted spin systems. Identifying a clear fingerprint of this chiral Hall effect (CHE) in discrete tight-binding models as well as ab-initio calculations is central in establishing a solid understanding of this new phenomenon closely tied to real space topology of magnetic textures. We provide robust numerical evidence for the CHE in a honeycomb lattice of canted spins and present a material candidate, SrRuO3. We uncover contributions to the Hall conductivity sensitive to the canting angle between neighboring spins which can be directly related to the imprinted vector chirality. Exploring the symmetry properties of the CHE we demonstrate the complex interplay of symmetry, topology and chirality in canted spin systems. [1]L .Smejkal et al., Science Advances 6 (2020) [2]L. Smejkal et al., Nature Physics 14, 242-251 (2018) [3]J. Kipp et al., Comm. Phys. 4, 99 (2021)

MA 2: Focus Session: Magnon Polarons - Magnon-Phonon Coupling and Spin Transport (joint session MA/HL)

The coupling of spin waves and atomic lattice vibrations in solid magnetic states, so-called magnon polarons (MPs), can have large impact on spin transport properties as recently explored for spin Seebeck effect, spin pumping and nonlocal spin transport. This resonant enhancement can be reached when the magnon dispersion is shifted by a magnetic field and crosses the phonon dispersion with sufficient overlap. While initially observed at low temperatures and large magnetic fields, further material and device developments have led to MPs at room temperature and moderate magnetic fields. Thus, MPs become important for the manipulation and amplification of spin currents in spintronic and spin caloritronic devices, e.g. by carrying the spins much further than using uncoupled magnons. This focus session highlights the main important research outcomes for MPs, state-of-the-art techniques to detect MPs, such as Brillouin light scattering, and to study MP transport, e.g. by spin Seebeck effect and nonlocal spin transport, as well as the investigation of MPs in different material classes such as garnets, ferrites and antiferromagnets. In addition, the excessive theoretical work on MPs performed recently is addressed in this focus session.

Organizer: Timo Kuschel (Bielefeld University)

Time: Monday 13:30–17:00 Location: H5

Invited Talk MA 2.1 Mon 13:30 H5

Magnon-polarons in magnetic insulators — •Benedetta Flebus — Boston College, Chestnull Hill, USA

We theoretically study the effects of strong magneto-elastic coupling on the transport properties of magnetic insulators. We develop a Boltzmann transport theory for the mixed magnon-phonon modes, i.e., magnon-polarons, and determine transport coefficients of the composite quasi-particles. Magnon-polaron formation causes anomalous features in the magnetic field and temperature dependence of the spin Seebeck effect when the disorder scattering in the magnetic and elastic subsystems is sufficiently different. We discuss how experimental data by Kikkawa et al. [PRL 117, 207203 (2016)] on yttrium iron garnet films can be explained by an acoustic quality that is much better than the magnetic quality of the material.

Invited Talk MA 2.2 Mon 14:00 H5

Spin-phonon coupling in non-local spin transport through magnetic insulators — •Rembert Duine — Institute for Theoretical Physics, Utrecht University, The Netherlands

Long-range spin transport through ferromagnetic and antiferromagnetic insulators has recently been demonstrated. In this talk I will discuss how spin-phonon interactions influence this transport. In the first part of the talk I will discuss how bulk spin-phonon interactions lead to magnon-polaron formation and how this composite boson influences the non-local transport. In the second part, I will discuss how spin-phonon interactions across an interface give rise to long-distance spin transport that is carried purely by phonons.

Invited Talk MA 2.3 Mon 14:30 H5

Double accumulation and anisotropic transport of magneto-elastic bosons in yttrium iron garnet films — •Alexander A. Serga — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern

Interaction between quasiparticles of a different nature, such as magnons and phonons, leads to mixing their properties and forming hybrid states in the areas of intersection of individual spectral branches. In garnet ferrite films, such hybridization results in a resonant increase in the efficiency of the spin Seebeck effect and the spontaneous bottleneck accumulation of hybrid magnetoelastic bosons—magnon polarons.

Similar to the Bose-Einstein magnon condensation (BEC), the latter phenomenon occurs in a yttrium iron garnet film exposed to microwaves. However, unlike the BEC, which is a consequence of the equilibrium Bose statistics, the bottleneck accumulation is determined by changing interparticle interactions. Studying the transport properties of accumulated quasiparticles, we found that such accumulation occurs in two frequency-distant groups: quasiphonons and quasimagnons. These quasiparticles propagate in the film plane as spatially localized beams with different group velocities. The developed theoretical model qualitatively describes the double accumulation effect, and the analysis of the two-dimensional quasiparticle spectrum makes it possible to determine the wavevectors and frequencies of each group.

Funded by the ERC Advanced Grant 694709 SuperMagnonics and by the DFG within TRR 173 – 268565370 (project B04).

MA 2.4 Mon 15:00 H5

enhancement of the spin seebeck effect by magnon-phonon resonance in a partially compensated magnet — •R. Ramos[1,2], T. Hioki[3,4], Y. Hashimoto[1], T. Kikkawa[1,3,4], P. Frey[5], A.J.E. Kreil[5], V.I. Vasyuchka[5], A.A. Serga[5], B. Hillebrands[5], and E. Saitoh[1,3,4] — [1]WPI AIMR, Tohoku University, Japan — [2]CIQUS, Departamento de Química-Física, Universidade de Santiago de Compostela, Spain — [3]Department of Applied Physics, The University of Tokyo, Japan. — [4]IMR, Tohoku University, Japan — [5]Fachbereich Physik and Landesforshungszentrum OPTIMAS, Technische Universität Kaiserslautern, Germany

The spin Seebeck effect (SSE) refers to the generation of a spin current in magnetic materials by the application of a thermal gradient. Recently, the effect of magnon-phonon hybridization, resulting from the crossing of the magnon and phonon dispersions, has been detected in the SSE and named magnon-polaron SSE. This is experimentally observed as spikes of the SSE-voltage at the magnetic field values for which the hybridization between the magnon and phonon dispersions is maximized over k-space. In this talk, we will report the detection of magnon-polaron SSE in a nonmagnetic-ion-substituted garnet system at room temperature and low magnetic fields [1]. The effect is 8 times larger than that observed in a YIG film. We show that the magnon dispersion can be strongly affected by the nonmagnetic-ion substitutions, thus resulting in a clear modification of the magnetic field condition for the observation of magnon-polarons. [1] R. Ramos et al. Nature Comm. 10, 5162 (2019).

Invited Talk MA 2.5 Mon 15:15 H5

Magnon polarons and the low-temperature spin-Seebeck effect — •Piet Brouwer and Rico Schmidt — Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

Using a simplified microscopic model of coupled spin and lattice excitations in a ferromagnetic insulator we evaluate the magnetic-field dependence of the longitudinal spin Seebeck effect at low temperatures. We find that at low temperatures, large magnetic fields, and for not-too-large system sizes the spin Seebeck effect is almost completely mediated by magnon polarons, superpositions of magnon and phonon excitations, with frequency close to the crossing points of magnon and phonon dispersions. We find an enhancement of the spin-Seebeck effect for “critical” values of the magnetic field, for which magnon and phonon dispersions touch. Such an enhancement of the longitudinal spin-Seebeck effect was observed experimentally by Kikkawa et al. [Phys. Rev. Lett. 117, 207203 (2016)]. We find that the existence of this enhancement is independent of the relative strength of magnon-impurity and phonon-impurity scattering.

Invited Talk MA 2.6 Mon 15:45 H5

Magnon-Polarons in different flavors: (anti)ferromagnetic to topological — •Akashdeep Kamra — Condensed Matter Physics Center (IFIMAC) and Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Due to magnetoelastic coupling, magnons and phonons in a magnet can combine to form hybrid quasiparticles, inheriting properties from both, called magnon-polarons. We will begin by examining and clarifying the essential requirements for their hybridization in terms of the spin conservation laws and the nature of the magnetoelastic coupling. This will allow us to deduce the properties, such as spin, of the magnon-polarons thus formed and provide guidance on how to engineer magnon-polarons. In carrying out this general discussion, we will analyze the cases of magnon-polarons in ferromagnets as examples. Then, we will apply the general principles developed to the cases of antiferromagnets and topological magnonic insulators thereby demonstrating magnon-polarons with novel, tunable, and chiral properties. We will conclude our discussion with recent experiments suggesting spin-phonon coupling to underlie collective quantum phenomena in the high-Tc superconductor YBCO.

References: [1] A. Kamra, H. Keshtgar, P. Yan, and G. E. W. Bauer. Phys. Rev. B 91, 104409 (2015). [2] H. T. Simensen, R. E. Troncoso, A. Kamra, and A. Brataas. Phys. Rev. B 99, 064421 (2019). [3] E. Thingstad, A. Kamra, A. Brataas, and A. Sudbø. Phys. Rev. Lett. 122, 107201 (2019).

Invited Talk MA 2.7 Mon 16:15 H5

Magnon polarons in antiferromagnetic insulator Cr_2O_3 — •Jing Shi — Department of Physics & Astronomy, University of California, Riverside, USA

While magnon polarons in ferrimagnetic materials have been experimentally investigated by various meanings including the spin Seebeck effect, nonlocal transport, inelastic neutron scattering, spin pumping, etc., similar hybridized excitations in antiferromagnets have not been well explored. For typical antiferromagnets, the magnon dispersion lies well above the acoustic phonon dispersion, which prevents the formation of magnon polarons under accessible magnetic fields. In this talk, I will first review the main magnon polaron results in yttrium iron garnet [1], a ferrimagnetic insulator. My focus will be on a special antiferromagnetic insulator: Cr_2O_3. In this uniaxial antiferromagnet, the left-handed magnon branch can be effectively lowered to zero at ~6 T, the spin-flop transition, allowing for thermodynamic measurements. In our study of Cr_2O_3 spin Seebeck effect [2], We observe magnon polaron anomalies right below the spin flop transition. where the left-handed magnon dispersion intersect both longitudinal and transverse acoustic phonon dispersions. I will present our experimental data and analysis in my talk.

[1] H.R. Man et al., Direct observation of magnon-phonon coupling in yttrium iron garnet. Phys. Rev B 96, 100406(R) (2017). [2] J.X. Li et al., Observation of magnon-polarons in a uniaxial antiferromagnetic insulator Cr_2O_3. Phys. Rev. Lett. 125, 217201(2020).

MA 2.8 Mon 16:45 H5

Revealing thermally driven distortion of magnon dispersion by spin Seebeck effect in $Gd_3Fe_5O_{12}$ — •Bin Yang[1], Si Yu Xia[1], Hui Zhao[1], Gan Liu[1], Jun Du[1], Ka Shen[2], Zhiyong Qiu[3], and Di Wu[1] — [1]National Laboratory of Solid State Microstructures, Jiangsu Provincial Key Laboratory for Nanotechnology, Collaborative Innovation Center of Advanced Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China — [2]Center for Advanced Quantum Studies and Department of Physics, Beijing Normal University, Beijing 100875, China — [3]School of Materials Science and Engineering, Dalian University of Technology, Dalian 116024, China

We report a systematic study of the temperature and field dependences of the spin Seebeck effect (SSE) in a bilayer of Pt/$Gd_3Fe_5O_{12}$. An anomalous structure is observed in the magnetic field dependent measurements at temperatures between ~60 and ~210 K.We attribute these anomalies to the contribution from the quasiparticles hybridized between the Gd moment dominated spin wave (α mode) and the transversal acoustic phonon, known as the magnon polarons, and explain these rich phenomena by an increase of the group velocity of the α-mode magnon with increasing temperature and the nonparabolic magnon dispersion of $Gd_3Fe_5O_{12}$. Our results demonstrate that the magnon polaron induced SSE is helpful for the investigation of the magnon dispersion evolution with a simple transport approach.

MA 3: Posters Magnetism I

Topics: Surface Magnetism (3.1-3.4), Thin Films: Magnetic Coupling Phenomena / Exchange Bias (3.5-3.11), Thin Films: Magnetic Anisotropy (3.12-3.13), Topological Insulators (3.14-3.15), Micro- and Nanostructured Magnetic Materials (3.16-3.20)

Time: Monday 13:30–16:30 Location: P

MA 3.1 Mon 13:30 P

Yu-Shiba-Rusinov states of Manganese atoms on proximitzed Silver layers — •Jennifer Hartfiel, Mira Kressler, Gaël Recht, and Katharina J. Franke — Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The adsorption of a magnetic adatom on a superconducting substrate perturbes the Cooper pair condensate in close proximity to the surface. The unpaired magnetic moment induces localized bound states, so-called Yu-Shiba-Rusinov (YSR) states, inside the superconducting energy gap, which can be probed by scanning tunneling spectroscopy (STS). The coupling strength between the magnetic moment of the impurity and the Cooper pairs determines the energy needed for tunneling into the YSR state.

In this work we perform STS measurements on Mn adatoms on Ag islands on Vanadium. Vanadium is very reactive and widely reconstructed by oxygen on the surface. This makes it difficult to investigate a possible adsorption-site dependence of the YSR energies. We passivate the surface by expitaxially grown silver monolayers. The Ag is proximitized by the superconducting substrate, and we observe YSR states for Mn on Ag/V. As the coupling of the magnetic impurity with the superconductor depends strongly on the adsorption geometry, we compare the YSR states for Mn atoms on two different crystal orientations of the Vanadium, which influences the structure of the Ag islands grown on top and, hence, the YSR states.

MA 3.2 Mon 13:30 P

Tailoring magnetic anisotropy by graphene-induced skyhook effect of 4f metals — •Alexander Herman[1], Stefan Kraus[2], Shigeru Tsukamoto[3], Lea Spieker[1], Tobias Lojewski[1], Damian Günzing[1], Tobias Hartl[2], Jan Gui-Hyon Dreiser[4], Bernard Delley[4], Katharina Ollefs[1], Thomas Michely[2], Nicolae Atodiresei[3], and Heiko Wende[1] — [1]Faculty of Physics and Center for Nanointegration, Duisburg-Essen — [2]II. Physikalisches Institut, Universität zu Köln — [3]Peter Grünberg Institute and Institute for Advanced Simulation, FZ Jülich — [4]SLS, Paul Scherrer Institut (CH)

From macroscopic heavy-duty permanent magnets to nanodevices the precise control of the magnetic properties in rare-earth metals is crucial for many applications used in our daily life. Therefore, a detailed understanding and manipulation of the 4f-metals magnetic properties represent the key to further boost the functionalization and efficiency of practical applications. We present a proof-of-concept surface-alloy system in which graphene induces a skyhook effect on a 4f metal and therefore modifies its magnetic properties. We demonstrate that by adsorbing graphene onto a long-range ordered two-dimensional dysprosium-iridium surface alloy, the magnetic 4f metal atoms are selectively lifted from the surface alloy and a giant magnetic anisotropy is introduced in dysprosium atoms as a result of manipulating its geometrical structure within the surface alloy. Our combined theoretical simulations and experimental measurements provide an easy and unambiguous understanding of its underlying mechanism. Financial support by DFG through projects WE 2623/17-1, MI 581/23-1, and AT 109/5-1.

MA 3.3 Mon 13:30 P

Step-edge-induced anisotropic chiral spin coupling in ultrathin magnetic films — Anika Schlenhoff, •Stefan Krause, and Roland Wiesendanger — Department of Physics, University of Hamburg, Germany

Step edges represent a local break of lateral symmetry in ultrathin magnetic films. In our experiments, we investigate the spin coupling across atomic step edges on Fe/W(110) by means of spin-polarized scanning tunneling microscopy and spectroscopy.

As we show in our experiments, atomic step edges induce a chiral spin coupling, with outreaching consequences on the local spin texture in the film [1]. Local modifications of the spin texture toward step edges separating double from single layer areas of Fe on W(110) are observed, and selection rules indicate a chiral spin coupling that significantly changes with the propagation along different crystallographic directions. The experimental results will be presented, and the findings are explained in terms of anisotropic Dzyaloshinskii-Moriya interaction arising from the broken lateral symmetry at atomic step edges.

Our experiments strongly indicate that surface roughness and interface quality on the atomic scale is of high relevance for spin manipulation and transmission in terms of tailored magnetic coupling for future spintronic applications.

[1] A. Schlenhoff, S. Krause, and R. Wiesendanger, Phys. Rev. Lett. **123**, 037201 (2019).

MA 3.4 Mon 13:30 P

Cation- and lattice-site-selective magnetic depth profiles of ultrathin Fe_3O_4(001) films — Tobias Pohlmann[1,2], •Timo Kuschel[3], Jari Rodewald[1], Jannis Thien[1], Kevin Ruwisch[1], Florian Bertram[2], Eugen Weschke[4], Padraic Shafer[5], Joachim Wollschläger[1], and Karsten Küpper[1] — [1]Uni Osnabrück, Germany — [2]DESY, Hamburg, Germany — [3]Uni Bielefeld, Germany — [4]HZB Bessy II, Berlin, Germany — [5]ALS, Berkeley, USA

We present x-ray magnetic circular dichroism (XMCD) and x-ray resonant magnetic reflectivity (XMRR) measurements on ultrathin Fe_3O_4(001) films to obtain magnetic depth profiles of the different cation species Fe^{2+}_{oct}, Fe^{3+}_{tet}, and Fe^{3+}_{oct} located on octahedral and tetrahedral sites of the inverse spinel structure of Fe_3O_4. Performing XRMR on the three resonant XMCD energies yields magnetic depth profiles that each correspond to one specific cation species.

The depth profiles of both Fe^{3+} cations reveal a (3.9±1.0)-Å-thick surface layer of enhanced magnetization, which is likely due to an excess of these ions at the expense of the Fe^{2+}_{oct} species in the surface region. The magnetically enhanced Fe^{3+}_{tet} layer is additionally shifted about 2.9±0.4 Å farther from the surface than the Fe^{3+}_{oct} layer [1].

Moreover, we compare the depth profiles with the recently revealed cation vacancy reconstruction of the Fe_3O_4(001) surface [2] as well as the unreconstructed Fe_3O_4(111) surface that is Fe_{oct}-terminated [3].

[1] T. Pohlmann et al., Phys. Rev. B 102, 220411(R) (2020)
[2] R. Bliem et al., Science 346, 1215 (2014)
[3] S. Brück et al., Appl. Phys. Lett. 100, 081603 (2012)

MA 3.5 Mon 13:30 P

Interlinking ferro- and antiferromagnetic thickness dependencies of macroscopic magnetic characteristics with microscopic properties of polycrystalline exchange-biased bilayers — •Maximilian Merkel, Meike Reginka, Rico Huhnstock, and Arno Ehresmann — Universität Kassel

A systematic investigation of the exchange bias shift and the coercive field exhibited by prototypical polycrystalline exchange-biased bilayers is conducted in dependence of the thicknesses of the participating ferro- and antiferromagnetic layer. Columnar grain growth is verified via thickness dependent grain size analysis by means of atomic force microscopy. Formulating analytic expressions for the named thickness dependencies allowed us to establish a quantitative link between the macroscopically observable magnetic characteristics and the microscopic properties. Relations depending on measurement conditions and parameters describing the microstructure of the granular antiferromagnetic layer in the context of a generalized description of polycrystalline exchange-bias systems were hereby thoroughly considered. This is facilitated by an extended time-dependent Stoner-Wohlfarth approach in combination with angular-resolved measurements of magnetization reversal curves utilizing magneto-optical Kerr magnetometry validating the consistency of the generalized model approach.

MA 3.6 Mon 13:30 P

Influence of strain on the magnetic ground state in multiferroic $BiFeO_3$ studied from First Principles — •Sebastian Meyer[1], Bin Xu[2,3], Matthieu Verstraete[1], Laurent Bellaiche[2], and Bertrand Dupé[1,4] — [1]Nanomat/Q-mat/CESAM, University of Liége, Belgium — [2]Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, USA — [3]Jiangsu Key Laboratory of Thin Films, School of Physical Science and Technology, Soochow University, China — [4]Fonds de la Recherche Scientifique (FNRS), Bruxelles, Belgium

We study the influence of compressive and tensile strain on the magnetic ground state in thin films of the multiferroic $BiFeO_3$ by means of density functional theory. Using two different methods, we determine the strength of the magnetic exchange, the Dzyaloshinskii-Moriya interaction and the anisotropy energies. The first one is based on the generalized Bloch theorem which allows the self-consistent computation of the total energy of spin spirals. This has already been applied to successfully determine the magnetic ground state in $R3c$ bulk $BiFeO_3$ [1]. The second one is based on the evaluation of a tight-binding Hamiltonian parameterized via Wannier functions and solved via Green functions methods as implemented in TB2J [2]. Using both methods, we explore the change of magnetic ground state of strained $BiFeO_3$ and compare the results with experimental findings.

[1] Xu, B., *et al.*, Phys. Rev. B **103**, 214423 (2021)
[2] He, Y., *et al.*, Comp. Phys. Comm. **264**, 107938 (2021)

MA 3.7 Mon 13:30 P

Tilted magnetization stripe domain reversal in Co/Pt multilayer systems — •Peter Heinig[1], Olav Hellwig[1,2], Ruslan Salikhov[2], Fabian Samad[2], Rico Ehrler[1], and Benny Böhm[1] — [1]Chemnitz University of Technology — [2]Helmholtz-Zentrum Dresden-Rossendorf

Co/Pt multilayer systems with total thickness above 10 nm are well-known for their highly periodic perpendicular stripe domain structures. Here we study $[Co(3.0\ nm)/Pt(0.6\ nm)]_X$ multilayers with constant Co and Pt thickness in the regime of tilted stripe domains, where we vary the number of repeats X to tune the remanent state from the well-known out-of-plane stripe domain via a tilted stripe domain to a purely in-plane domain state. Vibrating Sample Magnetometry (VSM) and Magnetic Force Microscopy (MFM) are used to study three characteristic samples with X = 22; 11 and 8, which represent the three above mentioned remanent states respectively. While for conventional perpendicular stripe domains the field reversal is characterized by irreversible hysteretic nucleation, propagation and annihilation of stripe domains across a broad field range, strikingly the tilted stripe domain regime reveals a collapse of all irreversible hysteretic switching down to a single point. The dramatically changed field reversal behavior will be discussed, also in the light of possible future applications.

MA 3.8 Mon 13:30 P

Nucleation site density & magnetization reversal in exchange-biased 1D nanostructures — •Sapida Akhundzada[1,3], Meike Reginka[1], Maximilian Merkel[1], Kristina Dingel[2,3], Bernhard Sick[2,3], Arno Ehresmann[1,3], and Michael Vogel[1,3] — [1]Institute of Physics & Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel — [2]Intelligent Embedded Systems, University of Kassel, Wilhelmshöher Allee 73, D-34121 Kassel — [3]AIM-ED - Joint Lab Helmholtzzentrum für Materialien & Energie, Hahn-Meitner-Platz 1, D-14109 Berlin

The interface-driven exchange bias (EB) effect [1] is a well-studied phenomenon observed in ferromagnetic (FM)/antiferromagnetic (AFM) thin film systems. In numerous studies, asymmetric hysteresis loops have been observed in EB thin films mainly caused by defects in the FM or AFM layer contributing to a locally inhomogeneous EB landscape. In full film samples, Romanens et al. [2] were able to correlate these asymmetries to higher domain nucleation densities for an antiparallel configuration of the applied field and the EB field. Here we report on the correlation between the nucleation site density and asymmetric remagnetization process in in-plane magnetized EB nanowires investigated by high-resolution optical Kerr microscopy. The influence of the structural dimensions, the EB material system, and additional modification of the interface by keV He ion bombardment are shown.

[1] W. H. Meiklejohn, J. Appl. Phys. 33, 1328 (1962)
[2] F. Romanens et al, Phys. Rev. B 72, 134410 (2005)

MA 3.9 Mon 13:30 P

Magnetic Coupling in YIG/GIG Heterostructures — •Sven Becker[1], Zengyao Ren[1,2,3], Felix Fuhrmann[1], Andrew Ross[1,4], Sally Lord[1,5], Shilei Ding[1,2,6], Rui Wu[1,7], Jinbo Yang[6], Jun Miao[3], Mathias Kläui[1,2,7], and Gerhard Jakob[1,2] — [1]University of Mainz, Germany — [2]Graduate School of Excellence 'MAINZ', Germany — [3]USTB, Beijing, China — [4]Université Paris-Saclay, France — [5]University of Manchester, UK — [6]Peking University, China — [7]University of Trondheim, Norway

We study the magnetic coupling in epitaxial $Y_3Fe_5O_{12}/Gd_3Fe_5O_{12}$ (YIG/GIG) heterostructures grown by pulsed laser deposition. From bulk sensitive magnetometry and surface sensitive spin Seebeck effect and spin Hall magnetoresistance measurements, we determine the alignment of the heterostructure magnetization as a function temperature and external magnetic field. The ferromagnetic coupling between the Fe sublattices of YIG and GIG dominates the overall behavior of the heterostructures. Because of the temperature-dependent gadolinium moment, a magnetic compensation point of the total bilayer system can be identified. This compensation point shifts to lower temperatures with increasing YIG thickness due the parallel alignment of the iron moments. We show that we can control the magnetic properties of the heterostructures by tuning the thickness of the individual layers, opening up a large playground for magnonic devices based on coupled magnetic insulators. These devices could potentially control the magnon transport analogously to electron transport in giant magnetoresistive devices.

MA 3.10 Mon 13:30 P

Growth, structure, and magnetic properties of artificially layered NiMn in contact to ferromagnetic Co on $Cu_3Au(001)$ — •Tauqir Shinwari[1], Ismet Gelen[1], Melek Villanueva[1], Ivar Kumberg[1], Yasser A. Shokr[1,2], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Faculty of Science, Department of Physics, Helwan University, 17119 Cairo, Egypt

Single-crystalline artificially layered [Ni/Mn] antiferromagnetic films with 1 atomic monolayer (ML) of Ni and 1, 2, or 3 ML of Mn have been deposited under ultrahigh-vacuum conditions on $Cu_3Au(001)$ and covered by ferromagnetic Co layers. Their structural and magnetic properties are characterized by low-energy electron diffraction (LEED) and magneto-optical Kerr effect (MOKE), respectively, and compared with disordered Ni_xMn_{100-x} alloy films with the same Ni/Mn ratio and the same film thickness. We find from LEED I(V) curves that the perpendicular interatomic lattice distance is decreased by 2% in the artificially layered [Ni/Mn] samples in comparison to the disordered Ni_xMn_{100-x} alloy films. This change in the structure causes higher coercivity, exchange bias, and stronger exchange coupling in artificially layered [Ni/Mn] samples compared to disordered Ni_xMn_{100-x} alloy films.

MA 3.11 Mon 13:30 P

Inverse proximity effects in superconductor/ferromagnet heterostructures studied by GISANS — •Annika Stellhorn[1,2], Emmanuel Kentzinger[1], Anirban Sarkar[1], Vitaliy Pipich[3], Kathryn Krycka[4], Patrick Schöffmann[1], Tanvi Bhatnagar-Schöffmann[1,5], and Thomas Brückel[1] — [1]Forschungszentrum Jülich GmbH, JCNS-2 and PGI-4, JARA-FIT, Jülich, GERMANY — [2]Lund University, Division of Synchrotron Radiation Research, Lund, Sweden — [3]Forschungszentrum Jülich GmbH, JCNS@MLZ, Garching, Germany — [4]National Institute of Standards and Technology, NIST-NCNR, Gaithersburg, USA — [5]Forschungszentrum Jülich GmbH, PGI-5, Jülich, GERMANY

Understanding the origin of proximity effects at the interfaces of superconducting and ferromagnetic materials is the key for an application in fluxonic devices and in spintronics. Depending on the ferromagnetic magnetocrystalline anisotropy, such proximity effects can lead to domain-wall-superconductivity or a generation of long-ranged spin-triplet Cooper pairs. This work presents a study of the depth-resolved lateral magnetic profile in the superconductor(S)/ferromagnet(F) thin film system Nb(S)/FePd(F) with perpendicular magnetic anisotropy by Grazing-Incidence Small-Angle Neutron Scattering (GISANS) with polarization analysis. In these systems, the transition from the normal-conducting state via a domain-wall-superconducting state to a complete-superconducting state is accompanied by an increase of the domain wall width.

MA 3.12 Mon 13:30 P

Impact of the separate variation of the sputter deposition pressure for seed and multilayer growth on the magnetic properties of Co/Pt multilayer films — •Rico Ehrler, Tino Uhlig, and Olav Hellwig — Chemnitz University of Technology, D-09107 Chemnitz, Germany

The pressure during the sputter deposition process greatly influences the structural as well as magnetic properties of Co/Pt multilayer films with perpendicular anisotropy. Already in 2013 Pierce et al. [1] tuned the lateral heterogeneity and structural order in such systems by changing the sputter deposition pressure for both the Pt seed as well as the multilayer simultaneously. By independent pressure variation of seed and multilayer we achieve an even higher degree of control over the magnetic properties. In a later work, a Ta adhesion layer between substrate and seed was used to achieve a highly oriented Pt(111) texture [2]. This is in accordance with our investigation, where the presence of such a layer greatly influences the growth of the seed.

In this study, a high and low deposition pressure was chosen independently for seed and multilayer, leading to 4 different seed/multilayer combinations. We repeated this variation with an added Ta adhesion layer between the substrate and the Pt seed and will highlight the impact of these systematic variations on the structural and magnetic properties.

[1] M. S. Pierce et al, Phys. Rev. B, vol. 87, no. 18, 2013
[2] Yu. Tsema et al., Appl. Phys. Lett., vol. 109, no. 7, 2016

MA 3.13 Mon 13:30 P

Effect of laser annealing on the magnetic properties of Co/Pt based multilayers — •Lokesh Rasabathina[1], Apoorva Sharma[1], Sandra Busse[3], Benny Böhm[1], Fabian Samad[1,2], Georgeta Salvan[1], Alexander Horn[3], and Olav Hellwig[1,2,4] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Laserinstitut Hochschule Mittweida, Schillerstraße 10, 09648 Mittweida, Germany — [4]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, 09107 Chemnitz, Germany

Two methods of laser annealing, namely, Continuous Wave (CW) and Pulsed Wave (PW) method, are used for modifying the magnetic properties of perpendicular magnetic anisotropy (PMA) multilayers in a controlled manner. For this we compare a set of two samples, a PMA $(Co/Pt)_{10}$ multilayer and an antiferromagnetically interlayer exchange coupled PMA $(Co/Pt)_4/Co/Ir/(Co/Pt)_5$ multilayer. Room temperature hysteresis loops using longitudinal MOKE magnetometry are measured for different laser annealing conditions. Thus, a relationship between the applied laser parameters and the magnetic properties is extracted, which provides insight into the processes that occur during the laser annealing process.

MA 3.14 Mon 13:30 P

Giant Topological Hall Effect in Noncollinear Phase of Two-dimensional Antiferromagnetic Topological Insulator MnBi4Te7 — •Subhajit Roychowdhury, Sukriti Singh, Satya N. Guin, Nitesh Kumar, Tirthankar Chakraborty, Walter Schnelle, Horst Borrmann, Chandra Shekhar, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Magnetic topological insulators provide an important platform for realizing several exotic quantum phenomena, such as the axion insulating state and quantum anomalous Hall effect, owing to the interplay between topology and magnetism. MnBi4Te7 is a two-dimensional Z_2 antiferromagnetic (AFM) topological insulator with a Néel temperature of ~13 K. In AFM materials, the topological Hall effect (THE) is observed owing to the existence of nontrivial spin structures. In this study, we observed that an unanticipated THE starts to develop in a MnBi4Te7 single crystal when the magnetic field is rotated away from the easy axis (c-axis) of the system. Furthermore, the THE resistivity reaches a giant value of ~7 microΩcm at 2 K when the angle between the magnetic field and c-axis is of 75°. This value is significantly higher than the values for previously reported systems with noncoplanar structures. The THE can be ascribed to the noncoplanar spin structure resulting from the canted state during the spin-flop transition in the ground AFM state of MnBi4Te7. The large THE at a relatively low applied field makes the MnBi4Te7 system a potential candidate for spintronic applications.

MA 3.15 Mon 13:30 P

High-throughput screening of the exchange interactions among magnetic impurities in a quantum spin Hall insulator — •Rubel Mozumder, Philipp Rüssmann, and Stefan Blügel — Peter Grünberg Institut (PGI) and Institute for Advanced simulation (IAS), Forschungszentrum Jülich, D-52424 Jülich, Germany

An internal magnetic field in Quantum Spin Hall Insulators (QSHI) breaks the time-reversal symmetry and transforms the QSHI into a Quantum Anomalous

Hall insulator (QAHI). This topological phase transition also transforms 1D helical edge states of a QSHI into 1D chiral states, which are topologically protected single spin-transport channels at the edges of QAHIs.

Here we present a high-throughput study of a large number of magnetic impurities (3*d* and 4*d* transition-metal elements) in different combinations, which are embedded into the QSHI Bi_2Te_3. For this, we extend the AiiDA-KKR package [1] that allows to run high-throughput *ab initio* calculations using the JuKKR code [https://jukkr.fz-juelich.de] that is based on full-potential relativistic all-electron density functional theory calculations within the Korringa-Kohn-Rostoker Green-function method. We extract Heisenberg exchange coupling parameters as well as Dzyaloshinskii-Moriya vectors for pairs of impurities to study the tendency toward stable ferromagnetic order, which is a prerequisite for the QAHI state. Furthermore, we investigate the effect of co-doping on the magnetic interactions.

[1] P. Rüßmann *et al.*, npj Comput Mater **7**, 13 (2021).

MA 3.16 Mon 13:30 P

Complex nanostructured magnetic thin films investigated by x-ray absorption spectroscopy — •Damian Günzing[1], Shalini Sharma[2,3], Alexander Zintler[3], Johanna Lill[1], Debora Motta Meira[4], Harish K Singh[3], Ruiwen Xie[3], Georgia Gkouzia[3], Márton Major[3], Iliya Radulov[3], Philipp Komissinskiy[3], Hongbin Zhang[3], Konstantin Skokov[3], Yukiko K Takahashi[2], Lambert Alff[3], Leopoldo Molina-Luna[3], Heiko Wende[1], and Katharina Ollefs[1] — [1]Faculty of Physics, University of Duisburg-Essen — [2]National Institute for Materials Science, Tsukuba — [3]Institute of Materials Science, Technical University of Darmstadt — [4]Sector 20, Advanced Photon Source, Argonne National Laboratory

Understanding the interplay of the structural phase composition and the corresponding magnetic properties is at the heart of hysteresis design of e.g. hard magnetic materials. Here, we investigated a $SmCo_5$ Sm_2Co_{17} nano composite film manufactured via MBE on an Al_2O_3 substrate without additional buffer layers [1]. We established a multi-absorber fitting and simulation method for non-destructive extended x-ray fine structure (EXAFS) spectra of complex magnetic materials to quantify the two phases, $SmCo_5$ and Sm_2Co_{17}. In combination with transmission electron microscopy and magnetometry we found that the high magnetization and strong perpendicular anistropy originates from the nanoscale composition of these two phases with coherent interfaces. (Supported by the DFG Project-ID 405553726*CRC 270).

[1] S. Sharma et al., *ACS Appl. Mater. Interfaces* (2021) 13, 27, 32415-32423

MA 3.17 Mon 13:30 P

Topographic and magnetic characterization of periodically curved organic/metallic hybrid thin film systems — •Christian Janzen[1], Sekvan Bagatur[2], Maximilian Merkel[1], Meike Reginka[1], Michael Vogel[1], Thomas Fuhrmann-Lieker[2], and Arno Ehresmann[1] — [1]Institute of Physics and Center for Interdisciplinary Nanostrcuture Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel — [2]Institute of Chemistry and CINSaT, University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

In this work, a low-molecular azo-glass material (AZOPD [1]) is structured by a two-beam-interference-patterning process. Thereby, a periodically curved topography with a structure height and a structure wavelength at the nanoscale is obtained, whereby the latter is constant over the sample area. The periodically curved organic layer is used as a topographic template for the deposition of a ferromagnetic thin film. Non-contact atomic force microscopy measurements were conducted in order to investigate the alteration of the topography after sputter deposition. By spatially resolved magneto-optical Kerr magnetometry, a direct correlation between the local topography of the heterostructure and its coercive field is observed. The occurence of an uniaxial magnetic anisotropy, originating from the periodically curved topography, is examined by varying the ferromagnetic layer thickness. Finally, the influence of the sample topography on the alignment of magnetic domains is investigated via Kerr-microscopy.

[1] Fuhrmann *et al.* Chem. Mater. 1999, 11, 8, 2226-2232

MA 3.18 Mon 13:30 P

Simulation of the FEBID process — •Alexander Kuprava[1] and Michael Huth[2] — [1]Goethe Universität Frankfurt, Germany — [2]Goethe Universität Frankfurt, Germany

Focused electron beam induced deposition is a direct-write nano-fabrication technology with unique advantages for free-form 3D deposition. However, a shape-true transfer from a 3D CAD model target structure to the actual nano-deposit is a non-trivial task. Here we present our modular computer simulation framework that was developed to simulate FEBID process in order to assist the study of the growth of 3D structures. The program includes an electron-beam generation and an electron-solid interaction module, a diffusion module and a reaction equation solver. A Monte Carlo (MC) simulation was utilized for scattered electron trajectories generation and inelastic electron-solid interaction on a cellular structured 3D grid. The simulation details are discussed which include applied structured grid-based simulation practices, the numerical solution of the reaction equation, the diffusion simulation concept and the MC simulation of primary and secondary electron flux. The program was used to simulate the growth of high aspect-ratio Pt-based nanoscale pillars with a stationary Gaussian electron beam using (CH3)3CpCH3Pt(IV) as a precursor. The simulation results were compared to the experimentally grown structures regarding shape trueness and growth rate.

MA 3.19 Mon 13:30 P

Spray deposition of ferromagnetic $SrFe_{12}O_{19}$ nanoplates colloid at Si and cellulose substrate — •Andrei Chumakov[1], Calvin Brett[1,2], Artem Eliseev[3], Evgeny Anokhin[3], Lev Trusov[3], Lewis Akinsinde[4], Marc Gensch[1,5], Dirk Menzel[6], Matthias Schwartzkopf[1], Wei Cao[5], Shanshan Yin[5], Manuel Scheel[5], Micheal Rübhausen[4], Peter Müller-Buschbaum[5,7], Daniel Soederberg[2], Andrei Eliseev[3], and Stephan V. Roth[1,2] — [1]DESY, Hamburg, Germany — [2]KTH RIT, Stockholm, Sweden — [3]MSU, Moscow, Russia — [4]CFEL, Universität Hamburg, Hamburg, Germany — [5]TU München, Garching, Germany — [6]TU Braunschweig, Braunschweig, Germany — [7]TU München, MLZ, Garching, Germany

Ferromagnetic $SrFe_{12}O_{19}$ nanoparticles with a hard magnetic moment perpendicular to their plane and stabilized by a positive charge can form a self-ordered coating under the influence of magnetic fields drying from dispersion. We investigated the film formation of a stable colloid dispersion of ferromagnetic nanoplates and nanoblocks onto a silicon substrate and cellulose nanofilm without and under the action of an external magnetic field during scalable layer-by-layer spraying. The formation of a film of ferromagnetic particles from an aqueous colloid makes it possible to form a stable magnetic coating of agglomerates of nanoparticles. An external magnetic field in the deposition process leads to the appearance of residual magnetization in the film. Particles with a smaller aspect ratio form a periodic structure of agglomerates of nanoparticles with signs of an artificial opal-like structure.

MA 3.20 Mon 13:30 P

Magnetization switching of dipolar coupled elongated permalloy nanostructures of high shape anisotropy — Neeti Keswani[1], Yoshikata Nakajima[2], Neha Chauhan[2], Tomofumi Ukai[2], Himadri Chakraborti[3], Kantimoy Das Gupta[3], Tatsuro Hanajiri[2], Sakthi Kumar[2], Yukio Ohno[4], Hideo Ohno[4], and •Pintu Das[1] — [1]Department of Physics, Indian Institute of Technology Delhi, New Delhi-110016 — [2]Bio Nano Electronics Research Centre, Toyo University, Kawagoe, Saitama-3508585, Japan — [3]Department of Physics, Indian Institute of Technology Bombay, Mumbai-400076 — [4]Research Institute of Electrical Communications, Tohoku University, Sendai, Japan - 9808577

Behavior of nanomagnets of strong shape anisotropy can be studied by modelling them as Ising-like macrospins. Due to the potential use of such macrospin-like nanomagnets in devices such as in nanomagnetic logic etc., a detailed understanding of the exact switching behavior of such nanomagnets coupled via dipolar interaction is essential.

In this work, we have used 2-dimensional electron gas based micro-Hall magnetometry in ballistic transport regime to measure the stray fields emanating from the lithographically patterned elongated nanomagnets of $Ni_{80}Fe_{20}$ arranged in a double ring like structure. Our results demonstrate that although the magnetic images of the nanomagnets show single-domain behavior, however, their switching process may involve formation of other complex structures such as magnetic vortices, etc. The experimental results are analyzed by performing micro-magnetic simulations for the nanostructures.

MA 4: Spin-Dependent 2D Phenomena

Time: Tuesday 10:00–11:15 Location: H5

Invited Talk MA 4.1 Tue 10:00 H5

2D Magnetic materials — •Alberto Morpurgo — University of Geneva

Exfoliation of thin crystals from van der Waals bonded parent compounds allows the realization of atomically thin layers, exhibiting new phenomena, properties and functionality. For atomically thin magnetic materials, this strategy has been followed only recently, and has led to multiple interesting results. In my talk I will mainly focus on the investigation of 2D semiconducting magnetic materials by means of transport measurements. I will discuss how we use atomically thin layers to realize tunnel barriers, and measure the temperature and magnetic field dependence of the tunneling resistance to extract detailed information about their magnetic phase diagram. In a first generation of experiments we have demonstrated the principle for diferent antiferromagnetic semiconductors (CrI_3, $CrCl_3$, $MnPS_3$), and extracted important microscopic information about the phase transitions occurring in these systems (and in some cases about the relevant exchnage integrals). More recently we have shown that the technique also works for ferromagnets such as $CrBr_3$, using which we are able to infer detailed information about the magnetic field and temperature dependence of the tubnneling resistance (both in the ferromagnetic and in the paramagnetic state).

MA 4.2 Tue 10:30 H5

Spin-polarised imaging and quasi-particle interference of the van-der-Waals ferromagnet Fe_3GeTe_2 — •Olivia Armitage[1], Christopher Trainer[1], Luke Rhodes[1], Harry Lane[2], Edmond Chan[2], Chris Stock[2], and Peter Wahl[1] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife, KY16 9SS, United Kingdom — [2]SUPA, School of Physics and Astronomy, University of Edinburgh, United Kingdom

Van-der-Waals ferromagnets have enabled the development of heterostructures with spintronics functionalities. However, information about the magnetic properties of these systems has come largely from macroscopic techniques, with little being known about the microscopic magnetic properties. Here, we use spin-polarised scanning tunnelling microscopy and quasi-particle interference imaging to study the magnetic and electronic properties of the metallic 2D vdW ferromagnet Fe_3GeTe_2. From comparison with Density Functional Theory calculations we can assign the quasi-particle interference to be dominated by spin-majority bands. We find a dimensional dichotomy of the bands at the Fermi energy: bands of minority character are predominantly two-dimensional in character, whereas the bands of majority character are three-dimensional. We expect that this will enable new design principles for spintronics devices.

MA 4.3 Tue 10:45 H5

Photocurrents in single-layer Fe3GeTe2 from first principles — •Maximilian Merte[1,2,3], Frank Freimuth[3,1], Theodoros Adamantopoulos[1], Dongwook Go[3,1], Tom Saunderson[3,1], Matthias Kläui[3], Stefan Blügel[1], and Yuriy Mokrousov[1,3] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Department of Physics, RWTH Aachen University, 52056 Aachen, Germany — [3]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

We present a method for calculating laser induced currents [1], which are of second order in the electric field, by means of Wannier interpolation. Our method can be applied as a post-processing tool to the wannier90code [2], which is compatible with many ab-initio codes. We apply the developed method to study photocurrents in a single-layer of the van der Waals layered crystal Fe3GeTe2, which act as 2D ferromagnetic metals whose properties are being intensively explored nowadays [3]. Our calculations predict a very sizeable magnitude of photocurrents in this material, whose sign and properties can be tuned by doping or by the frequency of the pulse. We also uncover the importance of the scattering effects which are naturally taken care of within the Keldysh formalism that we use as the ground framework for our method. We acknowledge funding from Deutsche Forschungsgemeinschaft (DFG) through SFB/TRR 173 and 288. Simulations were performed with computing resources granted by JARA-HPC from RWTH Aachen University and Forschungszentrum Jülich under projects jara0161, jiff40 and jias1a [4]

[1] Frank Freimuth et al., arXiv: 1710.10480 (2017)
[2] www.wannier.org
[3] Y. Deng et al., Nature 563, 94 (2018).
[4] Jülich Supercomputing Centre. (2018). JURECA: Modular supercomputer at Jülich Supercomputing Centre. Journal of large-scale research facilities, 4, A132. http://dx.doi.org/10.17815/jlsrf-4-121-1

MA 4.4 Tue 11:00 H5

Charge density waves as enablers for chiral magnetism in two-dimensional $CrTe_2$ — •Nihad AbuAwwad[1,2], Manuel dos Santos Dias[1], Sascha Brinker[1], and Samir Lounis[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany

The discovery of two-dimensional (2D) van der Waals magnets opened unprecedented opportunities for the fundamental exploration of magnetism in quantum materials and the realization of next generation spintronic devices. Recently, thin $CrTe_2$ films were demonstrated to be ferromagnetic up to room temperature, with an intriguing dependence of the easy axis on the thickness of the material [1,2]. Here, we demonstrate using first-principles that the charge-density waves characterizing a single $CrTe_2$ give rise to chiral magnetism through the emergence of the Dzyaloshinskii-Moriya interaction (DMI). Utilizing atomistic spin dynamics, we perform a detailed investigation of the complex magnetic properties pertaining to this 2D material impacted by the presence of various types of charge density waves.

–Work funded by the Palestinian-German Science Bridge (BMBF–01DH16027) and Priority Programme SPP 2244 2D Materials Physics of van der Waals Heterostructures of the DFG (project LO 1659/7-1).

[1] Zhang *et al.*, Nat. Commun. **12**, 2492 (2021); [2] Meng *et al.*, Nat. Commun. **12**, 809 (2021).

MA 5: Posters Magnetism II

Topics: Skyrmions (5.1-5.14), Non-Skyrmionic Magnetic Textures (5.15-5.20), Weyl Semimetals (5.21-5.22)

Time: Tuesday 10:00–13:00 Location: P

MA 5.1 Tue 10:00 P

Robust Formation of Nanoscale Magnetic Skyrmions in Easy-Plane Anisotropy Thin Film Multilayers with Low Damping — •Luis Flacke[1,2], Valentin Ahrens[3], Simon Mendisch[3], Lukas Körber[4,5], Tobias Böttcher[6], Elisabeth Meidinger[1,2], Misbah Yaqoob[1,2], Manuel Müller[1,2], Lukas Liensberger[1,2], Attila Kákay[4], Markus Becherer[3], Philipp Pirro[6], Matthias Althammer[1,2], Stephan Geprägs[1], Hans Huebl[1,2,7], Rudolf Gross[1,2,7], and Mathias Weiler[1,2,6] — [1]Walther-Meißner Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physics Department, Technical University of Munich, 85748 Garching, Germany — [3]Department of Electrical and Computer Engineering, Technical University of Munich, 80333 Munich, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [5]Fakultät Physik, Technische Universität Dresden, 01062 Dresden, Germany — [6]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — [7]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

We investigate magnetic superlattices based on the low-damping and high saturation magnetization binary alloy Co25Fe75. The formation of stable sub-100 nm diameter skyrmions is confirmed and analyzed by magnetic force microscopy within an $K_{\mathrm{eff}} < 0$. The relatively low damping of the superlattice spin dynamics is quantified by broadband ferromagnetic resonance measurements.

MA 5.2 Tue 10:00 P

Exchange- and Dzyaloshinskii-Moriya interactions in magnetic bilayers at surfaces — •Tim Drevelow, Mara Gutzeit, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany

Magnetic skyrmions in synthetic antiferromagnets exhibit favorable transport properties [1], e.g. the absence of the skyrmion Hall effect and have recently been stabilized at room temperature [2]. Here, we investigate synthetic antiferromagnets built from trilayers composed of Co and Fe layers coupled via a Rh spacer layer. *Ab initio* calculations using density functional theory were performed to obtain the strength of the inter- and intralayer exchange and Dzyaloshinskii-Moriya interactions which allows to parametrize an atomistic spin model. We studied freestanding trilayers as well as trilayers on the Ir(111) surface since both Rh/Co and Rh/Fe bilayers have previously been grown on this surface [3,4].

[1] Zhang *et al.* Nat. Com. **7**, 10293 (2016)
[2] Legrand *et al.* Nat. Mat. **19**, 34 (2020)
[3] Romming *et al.* Phys. Rev. Lett. **120**, 207201 (2018)
[4] Meyer *et al.* Nat. Com. **10**, 3823 (2019)

MA 5.3 Tue 10:00 P

The Skyrmion Radius Calculator — •Moritz Sallermann, Bernd Zimmermann, Fabian Lux, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The skyrmion radius is an important quantity for any skyrmion characterisation, motion and device concept. For technological applications – especially as a promising building block for future information technology – it is essential to determine those materials in which skyrmions assume a typical radius of 10 nm or even less.

We studied the energy contributions of the circular domain wall profile [1] in thin, infinite films of magnetic materials, employing the continuous, micromagnetic approximation. Notably, we also include the exact contribution of the magnetostatic interactions and thus go beyond the commonly applied thin-film

approximation. We confirm our findings by comparing them with exact micromagnetic calculations that do not depend on any choice of trial functions. We provide an easy to use and fast online tool, the Skyrmion Radius Calculator [2], which computes an approximation to the skyrmion radius in fractions of a second. It is based on the minimization of the energy of the ansatz profile. The agreement with full micromagnetic simulations can be estimated from the resulting profile parameters and is excellent as long as the skyrmions are of domain-wall character.

Acknowledgement: DFG through SPP-2137 & SFB-1238 (project C1).

[1] F. Büttner, I. Lemesh and G.S. Beach, Sci.Rep., 8(1) (2018)
[2] https://juspin.de/skyrmion-radius/

MA 5.4 Tue 10:00 P

Modification of the DMI by He$^+$ ion bombardment characterized by high-resolution optical Kerr microscopy — •Sapida Akhundzada[1], Florian Ott[1], Maxwell Li[2], Tim Mewes[3], Arno Ehresmann[1], Vincent Sokalski[2], and Michael Vogel[1] — [1]Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Kassel, Germany — [2]Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, USA — [3]Department of Physics and Astronomy, University of Alabama, Tuscaloosa, USA

The Dzyaloshinkii-Moriya interaction (DMI) is an antisymmetric exchange interaction arising, e.g., from interfaces between ferromagnets and heavy metals with large spin-orbit coupling [1]. The DMI is topologically stabilizing chiral spin-structures like skyrmions which are promising candidates for nonvolatile magnetic memory technologies [2]. It has been recently demonstrated that the DMI can be tuned by bombardment with accelerated ions [3]. While altering the interfaces between the different material layers in total, the sign and magnitude of the DMI can be manipulated [3]. In a systematic study, we modified the DMI by keV He ion bombardment in perpendicularly magnetized ferromagnetic/heavy metal multilayer system. In order to characterize the interfacial DMI, we characterized the field-driven, asymmetric growth of the magnetic domains by high-resolution Kerr microscopy.

[1] T. Moriya, Phys. Rev. Lett. 4, 228 (1960)
[2] A. Fert, V. Cros and J. Sampaio, Nat. Nanotechnol. 8, 152 (2013)
[3] H. T. Nembach, et al., arXiv:2008.06762 (2020)

MA 5.5 Tue 10:00 P

Stability of the skyrmion lattice in $Fe_{1-x}Co_xSi$ — •Carolina Burger[1], Andreas Bauer[1], Alfonso Chacon[1], Marco Halder[1], Jonas Kindervater[1], Sebastian Mühlbauer[2], André Heinemann[2], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, D-85748 Garching, Germany

We report measurements of the magnetization, susceptibility, and electrical transport on single-crystal $Fe_{1-x}Co_xSi$, complemented by small-angle neutron scattering. In small magnetic fields, this compound hosts a hexagonal lattice of topologically non-trivial skyrmions that may persist metastably down to lowest temperatures when field-cooled. We show that signatures characteristic of the skyrmion lattice survive field values up to the field-polarized regime as well as field inversion.

At low temperatures, the Hall effect is dominated by the anomalous contributions, with additional contributions emerging in the vicinity of the magnetic phase transitions hinting towards complex processes associated with the unwinding of the skyrmion lattice.

[1] A. Bauer, C. Pfleiderer, and M. Garst, Phys. Rev. B 93 (23), 235144 (2016), [2] A. Bauer, A. Chacon, M. Halder, C. Pfleiderer, Springer Series in Solid-State Sciences 192 (2018), [3] H. Oike, A. Kikkawa, N. Kanazawa, Y. Taguchi, M. Kawasaki, Y. Tokura, and F. Kagawa, Nature Phys. 12, 62 (2016)

MA 5.6 Tue 10:00 P

Topological Hall effect in thin films of noncollinear magnets — •Rebeca Ibarra[1,2], Anastasios Markou[1], Aleksandr Sukhanov[2], Dmytro Inosov[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Technical University Dresden, Germany

Topological spin textures in quantum materials are of great interest, along with the associate transport signatures, for next-generation spintronic applications. Recently, the tetragonal (t) Heusler compounds show to host elliptical skyrmions and antiskyrmions [1], and the hexagonal (h) half-Heusler compound MnPtGa displays noncollinear magnetism [2]. Spin chirality in metallic materials with noncoplanar spin structure gives rise to a Berry phase-induced topological Hall effect. In addition, neutron diffraction is a powerful technique to study the magnetic structure of these chiral materials.

Here, we study the noncollinear spin textures in high-quality epitaxial thin films of the t-Mn_2RhSn and h-MnPtGa compounds. In t-Mn_2RhSn, we observe topological Hall signatures of two distinct chiral spin textures. Interestingly, we show with single-crystal neutron diffraction that the h-MnPtGa undergoes a magnetic phase transition from ferromagnetic to in-plane canted antiferromagnetic. With our thin film method, we can access a novel and fundamental understanding of these compounds not possible with other methods.

[1] J. Jena *et al.*, Nat. Commun. **11**, 1115 (2020).
[2] J. A. Cooley *et al.*, Phys. Rev. Mater. **4**, 044405 (2020).

MA 5.7 Tue 10:00 P

Spin-transfer torque driven motion, deformation, and instabilities of magnetic skyrmions at high currents — •Jan Masell[1], Davi R. Rodrigues[2], and Karin Everschor-Sitte[2] — [1]RIKEN CEMS, Wako, Japan — [2]University of Duisburg-Essen, Duisburg, Germany

Magnetic skyrmions are whirls which are characterized by a topological winding number. They have gained massive attention due to this real-space topological property and other features like possible nanometer size, extraordinary stability, or easy manipulation by electrical currents or other means. Therefore, various proposals emerged how skyrmions might serve as mobile information carriers in future information technology.

When considering skyrmions driven by spin-transfer torque (STT), it is usually assumed that distortions due to the current are small.

We have simulated STT-driven skyrmions with ultra high precision and quantitatively studied the distortion by STT in the entire stability regime up to the ferromagnetic instability. We find analytical expressions for the distortion of skyrmions, which is quadratic in the current, as well as for the STT-induced elliptical instability which destroys the skyrmion. We show numerically that for large enough Gilbert damping, however, stable but distorted "shooting star" skyrmion solutions are possible in regimes even above the elliptical instability. [1]

[1] J. Masell, D. R. Rodrigues, B. F. McKeever & K. Everschor-Sitte, Phys. Rev. B **101**, 214428 (2020)

MA 5.8 Tue 10:00 P

Skyrmion movement in Ta/CoFeB/MgO-trilayers — •Hauke Lars Heyen[1], Jakob Walowski[1], Christian Denker[1], Malte Römer-Stumm[2], Markus Münzenberg[1], and Jeffrey McCord[2] — [1]Institut für Physik, Universität Greifswald, Felix-Hausdorff-Straße 6, 17489 Greifswald, Germany — [2]Christian-Albrechts-Universität zu Kiel, Institute for Materials Science, Nanoscale Magnetic Materials and Magnetic Domains, 24143 Kiel, Germany

Skyrmion manipulation and dynamics control are promising tools for the realization of racetrack memory devices to increase data storage densities.

We use current pulses to experimentally investigate skyrmion dynamics in Ta/CoFeB/MgO-trilayers. Layer thickness control in CoFeB layers in the picometer range generated by very small thickness gradients allows to produce layers exhibiting a transition region from in-plane to out-of-plane magnetic anisotropy along the sample. This enables fine adjustment for optimal skyrmion nucleation. Skyrmions are created in the demagnetized CoFeB layer using magnetic field pulses tilted slightly out of the plane direction. Afterwards stabilized by a small out-of-plane field, skyrmion dynamics are generated with microsecond current pulses and recorded by Kerr-microscopy.

By using a specially developed tracking software to follow the motion after each current pulse, we analyze the skyrmion dynamics. The movement shows a Skyrmion-Hall-effect and a superdiffusive distribution. Further the skyrmions seem to get stuck, generated or annihilated at pinning centers.

MA 5.9 Tue 10:00 P

Ab-initio investigation of intrinsic antiferromagnetic skyrmions in magnetic thin films — •Amal Aldarawsheh[1,2], Imara Fernandes[1], Sascha Brinker[1], Moritz Sallersmann[1], Muayyad Abusaa[3], and Samir Lounis[1,2] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany — [3]Physics Department, Arab American University, Jenin, Palestine.

Skyrmions are topologically protected spin textures that are envisioned to be the next generation of bits. However, conventional ferromagnetic (FM) skyrmions are deflected when an electric field is applied, which limits their use in spintronic devices. In contrast, antiferromagnetic (AFM) skyrmions, which consist of two FM solitons coupled antiferromagnitically, are predicted to have zero net magnus force [1], and this makes them promising candidates for spintronic racetrack memories. So far these have been stabilized in synthetic AFM structures [2], i.e. multilayers hosting FM skyrmions, which couple antiferromagnetically through a non-magnetic spacer. Using *ab initio* calculations in conjunction with atomistic spin dynamics, we investigate systematically and predict the presence of chiral intrinsic AFM structures in specific and realistic combination of thin films deposited on heavy substrates.

[1] X. Zhang *et al.* Sci. Rep. **6**, 24795 (2016), [2] Legrand *et al.* Nat. Mat., **19**, 34 (2020). Work funded by the PGSB (BMBF–01DH16027) and Horizon 2020–ERC (CoG 681405–DYNASORE).

MA 5.10 Tue 10:00 P

First-principles study of DMI mechanisms and exchange frustration in Rh/Co/Fe/Ir multilayers — •Felix Nickel, Sebastian Meyer, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel

Magnetic skyrmions are promising for the usage in data storage and logic devices. Materials, which can host small diameter skyrmions in zero magnetic field at room temperature, are suitable for such applications. Recently, it has been shown that ultrathin Rh/Co films on Ir(111) exhibit skyrmions with diameters below 10 nm at zero magnetic field [1]. On the other hand, room temperature skyrmions with diameters of 30 nm - 90 nm have been found in magnetic multilayers [2].The Dzyaloshinskii-Moriya Interaction (DMI), exchange frustration and magnetocrystalline anisotropy are the main characteristics that make materials capable of hosting such complex spin structures. We performed density functional theory calculations for different transition-metal multilayer systems consisting of Co, Fe, Ir and Rh and determined those magnetic interactions to investigate if properties of ultra thin film systems, like in Ref. [1], can be transferred to multilayer systems. We present how the magnetic interactions depend on the structural properties of the multilayer systems. Further we predict multilayers which are very promising for the stabilisation of magnetic skyrmions.

[1] Meyer *et al.*, Nat. Commun. **10**, 3823 (2019)
[2] Moreau-Luchaire *et al.*, Nat. Nanotechnol. **11**, 444 (2016)

MA 5.11 Tue 10:00 P

Skyrmion braids — Fengshan Zheng[1], Filipp N. Rybakov[2], •Nikolai S. Kiselev[3], Dongsheng Song[1,4], András Kovács[1], Haifeng Du[5], Stefan Blügel[3], and Rafal E. Dunin-Borkowski[1] — [1]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Gr\"unberg Institute, Forschungszentrum J\"ulich, 52425 J\"ulich, Germany — [2]Department of Physics, KTH-Royal Institute of Technology, Stockholm, SE-10691 Sweden — [3]Peter Gr\"unberg Institute and Institute for Advanced Simulation, Forschungszentrum J\"ulich and JARA, 52425 J\"ulich, Germany — [4]Institutes of Physical Science and Information Technology, Anhui University, Hefei 230601, China — [5]High Magnetic Field Laboratory, Chinese Academy of Science (CAS), Hefei, Anhui Province 230031, China

Skyrmions are vortex-like spin textures that form strings in magnetic crystals. Due to the analogy to elastic strings, skyrmion strings are naturally expected to braid and form complex three-dimensional patterns, but this phenomenon has not been explored yet. We found that skyrmion strings can form braids in cubic crystals of chiral magnets [1]. Our finding is confirmed by direct observations of skyrmion braids in B20-type FeGe using transmission electron microscopy. The theoretical analysis predicts that the discovered phenomenon is general for a wide family of chiral magnets. These findings have important implications for skyrmionics and propose a solid-state framework for applications of the mathematical theory of braids.

[1] F. Zheng et al., arXiv:2104.01682.

MA 5.12 Tue 10:00 P

Antiskyrmions and sawtooth surface textures in an S4 symmetric magnet — Kosuke Karube[1], Licong Peng[1], •Jan Masell[1], Xiuzhen Yu[1], Fumitaka Kagawa[1,2], Yoshinori Tokura[1,2], and Yasujiro Taguchi[1] — [1]RIKEN CEMS, Wako, Japan — [2]University of Tokyo, Tokyo, Japan

Magnetic skyrmions are vortex-like textures in the magnetization. By now, skyrmions are found in many systems ranging from bulk chiral magnets to thin films and monolayers. Their anti-vortex-like anti-particles, consequently dubbed "antiskyrmions", were theoretically predicted to exist in magnets with D_{2d} or S_4 symmetry [1], but were observed only in a family of D_{2d}-symmetric Heuslers. [2]

We report the first observation of antiskyrmions in a magnet with S_4 symmetry. We prepared Pd-doped Schreibersite which shows a weak uniaxial anisotropy and weak antisymmetric DMI. Thus, domain walls with opposite handedness are stabilized along two orthogonal directions. In thin films, LTEM reveals square-shaped antiskyrmions, elliptical skyrmions, and trivial bubbles, as a consequence of dipolar interactions. For thicker systems, MFM shows that the domain wall textures fractalize with sawtooth patterns. These novel patterns arise from the weak antisymmetric DMI in combination with dominant dipolar interactions, as shown by our micromagnetic simulations. [3]

[1] A.N. Bogdanov & D.A. Yablonskii, JETP **68,** 101-103 (1989)
[2] A.K. Nayak *et al.*, Nature **548,** 561-566 (2017)
[3] K. Karube, L.C. Peng, J. Masell, *et al.*, Nature Materials **20,** 335-340 (2021)

MA 5.13 Tue 10:00 P

Real-Space Observation of Topological Defects in Extended Skyrmion-Strings — •Jan Masell[1], Xiuzhen Yu[1], Fehmi S. Yasin[1], Kosuke Karube[1], Naoya Kanazawa[2], Kiyomi Nakajima[1], Takuro Nagai[3], Koji Kimoto[3], Wataru Koshibae[1], Yasujiro Taguchi[1], Naoto Nagaosa[1,2], and Yoshinori Tokura[1,2] — [1]RIKEN CEMS, Wako, Japan — [2]University of Tokyo, Tokyo, Japan — [3]National Institute for Materials Science, Tsukuba, Japan

Skyrmions are whirls in the magnetization which are characterized by a 2d topological winding number. Due to their topology, large skyrmions are protected by a high energy barrier [1] which makes them interesting objects for potential future applications. However, in 3d bulk materials or thin films, skyrmions are strings (SkS) which can have singular topological defects [2], known as Bloch points.

We use Lorentz Transmission Microscopy (LTEM) on thin films of chiral magnets to obtain a sideview of SkS that extend in the film plane. We obtain high resolution images of various defects, including Bloch points which terminate SkS or fuse them, but also SkS which annihilate smoothly by escaping through the surface. These objects can be discerned by comparing them to the results of micromagnetic simulations. [3]

[1] B. Heil, A. Rosch & J. Masell, Phys. Rev. B **100,** 134424 (2019)
[2] P. Milde *et al.*, Science **340**, 1076-1080 (2013)
[3] X.Z. Yu*, J. Masell* *et al.*, Nano Lett. **20,** 7313-7320 (2020)

MA 5.14 Tue 10:00 P

Mode following method for magnetic systems — •Stephan von Malottki[1,2], Moritz A. Goerzen[2], Hendrik Schrautzer[1,2], Pavel F. Bessarab[1], and Stefan Heinze[2] — [1]Science Institute, University of Iceland, Reykjavík — [2]ITAP, University of Kiel, Germany

The average lifetime of metastable magnetic states is commonly determined by harmonic transition state theory (HTST) [1] or the related Langer's theory [2], resulting in an Arrhenius-law depending on the thermal energy, the energy barrier and the pre-exponential factor. The latter contains information about the dynamics and entropic effects of the transition and is often challenging to obtain. In the past, the application of HTST calculations to magnetic skyrmions has been limited to cases in which the harmonic and zero-mode approximations are justified [1-3]. Other cases, such as the collapse of magnetic skyrmions via the chimera transition [2-4] or the collapse of antiskyrmions [4] were not always accessible. Here, we present a numerical method to evaluate the entropic contribution of individual Eigenmodes beyond the harmonic approximation. With this method, not only the quality of the harmonic and zero-mode approximations can be evaluated, but also the direct numerical calculation of the entropic contributions becomes feasible, which allows access to intermediate temperature regimes that could not be treated with conventional HTST.

[1] P. Bessarab *et al.* Sci. Rep. **8**, 3433 (2018) [2] L. Desplat *et al.* PRB **99**, 174409 (2019) [3] F. Muckel *et al.* Nat. Phys. **17**, 395-402 (2021) [4] S. Meyer *et al.* Nat. Commun. **10** 3823, (2019)

MA 5.15 Tue 10:00 P

Single-Crystal Growth and Low-Temperature Properties of Er_2 — •Christoph Resch[1], Georg Benka[1,2], Andreas Bauer[1], and Christian Pfleiderer[1] — [1]Physik Department E51, Technische Universität München, 85748 Garching, Germany — [2]Kiutra GmbH Rupert-Mayer-Str. 4481379 Munich, Germany

Single crystals of the hexagonal rare-earth diboride ErB_2 were synthesized by means of the self-adjusted flux travelling solvent optical floating zone technique. The magnetic phase diagram was inferred from measurements of the magnetization and the ac susceptibility as a function of magnetic field and temperature for fields up to 14 T applied along major crystallographic axes. We find behavior characteristic of a hard-axis-easy-plane antiferromagnet. Magnetoresistivity and hall effect measurements up to 20 T exhibit a field dependence that may not be accounted for by standard normal and anomalous contributions, suggesting non-collinear antiferromagnetic order as potential origin.

MA 5.16 Tue 10:00 P

Topological-chiral magnetic interactions in ultrathin films at surfaces — •Soumyajyoti Haldar[1], Sebastian Meyer[2], André Kubetzka[3], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstr. 15, 24098 Kiel, Germany — [2]Nanomat/Q-mat/CESAM, Université de Liège, B-4000 Sart Tilman, Belgium — [3]Department of Physics, University of Hamburg, 20355 Hamburg, Germany

Non-collinear spin structures are of fundamental interest in magnetism since they allow to obtain insight into the underlying microscopic interactions and are promising for spintronic applications [1,2]. Here, we demonstrate that recently proposed topological-chiral magnetic interactions [3] can play a key role for magnetic ground states in ultrathin films at surfaces [4]. Based on density functional theory we show that significant chiral-chiral interactions occur in hexagonal Mn monolayers due to large topological orbital moments which interact with the emergent magnetic field. Due to the competition with higher-order exchange interactions superposition states of spin spirals such as the 2Q state or a distorted 3Q state can arise. Simulations of spin-polarized scanning tunneling microscopy images suggest that the distorted 3Q state could be the magnetic ground state of a Mn monolayer on Re(0001).

[1] A. Fert *et al.*, Nat. Rev. Mater. **2**, 17031 (2017).
[2] J. Grollier *et al.*, Nat. Electron. **3**, 360 (2020).
[3] S. Grytsiuk *et al.*, Nat. Commun. **11**, 511 (2020).
[4] S. Haldar *et al.*, arXiv:2106.08622 (2021).

MA 5.17 Tue 10:00 P

Creation of reconfigurable stray field landscapes in synthetic antiferromagnets via focused ion beam irradiation — •Fabian Samad[1,2], Gregor Hlawacek[1], Sri Sai Phani Kanth Arekapudi[2], Xiaomo Xu[1], Leopold Koch[2], Miriam Lenz[1], and Olav Hellwig[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany

Synthetic antiferromagnets (SAFs) with perpendicular magnetic anisotropy (PMA) can exhibit different magnetic phases depending on the magnetic history and energy balance [1]. By using focused He^+ ion beam (FIB) irradiation, the antiferromagnetic (AF) interlayer exchange coupling (IEC) and PMA can be reduced on a lateral (sub-)micron scale, such that different magnetic textures can be "written" with FIB [2,3]. Due to the depth-dependent ion damage, AF domains are stabilized at low fluences, typically around 10 ions/nm^2. When using a fluence gradient, the AF domains can be further manipulated in a directional fashion by applying external magnetic fields. Thus, a well-defined and reconfigurable stray field landscape is created, which can act on a suitable functional overlayer, such as a spin wave conducting or superconducting layer.

[1] Hellwig et al., J. Magn. Magn. Mater. 319, 13 (2007)
[2] Koch et al., Phys. Rev. Applied 13, 024029 (2020)
[3] Samad et al., Appl. Phys. Lett. 119 (2021)

MA 5.18 Tue 10:00 P

Ab initio exploration of hopfion hosting magnets — •Imara Lima Fernandes, Roman Kováčik, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Topological magnetic textures are currently of great interest in condensed matter physics due to their rich science and potential applications in information technology. In contrast to two-dimensional magnetic skyrmions, which are currently under intense scrutiny both theoretically and experimentally, their three-dimensional (3D) counterpart, known as Hopfions, were only recently observed experimentally [1]. Hopfions are stable solutions of the magnetization field with a knotted topological structure. In particular, their simplest spin texture can be described as a closed torus with a topologically nontrivial spin texture in the cross-section profile.

In the current work, using *ab initio* calculations, we explore suitable classes of materials to host magnetic hopfions based on analytical conditions of Heisenberg exchange parameters derived in Ref. [2]. We address systematically the case of chemical disorder and temperature in order to approach the optimal magnetic parameter field. The present study may give a guidance to identify suitable materials.

– Funding is provided by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant 856538 – 3D MAGiC).

[1] Kent, N. *et al*, Nat. Commun. **12**, 1562 (2021).
[2] Rybakov, F. N. *et al*, arXiv:1904.00250

MA 5.19 Tue 10:00 P

Combing the helical phase of chiral magnets with electric currents — •Jan Masell[1], Xiuzhen Yu[1], Naoya Kanazawa[2], Yoshinori Tokura[1,2], and Naoto Nagaosa[1,2] — [1]RIKEN CEMS, Wako, Japan — [2]University of Tokyo, Tokyo, Japan

In chiral magnets, the competition between the ferromagnetic exchange interaction and the small Dzyaloshinskii-Moriya interaction can form long-ranged helical modulations as the ground state. This helical phase has been extensively studied and chiral magnets gained extra attention when the skyrmion lattice was discovered in the chiral magnet MnSi a decade ago. However, in contrast to particle-like skyrmions, the helical phase seemed useless for spintronic applications as it is strongly pinned and hard to manipulate.

We have recently managed to unpin the helical phase in thin films of the chiral magnet FeGe by using electrical currents. Our theoretical analytical and numerical analysis predicts that the unpinned helical phase shows a variety of interesting dynamical phenomena, including distinct reorientation processes which can be driven by defects deep in the bulk or by the edge of the material, and predict numerous instabilities. Our results pave the way for "helitronics" and potential application in memory devices or unconventional computing.

[1] J. Masell, X.Z. Yu, N. Kanazawa, Y. Tokura & N. Nagaosa, Phys. Rev. B **102,** 180402(R) (2020)

MA 5.20 Tue 10:00 P

Magnetic ordering in $CePdAl_3$ and $CePtAl_3$ — •Michal Stekiel[1], Petr Cermak[4,5], Wolfgang Simeth[1,2], Martin Meven[4,3], Christian Franz[1,4], Stefan Weber[1], Rudolf Schönmann[1], Vivek Kumar[1], Kirill Nemkovskiy[4], Hao Deng[4,3], Andreas Bauer[1], Christian Pfleiderer[1], and Astrid Schneidewind[4] — [1]Technische Universität München, Garching, Germany — [2]Paul-Scherrer-Institut, Villigen, Switzerland — [3]RWTH Aachen at MLZ, Garching, Germany — [4]JCNS at MLZ, Garching, Germany — [5]Charles University, Praha, Czech Republic

In cerium-based intermetallic compounds the interplay of localized 4f electrons with itinerant d electrons may result in a wide range of magnetic and electronic ordering phenomena. Here, we report a comprehensive neutron diffraction study on single crystals of the non-centrosymmetric compounds $CePdAl_3$, crystallizing in the orthorhombic space group $Cmc2_1$, and $CePtAl_3$, crystallizing in the tetragonal space group $I4/mmm$. In $CePdAl_3$, a collinear antiferromagnetic structure is observed below $T_N = 5.3$ K with an ordered moment of 1.64 μ_B/Ce pointing along the a direction. In $CePtAl_3$, an amplitude-modulated cycloidal structure with an ordering vector ($\frac{2}{3}00$) emerges below $T_N = 3.2$ K. A symmetry analysis and its connection to the magnetic structures of measured compounds will be presented.

MA 5.21 Tue 10:00 P

Spin and orbital texture of the Weyl semimetal $MoTe_2$ studied by spin-resolved momentum microscopy — •Kenta Hagiwara[1], Xin Liang Tan[1], Philipp Rüssmann[1], Ying-Jiun Chen[1,2], Koji Fukushima[3], Keiji Ueno[3], Vitaliy Feyer[1], Shigemasa Suga[1,4], Stefan Blügel[1], Claus M. Schneider[1,2], and Christian Tusche[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg — [3]Saitama University, 338-8570, Saitama, Japan — [4]Osaka University, 567-0047, Osaka, Japan

Weyl semimetals host chiral fermions in solids as a pair of non-degenerate linear dispersions with band crossing points in their bulk electronic structure. These Weyl points are protected by topology, forming a Fermi arc, which is a connection between a pair of Weyl points with opposite chirality at the surface. Momentum microscopy provides two dimensional photoelectron maps of the in-plane crystal momentum over the whole Brillouin zone, simultaneously. Together with an imaging spin filter, we have revealed the spin-resolved electronic structure of the type-II Weyl semimetal $1T_d$ $MoTe_2$ in the full Brillouin zone. Supported by first-principles calculations, we clarified the spin texture and the orbital texture of the Weyl cones, which reflect the chirality of the Weyl points. We give evidence that a pair of Weyl cones exhibits a strong circular dichroism with reversed sign, indicating the different charge of the respective Weyl points in the Fermi surface.

MA 5.22 Tue 10:00 P

Giant anomalous Hall and Nernst eff ect in magnetic cubic Heusler compounds — •Jonathan Noky[1], Yang Zhang[2], Claudia Felser[1], and Yan Sun[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Massachusetts Institute of Technology, Cambridge, USA

There is an ongoing search for materials with large anomalous Hall and Nernst effects. These effects can be utilized in applications for data storage, thermoelectric power generation, and a high temperature quantum anomalous Hall effect, when preparing them as thin films. A promising class of materials for this purpose are the Heusler compounds because they can be grown in thin films and have a high Curie temperature. In these systems, the interplay between magnetism and topological band structures leads to a strongly enhanced Berry curvature. This can consequently create large anomalous Hall and Nernst effects.

In this work, we provide a comprehensive study of the intrinsic anomalous transport properties for magnetic cubic full Heusler compounds and we illustrate that several Heusler compounds outperform the best so far reported materials. Additionally, the results reveal the general importance of mirror planes in combination with magnetism for giant anomalous Hall and Nernst effects, which should be valid for all linear responses (spin Hall effect, spin orbital torque, etc.) dominated by intrinsic contributions.

MA 6: Focus Session: Spin-Charge Interconversion (joint session MA/HL)

While classical spintronics has traditionally relied on ferromagnetic metals as spin generators and spin detectors, a new approach called spin-orbitronics exploits the interplay between charge and spin currents enabled by the spin-orbit coupling (SOC) in non-magnetic systems. Efficient spin-charge interconversion can be realized through the direct and inverse Edelstein effects at interfaces where broken inversion symmetry induces a Rashba SOC. Although the simple Rashba picture of split parabolic bands is usually used to interpret such experiments, it fails to explain the largest conversion effects and their relation to the actual electronic structure.

Organizer: Ingrid Mertig (University Halle-Wittenberg)

Time: Tuesday 13:30–16:45 Location: H5

Invited Talk MA 6.1 Tue 13:30 H5

Spin-charge interconversion with oxide 2-dimensional electron gases — •Manuel Bibes — Unité Mixte de Physique CNRS/Thales

Oxide 2-dimensional electron gases (2DEGs) display a wide range of functionalities including Rashba spin-orbit coupling (SOC), which offers exciting opportunities for spintronics. In this talk, I will show that the 2DEG that forms at the interface of SrTiO3 (STO) with LaAlO3[1] or reactive metals such as Al[2,3] may be exploited to efficiently interconvert spin and charge currents. By applying a gate voltage, we tune the position of the Fermi level in the complex multi-orbital structure of STO, which results in a strong variation of the conversion amplitude[4]. This can be related to the band structure through ARPES experiment and tight-binding calculations. I will present results from both spin-charge conversion where spins are injected by spin pumping in a FMR cavity and detected as a transverse voltage[5], and from charge-spin conversion probed through the bilinear magnetoresistance (BMR). Using a semi-classical model, the analysis of the BMR amplitude yields a good estimate of the Rashba coefficient[6]. In a second part, I will present gate-controlled, all-electrical spin current generation and detection in planar nanodevices only based on a STO 2DEGs[7].

[1] Ohtomo et al, Nature 2004, 427, 423. [2] Rödel et al, Adv. Mater. 2016, 28, 1976. [3] Vicente-Arche et al, PR Mater. 2021, 5, 064005. [4] Lesne et al, Nat. Mater 2016, 15, 1261. [5] Vaz et al, Nat. Mater. 2019, 18, 1187. [6] Vaz et al, PR Mater. 2020, 4, 071001. [7] Trier et al, Nano Lett. 2020, 20, 395.

Invited Talk MA 6.2 Tue 14:00 H5

Spin-to-charge current conversion for logic devices — •Felix Casanova — CIC nanoGUNE, San Sebastian, Basque Country, Spain

The integration of logic and memory in spin-based devices, such as the recent MESO proposal by Intel [1], could represent a post-CMOS paradigm. A key player is the spin Hall effect (SHE), which allows to electrically create or detect pure spin currents without using ferromagnets (FM). Understanding the different mechanisms giving rise to SHE allows to optimize spin-to-charge conversion (SCC) in heavy metals. With this knowledge, we developed a novel and simple FM/Pt nanodevice to readout the in-plane magnetic state of the FM electrode using SHE [2]. The spin-orbit based detection allows us to independently enhance the output voltage (needed to read the in-plane magnetization) and the output current (needed for cascading circuit elements) with downscaling of different device dimensions, which are necessary conditions for implementing the MESO logic [1].

Finally, I will present a radically different approach to further enhance SCC. By engineering a van der Waals heterostructure which combines graphene with a transition metal dichalcogenide, we first demonstrated SHE in graphene due to spin-orbit proximity [3]. The combination of long-distance spin transport and SHE in the same material gives rise to an unprecedented SCC efficiency, making graphene-based systems excellent candidates for MESO logic [1,2].

[1] Manipatruni et al., Nature 565, 35 (2019); [2] Pham et al., Nature Electron. 3, 309 (2020); [3] Safeer et al., Nano Lett. 19, 1074 (2019); Herling et al., APL Mater. 8, 071103 (2020).

Invited Talk MA 6.3 Tue 14:30 H5

Electrical and thermal generation of spin currents by magnetic graphene — •B.J van Wees[1], T.S. Ghiasi[1], A.A. Kaverzin[1], D.K. de Wal[1], A.H. Dismukes[2], and Bart Wees[2] — [1]Zernike Institute for Advanced Materials, Groningen, The Netherlands — [2]Department of Chemistry, Colombia University, New York, NY, USA

I will introduce proximity effects in Van der Waals heterostructures of graphene and materials with strong spin orbit interaction or magnetic 2D materials. Then I will discuss recent experiments [1] where we demonstrate with (non)local spin transport experiments that the proximity of the antiferromagnet CrSBr introduces a strong spin dependent conductivity (with a polarization of about 24%) in (bilayer) graphene. The strength of the exchange field is estimated to be about 170T, implying that the graphene has become magnetic by proximity. This also resulted in the observation of a spin-dependent Seebeck effect. These results were recently confirmed using non-magnetic injector/detector electrodes [2] Fimally I will indicate some new (device) functionalities made possible by this strong proximity inducedspin-charge coupling in graphene [1] T.S. Ghiasi et al., Nature Nanotech. 16, 788, Vol 18, 2021 [2] A.A. kaverzin et al., in preparation

15 min. break.

Invited Talk MA 6.4 Tue 15:15 H5

Ferroelectric switching of spin-to-charge conversion in GeTe — •Christian Rinaldi — Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy

Scalable and energy efficient magneto-electric spin-orbit (MESO) logic has been recently proposed by Intel as technologically suitable computing alternative to CMOS devices, towards attojoule electronics [1]. The MESO device comprises a magnetoelectric unit to drive a magnetic memory, while the read-out is perfomed exploiting spin-to-charge conversion in materials with large spin-orbit coupling.

Here we show that the ferroelectric Rashba semiconductor germanium telluride offers memory as well as spin-orbit read-out in a single material compatible with silicon, thus offering the opportunity for a great simplification of the MESO structure. Here we first demonstrate the robust control of ferroelectricity through gating. Then, by spin pumping measurements in Fe/GeTe, we reveal the ferroelectric control of its sizeable spin-to-charge conversion. These results pave the way to low power spin-orbit logic devices beyond-CMOS. [1] S. Manipatruni, Nature 565, 35 (2019); [2] S. Varotto et al., arXiv preprint, arXiv:2103.07646 (2021).

Invited Talk MA 6.5 Tue 15:45 H5

Theory of spin and orbital Edelstein effects in a topological oxide two-dimensional electron gas — •Annika Johansson[1], Börge Göbel[1,2], Jürgen Henk[1], Manuel Bibes[3], and Ingrid Mertig[1] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]Unité Mixte de Physique CNRS/Thales, Université Paris-Sud, Université Paris-Saclay, Palaiseau, France

$SrTiO_3$ (STO)-based two-dimensional electron gases (2DEGs) provide a highly efficient spin-to-charge conversion [1], also known as inverse Edelstein effect [2,3]. Recently, an extremely large spin-to-charge conversion efficiency was demonstrated in the 2DEG at the interface between STO and Al [4]. The application of a gate voltage leads to a strong variation and even sign changes of the spin-to-charge conversion.

We explain this unconventional gate dependence of the (inverse) spin Edelstein effect from a theoretical perspective by Boltzmann transport calculations within a multiorbital tight-binding model. Further, we report on the electrically induced magnetization originating from the orbital moments, known as orbital Edelstein effect [5]. At STO interfaces the orbital Edelstein effect exceeds the spin Edelstein effect by more than one order of magnitude.

[1] E. Lesne *et al.*, Nat. Mater. **15**, 1261 (2016)
[2] V. M. Edelstein, Solid State Commun., **73**, 233 (1990)
[3] K. Shen *et al.*, Phys. Rev. Lett. **112**, 096601 (2014)
[4] D. Vaz *et al.*, Nature Materials **18**, 1187 (2019)
[5] A. Johansson *et al.*, Phys. Rev. Research **3**, 013275 (2021)

Invited Talk MA 6.6 Tue 16:15 H5

Nonlinear magnetoresistance and Hall effect from spin-momentum locking — •Giovanni Vignale — University of Missouri

Surface states of topological insulators exhibit the phenomenon of spin-momentum locking, whereby the orientation of an electron spin is determined by its momentum. Recently a link has been discovered between the spin texture of these states and a new type of nonlinear magnetoresistance, which depends on the relative orientation of the current with respect to the magnetic field as well as the crystallographic axes, and scales linearly with both the applied electric and magnetic fields. The nonlinear magnetoresistance originates from the conversion of a non-equilibrium spin current into a charge current under the application of an external magnetic field. Additionally, it has been found that the nonlinear planar Hall effect, manifested as a transverse component of the nonlinear current, exhibits a Pi/2 phase shift with respect to the nonlinear longitudinal current, in marked contrast to the usual Pi/4 phase difference that exists between the linear planar Hall current and the linear longitudinal current in typical topological insulators and transition metal ferromagnets. In this talk I review the development of the theory vis-a-vis experiments done on the surface of topological insulator Bi_2Se_3 films and other materials.

MA 7: Skyrmions I (joint session MA/KFM)

Time: Wednesday 10:00–13:15 Location: H5

Invited Talk MA 7.1 Wed 10:00 H5

Anatomy of skyrmion-defect interactions and their impact on detection protocols — •Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany

Magnetic skyrmions are topological swirling spin-textures with enormous potential for new technologies that store, transport and read information. However, imperfections intrinsic to any real device lead to pinning or repulsion of skyrmions, generate complexity in their motion and challenge their application as future bits of information. I will discuss our first-principles investigations of the electronic, magnetic and transport properties of single skyrmions interacting with 3d and 4d impurities embedded in PdFe/Ir(111). We found that the skyrmions energy landscapes have a universal shape as function of the defect's electron filling, enabling predictions of the repulsive or attractive nature of the impurity [1]. This finding can be used to design complex energy profiles with targeted properties via atom-by-atom manufacturing of multi-atomic defects [2,3]. Finally, I address how the latter affect the electronic structure and the chiral orbital magnetism, with consequences for the efficiency of skyrmion detection protocols [4], either all-electrical or optical.

– Work funded by Horizon 2020–ERC (CoG 681405–DYNASORE).

[1] Fernandes et al., Nat. Commun. 9, 4395 (2018); [2] Arjana et al. Sci. Rep. 10, 14655 (2020); [3] Fernandes et al., JPCM 32, 425802 (2020); [4] Fernandes et al., Nat. Commun. 11, 1602 (2020).

MA 7.2 Wed 10:30 H5

In the eye of the storm – A high resolution view at the details of the 3D magnetic texture of Skymions tubes — S. Schneider[1,2], D. Wolf[2], A. Lubk[2], U.K. Rössler[1], A. Kovács[3], M. Schmidt[4], R.E. Dunin-Borkowski[3], B. Büchner[2], and •B. Rellinghaus[1] — [1]Dresden Center for Nanoanalysis, TU Dresden, Dresden, Germany — [2]IFW Dresden, Dresden, Germany — [3]FZ Jülich, Jülich, Germany — [4]MPI CPfS, Dresden, Germany

Low temperature holographic vector field electron tomography in an external magnetic field was used to quantitatively reconstruct the 3D magnetic texture of skyrmion tubes (SkTs) in an FeGe needle [1]. The resulting high-resolution 3D magnetic images reveal various previously unseen details of the SkTs in FeGe. Our findings include the occurrence of local deviations from a homogeneous Bloch character within the tubes. They highlight the collapse of the skyrmion texture upon approaching the surfaces of the needle, provide evidence for the coexistence of longitudinal and transverse skyrmion textures, and reveal an axial modulation of the SkTs that is found to be strongly correlated among neighboring tubes in the needle. Based on the quantitative 3D magnetic induction data, we have calculated spatially resolved energy density maps across the SkTs that provide experimental evidence for the energetic stabilization of these magnetic solitons through an energy gain due to the Dzyaloshinskii-Moryia interaction, which overcompensates the exchange energy in the tube centers. Details of the novel experimental setup and limitations of the approach will be discussed.

[1] D. Wolf et al., arXiv:2101.12630 [cond-mat.mtrl-sci]

MA 7.3 Wed 10:45 H5

Real-space observation of skyrmion dynamics in an insulating magnet with a small heat gradient — Xiuzhen Yu[1], Fumitaka Kagawa[1,2], Shinichiro Seki[2], Masashi Kubota[1], •Jan Masell[1], Fehmi S. Yasin[1], Kiyomi Nakajima[1], Masao Nakamura[1], Masashi Kawasaki[1,2], Naoto Nagaosa[1,2], and Yoshinori Tokura[1,2] — [1]RIKEN CEMS, Wako, Japan — [2]University of Tokyo, Tokyo, Japan

Magnetic skyrmions are whirls in the magnetization with a non-trivial real-space topology. They are frequently discussed as potential building blocks for future information technology devices due to their topological protection and high mobility: Skyrmions can be moved by electrical currents and magnetic field gradients. It was also proposed to move skyrmions by magnons or thermal gradients [1].

We report the first observation of skyrmion dynamics in a linear thermal gradient. While nanometer-sized skyrmions remain pinned even with large thermal gradients [2], we observe a depinning threshold on the order of only 10 K/m in the insulating chiral magnet Cu_2OSeO_3 where skyrmions are 60nm large and the Gilbert damping is low. The observed velocity on the scale of 1μm/s agrees with our estimates for skyrmion motion due to a thermally activated magnon current.

[1] L. Kong & J. Zang, PRL **111,** 067203 (2013)
[2] M. Hirschberger, J. Masell, *et al.*, PRL **125,** 076602 (2020)
[3] X.Z. Yu, J. Masell, *et al.*, preprint:
https://doi.org/10.21203/rs.3.rs-156692/v1

MA 7.4 Wed 11:00 H5

Screw dislocations in chiral magnets — •Maria Azhar[1], Volodymyr Kravchuk[1,2], and Markus Garst[1] — [1]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Bogolyubov Institute for Theoretical Physics of National Academy of Sciences of Ukraine, 03680 Kyiv, Ukraine

The Dyzaloshinskii-Moriya interaction stabilizes helimagnetic order in cubic chiral magnets for a large range of temperatures and applied magnetic field. In this helimagnetic phase the magnetization varies only along the helix axis, that is aligned with the applied field, giving rise to a one-dimensional periodic magnetic texture. This texture shares many similarities with generic lamellar order like cholesteric liquid crystals, for example, it possesses disclination and dislocation defects [1]. Here, we investigate both analytically and numerically screw dislocations of helimagnetic order. Whereas the far-field of these defects is universal, we find that various core structures can be realized even for the same Burgers vector of the screw dislocation. In particular, we identify screw dislocations with smooth magnetic core structures, that close to the transition to the field-polarized phase continuously connect either to vortices of the XY-order parameter or to skyrmion strings. In addition, close to zero fields we find singular core structure comprising a chain of Bloch points with alternating topological charge. [1] P. Schoenherr et al. Nature Physics 14, 465 (2018).

MA 7.5 Wed 11:15 H5

Skyrmion Diffusion in Confined Geometries — •Jan Rothörl[1], Chengkun Song[2], Nico Kerber[1], Yuqing Ge[1], Klaus Raab[1], Boris Seng[3], Maarten Alexander Brems[1], Florian Dittrich[1], Robert Reeve[1], Jianbo Wang[2], Qingfang Liu[2], Peter Virnau[1], and Mathias Kläui[1] — [1]Institute of Physics Johannes Gutenberg-University Mainz — [2]Key Laboratory for Magnetism and Magnetic Materials of the Ministry of Education Lanzhou University China — [3]Institut Jean Lamour Université de Lorraine France

Magnetic skyrmions are topologically stabilized quasi-two-dimensional whirls of magnetization. Diffusion of skyrmions in continuous films [1] can be exploited for novel computing approaches, which often require understanding the behavior of skyrmions in confined geometries. We were studying this behavior in different confined geometries like circles, triangles and squares using experiments and coarse-grained computer simulations. Our results indicate that mobility is not only governed by skyrmion density but also by the interplay between skyrmion numbers and geometry. For triangular or square geometries, we found that this behavior is drastically dependent on the commensurability of the skyrmion number with the shape of the confinement [2].

[1] Zázvorka et al., Nat. Nanotechnol. 14, 658 (2019) [2] Song et al., Adv. Funct. Mater. 31, 2010793 (2021)

MA 7.6 Wed 11:30 H5

Effects of interlayer exchange on collapse mechanisms and stability of magnetic skyrmions — •Hendrik Schrautzer[1,2], Stephan von Malottki[1,2], Pavel F. Bessarab[2,3], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel,Germany — [2]University of Iceland, Reykjavik, Iceland — [3]ITMO University, St. Petersburg, Russia

Despite the great success of realizing magnetic skyrmions in multilayers, even at room temperature [1], very little is known about the thermal stability of skyrmions in these systems. In this study, we investigate by means of minimum energy path calculations and harmonic transition state theory the skyrmion decay mechanisms, corresponding energy barriers, and thermal collapse rates in systems incorporating several magnetic monolayers as a function of interlayer exchange coupling (IEC). The magnetic interactions within each layer are chosen so as to mimic the well-established Pd/Fe/Ir(111) system parametrized by first principles density functional theory calculations. We find that skyrmions in different monolayers collapse successively (simultaneously) for weak (strong) IEC. For intermediate IEC regime, we find a rich diversity of decay mechanisms, including the chimera collapse stabilized by IEC. Counter-intuitively, an optimal value of the IEC strength exists for a certain stacking of the magnetic layers. It corresponds to maximum skyrmion stability. We use the determined skyrmion collapse mechanisms to ultimately evaluate the skyrmion lifetime in magnetic multilayers.

[1] Moreau-Luchaire, *et al.*, Nat. Nanotechnol. 11, 444 (2016).

MA 7.7 Wed 11:45 H5

Exploring the phase diagram of thin film MnSi — •Grace Causer[1], Maria Azhar[2], Alfonso Chacon[1], Andreas Bauer[1], Thorsten Hesjedal[3], Markus Garst[2], and Christian Pfleiderer[1] — [1]Physics Department, Technical University of Munich, Garching, Germany — [2]Institute for Theoretical Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Clarendon Laboratory, University of Oxford, Oxford, United Kingdom

We have charted the magnetic phase diagram of thin film MnSi grown on a Si substrate via the magnetisation, magnetic susceptibility, planar Hall, and small-angle neutron scattering data, tracking carefully the field and temperature history. Our experimental results are supported by micromagnetic simulations, which jointly reveal a magnetic phase diagram dominated by a field-induced unwinding of an out-of-plane propagating helical wavevector. Below 2 K a discrete phase regime can be discerned unambiguously. These observations provide insights into the integral role of magnetic anisotropy and dimensionality on the low-temperature phase diagram of thin film MnSi.

MA 7.8 Wed 12:00 H5

Optimizing the skyrmion profile for technological applications — •Markus Hoffmann, Sarina Lebs, Moritz Sallermann, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Chiral magnetic skyrmions are of great scientific interest and of potential relevance in information technology. Important properties – such as their lifetime, mobility, and robustness with respect to external influences – depend hereby on the specific application. Thus, skyrmion properties must be tuned to outperform existing technologies.

Based on a combination of micromagnetic arguments and atomistic spin-dynamics simulations carried out with `Spirit` (https://spirit-code.github.io), we investigate the dependence of aforementioned properties on the skyrmion profile, *i.e.*, on the spatial dependence of the magnetization field, and analyze how the skyrmion profile can be tuned to optimize the skyrmion's properties. To obtain static properties, we perform LLG and GNEB simulations, which provide us the energy barrier and the corresponding saddle point structure, and combine those with HTST calculations to determine the lifetime prefactor [1]. Additionally, we perform LLG simulations to investigate the dynamics of skyrmions, including their velocity as well as the skyrmion Hall angle.

We acknowledge funding from the DARPA TEE program through grant MIPR (#HR0011831554) from DOI, and DFG through SPP-2137 and SFB-1238 (project C1).

[1] M. Hoffmann *et al.*, Phys. Rev. Lett. **124**, 247201 (2020).

MA 7.9 Wed 12:15 H5

Emergence of Magnetic Skyrmions in Ultrathin Films of Manganese on W(001) at High Magnetic Fields — •Reiner Brüning, Kirsten von Bergmann, André Kubetzka, and Roland Wiesendanger — Festkörper- und Nanostrukturphysik, Hamburg, Deutschland

Topological spin textures like skyrmions with diameters on the order of a few nanometers are promising objects for the application in the field of spintronics. Whereas typical skyrmion systems like Pd/Fe bilayers on Ir(111) [1] have a hexagonal crystal symmetry, here, we investigate a monolayer of Mn on the square lattice of W(001) using spin-polarized scanning tunneling microscopy at 4.2 K. In absence of an external magnetic field, the known magnetic ground state of a 2.2 nm spin spiral is observed [2]. Between 90° rotational domains two types of magnetic domain walls can be identified.

The measurements at 9 T show that the external magnetic field leads to a decrease in the size of the domains and initializes the transition from the spin spiral to small skyrmion areas which results in a coexistence state of the spin spiral and skyrmion phase. Inside the small skyrmionic areas, the skyrmions arrange in a hexagonal-like order, in agreement with recent simulations [3]. By high voltage pulses of 1-2 V, we can locally induce transitions between spiral phase and skyrmion phase.

[1] N. Romming *et al*., Science, **341**, (2013)
[2] P. Ferriani *et al*., Phys. Rev. Lett. **101**, 027201 (2008)
[3] A. K. Nandy *et al*., Phys. Rev. Lett. **116**, 177202 (2016)

MA 7.10 Wed 12:30 H5

Application of Thermal and Induced Skyrmion Diffusion in Non-Conventional Computing — •Maarten A. Brems, Mathias Kläui, and Peter Virnau — Institute of Physics, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany

Magnetic skyrmions are two-dimensional magnetic quasi-particles with interesting properties for possible future applications in memory storage devices and non-conventional computing. We have shown that skyrmions in thin film magnetic multilayers exhibit thermal diffusion [1]. These properties make skyrmions promising candidates for signal carriers (tokens) in Brownian computing, which exploits thermal fluctuation for computations. We design a crossing-free layout for a composite half-adder module to overcome the problem that crossings generate for the fabrication of circuits [2]. To address the key issue of slow computation based on thermal excitations, we propose to combine artificial diffusion induced by an external excitation mechanism [2,3]. For magnetic skyrmions, induced diffusion by spin-orbit torques or other mechanisms can increase the computation speed by several orders of magnitude. This method can be employed to accelerate conventional Brownian computing as necessary and thereby greatly enhance the application scenarios of token-based computing for instance for low power devices such as autonomous sensors.

[1] J. Zázvorka et al., Nat. Nanotechnol. 14, 658 (2019). [2] M. A. Brems, P. Virnau and M. Kläui, ArXiv: 2107.02097 [Cond-Mat] (2021). [3] M. A. Brems, P. Virnau and M. Kläui, European patent disclosure, EP21164676.5 (2021).

MA 7.11 Wed 12:45 H5

Solitary-waves excitations and current-induced instabilities of skyrmion strings — •Volodymyr Kravchuk[1,3], Shun Okumura[2], and Markus Garst[1] — [1]Karlsruhe Institute of Technology, Germany. — [2]The University of Tokyo, Japan. — [3]Bogolyubov Institute for Theoretical Physics, Kyiv, Ukraine

Field-polarized chiral magnets possess topological line excitations where the magnetization within each cross-section perpendicular to the applied field forms a skyrmion texture. We introduce and discuss an effective field-theoretical description for the low-energy dynamics of such a skyrmion string. It predicts, in particular, that skyrmion strings support solitary waves that propagate along the string while maintaining their shape. Using integrals of motion, we derive the profile of these waves analytically, and we find quantitative agreement with numerical micromagnetic simulations [1]. In addition, we discuss the influence of a spin-polarized current on the string. Whereas it is well-known that a current flowing perpendicular to the string results in a skyrmion string motion, we demonstrate that a longitudinal current destabilizes the string. This destabilization occurs via the pumping of the Goldstone mode of the string that results in a helical-shaped string deformation that increases with time. Whereas in a clean system an infinitesimal current suffices, a finite threshold current is required to destabilize the string in the presence of disorder. Moreover, we show that this current-induced instability also holds for skyrmion lattices.

[1] V. Kravchuk, U. Rößler, J. van den Brink, M. Garst, PRB, 102, 220408(R) (2020).

MA 7.12 Wed 13:00 H5

Magnetoelastic coupling and phases in the skyrmion lattice magnet Gd_2PdSi_3 discovered by high-resolution dilatometry — •Sven Spachmann[1], Rüdiger Klingeler[1], Ahmed Elghandour[1], Matthias Frontzek[2], and Wolfgang Löser[3] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Oak Ridge National Laboratory, Oak Ridge, USA — [3]Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany

We report high-resolution capacitance dilatometry measurements on single crystals of the centrosymmetric skyrmion-hosting intermetallic Gd_2PdSi_3 in magnetic fields up to 15 T which are complemented by specific heat and magnetization studies. Our data enable us to complete the magnetic phase diagram and to establish yet unreported phase boundaries. We find strong magnetoelastic effects associated with antiferromagnetic order at T_{N1}= 22.3 K and T_{N2} = 19.7 K as well as an additional feature at $T^* \approx 13$ K. Grüneisen analysis shows the onset of magnetic contributions around 60 K, i.e., well above T_{N1}, and strong field effects in an applied magnetic field of 15 T are found up to 200 K (150 K) for B ∥ c (B ∥ a^*, i.e., B ⊥ c). Our data allow us to extract the uniaxial pressure dependence of the different phase boundaries. We elucidate thermodynamic properties of the recently discovered skyrmion lattice phase and show that it is strongly enhanced by uniaxial pressure.

MA 8: INNOMAG e.V. Dissertationspreis / Ph.D. Thesis Prize (2020)

The Working Group Magnetism (Arbeitsgemeinschaft Magnetismus der DPG) awards a dissertation prize whose aim is to recognise outstanding research done within the framework of a doctorate and communication of this research in an excellent way, both verbally and in writing. The prize is kindly supported by INNOMAG e.V. In this finalists session, pre-selected nominees will present and defend their dissertation. Afterwards, the prize committee decides on the winner of the INNOMAG e.V. Dissertation Prize 2020 and the award of 1000 EURO.

Time: Wednesday 10:00–12:10 Location: H2

MA 8.1 Wed 10:00 H2

Spin-orbit driven transport: Edelstein effect in Rashba systems and topological materials — •Annika Johansson — Martin Luther University Halle-Wittenberg, Halle, Germany

A charge current driven through a system with broken inversion symmetry can generate a spatially homogeneous spin polarization. This phenomenon is known as Edelstein effect [1,2]. Using semiclassical Boltzmann transport theory, I investigate the Edelstein effect in two- and three-dimensional Rashba systems and topological materials. Whereas the current-induced spin density in conventional isotropic Rashba systems is in-plane and perpendicular to the charge current, I show that the direction as well as the magnitude of the induced spin density can be strongly modified in systems with reduced symmetry, which provides new opportunities to control and manipulate the electrically induced magnetization [3].

Further, I predict a highly efficient Edelstein effect in three-dimensional Weyl semimetals, mainly originating from their topological surface states due to their favorable Fermi surface geometry, their strong spin polarization and the enhanced momentum relaxation time [4]. In comparison to Rashba systems, the Edelstein effect in Weyl semimetals is enhanced by at least one order of magnitude.

[1] A. Aronov and Y. Lyanda-Geller, JETP Lett. **50**, 431 (1989).
[2] V. Edelstein, Solid State Commun. **73**, 233 (1990).
[3] A. Johansson et al., Phys. Rev. B **93**, 195440 (2016).
[4] A. Johansson et al., Phys. Rev. B **97**, 085417 (2018).

MA 8.2 Wed 10:25 H2

Highly Efficient Domain Wall Motion in Ferrimagnetic Bi-layer Systems at the Angular Momentum Compensation Temperature — •Robin Bläsing — RWTH Aachen University, Aachen, Germany

Within the last decade, the efficiency of current-induced motion of magnetic domain walls (DWs) has been enhanced tremendously by utilizing the exchange coupling torque (ECT) in synthetic antiferromagnetic structures. The focus of the present study is on exploring this mechanism in ferrimagnetic layers consisting of a transition metal layer and a rare earth metal layer which couple antiferromagnetically. The DWs are moved by nanosecond-long current pulses and their velocity is determined by using Kerr microscopy at various temperatures. It is shown here that the motion is most efficient at a certain temperature T_A at which the angular momenta of both layers compensate each other and the ECT is maximized. Since the device temperature is significantly increased by the current pulses, taking into account Joule heating is of major importance when determining T_A. The results of current-induced domain wall motion in the present thesis can be used for the development of novel storage devices and improving their efficiency.

MA 8.3 Wed 10:50 H2

Spintronics with Terahertz Radiation: Probing and driving spins at highest frequencies — •Tom Sebastian Seifert — Freie Universität Berlin, Berlin, Germany

Spin-orbit interaction (SOI) will be of central importance for future spin-based electronics (spintronics) as it permits, for example, the conversion of charge into spin currents and vice versa via the spin Hall effect. It is highly interesting to study spin dynamics at terahertz (THz) frequencies because spintronic devices should eventually operate at THz rates. In our experiments, we employ femtosecond optical and THz pulses to trigger ultrafast spin and charge dynamics in magnetic thin-film stacks featuring a strong SOI. In particular, we study THz emission from multilayers consisting of magnetic and a nonmagnetic materials [1,2,3]. By varying the magnetic layer material, we aim at identifying the different mechanisms that can lead to the ultrafast generation of spin currents. Such mechanisms include spin-voltage-driven transport [4] by conduction-band electrons in metal-metal stacks and magnon-mediated transfer of spin angular momentum in insulator-metal stacks [5]. Finally, we turn from probing to driving spins at highest speeds by demonstrating the picosecond writing speed of an antiferromagnetic memory element based on CuMnAs employing strong THz pulses[6]. References: [1] T. Seifert et al., Nat. Phot. 10 (2016). [2] T. Kampfrath et al., Nat. Nanotech. 8 (2013). [3] T. Seifert et al., APL, 110, 252402 (2017). [4] R. Rouzegar et al., ArXiv 2103.11710 (2021) [5] T. Seifert et al., Nat. Commun. 9 (2018). [6] K. Olejnik et al., Science Adv. 4 (2018).

MA 8.4 Wed 11:15 H2

Linear and nonlinear spin waves in nanoscale magnonic structures for data processing — •Qi Wang — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, D-67663 Kaiserslautern, Germany

Spin waves, and their quanta magnons, attract attention as novel data carriers instead of electrons in future low-energy data processing units due to their short wavelength, low losses, and abundant nonlinear phenomena. Although separated spin-wave logic gates have already been demonstrated, the smallest sizes of these elements are in the ranges of a few micrometers and are not competitive with the current state-of-the-art CMOS technology. Moreover, the realization of an integrated magnonic circuit is still an unresolved challenge.

The objective of this talk is to present a nanoscale magnon directional coupler as a universal data processing unit for performing different logic operations and suitable for the integration into a magnonic circuit. First, the spin-wave characteristics in the nanoscale waveguides were studied theoretically and experimentally. Based on this knowledge, a nanoscale directional coupler was designed and its linear and nonlinear functionalities were studied using Brillouin Light Scattering spectroscopy. Following, the first integrated magnonic circuit consisting of two couplers and performing half-adder functionality was studied numerically. Finally, we introduced the inverse-design method into the field of magnonics and demonstrated its high performance, flexibility, and potential. These studies were supported by ERC StG MagnonCircuits.

Short break followed by bestowal of INNOMAG e.V. Dissertationspreis / Ph.D. Thesis Prize (2020)

MA 9: INNOMAG e.V. Diploma/Master Prize (2021)

Die Arbeitsgemeinschaft Magnetismus der DPG hat einen Diplom-/Masterpreis ausgeschrieben, welcher auf der Online-Tagung der DPG 2021 vergeben wird. Ziel des Preises ist die Anerkennung herausragender Forschung im Rahmen einer Diplom-/Masterarbeit und deren exzellente Vermittlung in Wort und Schrift. Im Rahmen dieser Sitzung tragen die besten der für ihre an einer deutschen Hochschule durchgeführten Masterarbeit Nominierten vor. Im direkten Anschluss entscheidet das Preiskommittee über den Gewinner bzw. die Gewinnerin des INNOMAG e.V. Diplom/Master-Preises 2021 in Höhe von 500 EURO. Talks will be given in English!

Time: Wednesday 12:30–14:20 Location: H2

MA 9.1 Wed 12:30 H2

Orbital Magnetic Moment of Magnons — •Robin R. Neumann[1], Alexander Mook[1,2], Jürgen Henk[1], and Ingrid Mertig[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Department of Physics, University of Basel, Basel, Switzerland

It is commonly accepted that magnons—collective excitations in a magnetically ordered system—carry a spin of $1\hbar$ or, phrased differently, a magnetic moment of $g\mu_B$. In this talk, I demonstrate that magnons carry magnetic moment beyond their spin magnetic moment. Our rigorous quantum theory uncovers a magnonic orbital magnetic moment brought about by spin-orbit coupling. We apply our theory to two paradigmatic systems where the notion of orbital moments manifests itself in novel fundamental physics rather than just quantitative differences. In a coplanar antiferromagnet on the two-dimensional kagome lattice the orbital magnetic moment gives rise to an orbital magnetization. While the spin magnetization is oriented in the kagome plane, the orbital magnetization also has a finite out-of-plane component leading to 'orbital weak ferromagnetism.' The insulating collinear pyrochlore ferromagnet $Lu_2V_2O_7$ exhibits a 'magnonic orbital Nernst effects,' i. e. transversal currents of orbital magnetic moment induced by a temperature gradient. The orbital magnetization and the orbital Nernst effect in magnetic insulators are two signatures of the orbital magnetic moment of magnons.

MA 9.2 Wed 12:50 H2

Angle-Dependent Magnetotransport in Semimetals — •Felix Spathelf[1,2,3], Benoît Fauqué[2], and Kamran Behnia[1] — [1]LPEM (CNRS), ESPCI Paris, Université PSL, Paris, France — [2]JEIP, USR 3573 CNRS, Collège de France, Université PSL, Paris, France — [3]Universität Heidelberg

We report on studies of the electrical and thermoelectric transport properties of semimetals with high mobilities at temperatures down to 2 K and in magnetic fields up to 13.8 T to understand their remarkable amplitude. The Seebeck effect, magnetoresistance and the Hall effect of bismuth were measured and compared to the results of a theoretical model, which was developed on the basis of semiclassical theory. The model perfectly describes the zero field Seebeck coefficient from 10 K to 300 K and agrees well with experimental data in a large part of the (T, B, Θ)-space. It is shown that the contribution of the Nernst coefficient to the Seebeck effect has to be taken into account when explaining the latter. In addition, the Seebeck effect of bismuth is at least up to a temperature of 120 K significantly affected by Landau quantisation. Furthermore, the influence of the sample shape on the angle-dependent magnetoresistance is studied in bismuth and antimony. At 40 K, magnetoresistance shows the symmetry inherited from the Fermi surface topology. Upon cooling below 20 K, this symmetry is lost in bismuth, but not in antimony. The loss of symmetry is sample-dependent and can be traced back to a robust surface contribution to conductivity. Besides, the highest magnetoresistance ever observed was measured in bismuth, amounting to $1.56 \cdot 10^8$ under a magnetic field of 12.8 T.

MA 9.3 Wed 13:10 H2

Optimizing the magnetocaloric effect in all-d-metal Ni-Co-Mn-Ti Heusler alloys — •Benedikt Beckmann and Oliver Gutfleisch — TU Darmstadt, 64287 Darmstadt, Germany

Magnetocaloric refrigeration is a promising cooling technology which could be an environmentally friendly and more energy efficient alternative to conventional vapor compression refrigeration. Among magnetocaloric materials, Ni-Mn based Heusler alloys, showing a first-order magnetostructural phase transition, are promising candidates. In this study, a systematic analysis of all-d-metal $Ni_{50-x}Co_xMn_{50-y}Ti_y$ Heusler alloys is carried out [1]. Due to their enhanced mechanical stability, these alloys can also be utilized in cooling cycles that apply magnetic field and pressure as external stimuli to induce the phase transition. A systematic heat treatment optimization is carried out, resulting in a substantial decrease of the transition width down to only 4 K. The microstructural differences between as-cast and differently annealed alloys are analyzed in detail by *in-situ* polarized light microscopy. As a result, large isothermal entropy changes up to 38 $Jkg^{-1}K^{-1}$ are achieved in 2 T. The adiabatic temperature change is measured directly for this material system and values up to -3.8 K for the first field application and -0.8 K under cyclic conditions are obtained in moderate magnetic field changes of 1.93 T.

We acknowledge financial support from DFG (CRC/TRR 270) and ERC (Adv. Grant No. 743116).

[1] A. Taubel & B. Beckmann et al., Acta Materialia 201, 425-434 (2021)

MA 9.4 Wed 13:30 H2

High-Resolution Dilatometry Studies on Transition Metal Oxides — •Marco Hoffmann, Kaustav Dey, Sven Spachmann, and Rüdiger Klingeler — Kirchhoff Institute for Physics, Heidelberg University, INF 227, D-69120 Heidelberg, Germany

The thermodynamic properties of the transition metal oxides $CoTiO_3$ and $R_4Ni_3O_{10}$ (R = La, Pr, Nd) were studied by means of high-resolution capacitance dilatometry. Thermal expansion and magnetostriction measurements were performed in temperatures down to 2 K and fields up to 15 T. For $CoTiO_3$ a strong magnetoelastic coupling is found and its phase diagram is constructed [1]. A phenomenological domain model is applied to explain its magnetostriction and magnetization data. Furthermore, a hydrostatic pressure dependence of the Néel temperature (T_N = 37 K) of dT_N/dp = 0.8 K/GPa is derived by a Grüneisen analysis. This analysis also shows a single dominant energy scale in $CoTiO_3$ below 50 K. For the $R_4Ni_3O_{10}$ compounds, on the other hand, Grüneisen analyses indicate competing interactions just below the metal-to-metal transition temperatures T_M and pressure dependencies of dT_M/dp = −8 K/GPa, −4 K/GPa and −3 K/GPa for R = La, Pr, Nd, respectively [2]. Clear anomalies in the thermal expansion at T_M for all three compounds show strong coupling between the electronic and lattice degrees of freedom. [1] M. Hoffmann, K. Dey, J. Werner, R. Bag, J. Kaiser, H. Wadepohl, Y. Skourski, M. Abdel-Hafiez, S. Singh, and R. Klingeler, Phys. Rev. B (accepted 2021) [2] D. Rout, S. R. Mudi, M. Hoffmann, S. Spachmann, R. Klingeler, and S. Singh, Phys. Rev. B **102**, 195144 (2020).

Short break followed by bestowal of INNOMAG e.V. Diploma/Master Prize (2021)

MA 10: Focus Session: Higher-Order Magnetic Interactions - Implications in 2D and 3D Magnetism I

Materials in which the magnetic moments order or cooperate in unusual ways underpin a plethora of physical phenomena, from strong magnetoelectric effects to topological quasiparticles, thus holding great promise for future spintronic and quantum computing applications. Magnetic interactions are the fundamental quantities that explain the complex magnetic phase diagrams and exotic excitation spectra of these intriguing materials. Recent theoretical and experimental developments have led to a realization of a pivotal role played by higher-order magnetic interactions in stabilizing intricate magnetic structures. The 4-spin 3-site interaction stabilizes an up-up-down-down state, which can become chiral. Theoretically, novel 4-spin chiral interactions and even 6-spin (chiral-chiral) couplings might explain the emergence of complex short-period 3D magnetic structures, and could open a path to the discovery of materials hosting 3D topological magnetization textures, such as magnetic hopfions. Experimentally, 4-spin interactions are conjectured to play a central role in skyrmions lattice formation in frustrated centrosymmetric materials. This area of research will make a strong impact in the field of magnetism in the upcoming years.

Organizers: Samir Lounis (University of Duisburg-Essen and Forschungszentrum Jülich), Manuel dos Santos Dias and Stefan Blügel (Forschungszentrum Jülich), Jonathan White (Paul Scherrer Institut)

Time: Wednesday 13:30–16:30 Location: H5

Invited Talk MA 10.1 Wed 13:30 H5

Topological spin crystals stabilized by itinerant frustration — •Yukitoshi Motome — The University of Tokyo, Tokyo, Japan

Topological spin crystals, which are periodic arrays of topological spin textures such as vortices, skyrmions, and hedgehogs, have attracted numerous attention for the potential use of their magnetic, transport, and optical properties for future spintronics and quantum computing. For materializing such unconventional magnetism, it is crucially important to understand the relevant magnetic interactions. Widely known is the Dzyaloshinskii-Moriya interaction, which stabilizes swirling spin textures in competition with ferromagnetic exchange interactions. Here, we theoretically study a different mechanism driven by effective magnetic interactions arising from itinerant nature of electrons. We show that, in addition to the well-known Ruderman-Kittel-Kasuya-Yosida interaction, multiple-spin interactions naturally arise as higher-order contributions from the spin-charge coupling in itinerant magnets. They are intrinsically long-ranged and have characteristic wave numbers specified by the Fermi surfaces, like the Ruderman-Kittel-Kasuya-Yosida interaction. We find that frustration among such long-range multiple-spin interactions, which we call itinerant frustration, can stabilize a variety of topological spin crystals with unique features, even in centrosymmetric systems where the Dzyaloshinskii-Moriya interaction is absent. We discuss our results with recent advances in experiments.

Invited Talk MA 10.2 Wed 14:00 H5

Formation of spin-hedgehog lattices and giant topological transport properties in chiral magnets — •Naoya Kanazawa — University of Tokyo, Tokyo, Japan

The last few years have seen remarkable progress in the discovery of versatile topological spin crystals with different topology, dimensionality and density. In parallel, the crucial role of higher-order magnetic interactions among multiple spins has been gradually recognized. In this talk, we report the formation of three-dimensional topological spin texture, i.e., the lattices of spin hedgehogs in a chiral magnet MnGe and its relatives. Their nature of twisting spins in short periods imply the relevance of such higher-order interactions. We also introduce various giant transport properties, such as topological Hall and thermoelectric effects, which may originate from the effective monopole field and dynamical fluctuations of spin hedgehogs.

This work is done in collaboration with K. Akiba, T. Arima, R. Arita, S. Awaji, C. D. Dewhurst, Y. Fujishiro, M. Ichikawa, K. Ishizaka, H. Ishizuka, F. Kagawa, K. Kakurai, Y. Kawamura, M. Kawasaki, A. Kikkawa, S. Kimura, K. Kindo, T. Koretsune, A. Kitaori, Y. Kozuka, R. Kurihara, A. Matsuo, H. Mitamura, A. Miyake, D. Morikawa, T. Nakajima, A. Nakamura, N. Nagaosa, K. Ohishi, H. M. Rønnow, K. Shibata, T. Shimojima, J. Shiogai, Y. Taguchi, M. Tokunaga, Y. Tokura, A. Tsukazaki, V. Ukleev, J. S. White, X. Z. Yu.

Invited Talk MA 10.3 Wed 14:30 H5

Topological-chiral magnetic interactions driven by emergent orbital magnetism — •Sergii Grytsiuk[1], Jan-Philipp Hanke[1], Markus Hoffmann[1], Juba Bouaziz[1], Olena Gomonay[2], Gustav Bihlmayer[1], Samir Lounis[1], Yuriy Mokrousov[1,2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

Based on microscopic arguments and a systematic total energy expansion, further validated by electronic structure calculations, we discover a new class of magnetic interactions of chiral nature originating from the so-called topological orbital moment (TOM) of electrons in non-coplanar magnets [1]. The

TOMs, $\mathbf{L}^{TO}$, emerge from the scalar spin chirality of three magnetic moments, $\mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$. As a result of a six-spin– or a four-spin interaction, they can interact with each other and interact with the spins of the underlying lattice. In the context of B20-type chiral magnet MnGe, these novel interactions can dominate over the Dzyaloshinskii-Moriya interaction in selecting the chiral ground state, providing possibly a key for solving the open question of the recently observed complex 3D magnetic structures. By providing a mechanism for the physical realization of the Faddeev model with hopfion solutions, topological-chiral interactions might play a key role in triggering the formation of 3D magnetic solitons without the assistance of an external magnetic field.

[1] S. Grytsiuk *et al.*, Nature Commun **11**, 511 (2020).

15 min. break.

Invited Talk MA 10.4 Wed 15:15 H5

Complex spin structures in thin transition metals films and their oxides — •Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Germany

The term “magnetism” subsumes a plethora of interactions originating from various physical mechanisms. Their competition often results in highly complex spin structures, such that the specific origin is masked and can only be unraveled by combining experiment and theory. For example, for an Fe monolayer on Rh(111) an up-up-down-down (↑↑↓↓) spin structure was predicted by DFT [1] which was only later understood to originate from the previously unconsidered four-spin–three-site beyond-Heisenberg interaction [2]. We could indeed confirm this ↑↑↓↓ spin structure experimentally by spin-polarized STM. Three orientational domains were observed, the field-dependent behavior of which is surprisingly complex, potentially due to uncompensated spins at domain boundaries. Furthermore, in a recent survey of submonolayer transition metal oxides on Ir and Pt(001) we observed highly complex spin structures which appears to be driven by a Dzyaloshinskii-Moriya-enhanced Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [3]. However, the orientation of the Dzyaloshinskii-Moriya vector and the observation of a long-wavelength spin rotation have not yet been adequately explained [4].

[1] A. Al-Zubi *et al.*, Phys. Status Solidi B **248**, 2242 (2011)
[2] A. Krönlein *et al.*, Phys. Rev. Lett. **120**, 207202 (2018)
[3] M. Schmitt *et al.*, Nature Comm. **10**, 2610 (2019)
[4] M. Schmitt *et al.*, Phys. Rev. B **100**, 054431 (2019)

MA 10.5 Wed 15:45 H5

Two-dimensional atomic-scale spin textures in Fe monolayers — André Kubetzka, Roland Wiesendanger, and •Kirsten von Bergmann — Department of Physics, University of Hamburg, Germany

Higher-order interactions can induce two-dimensionally modulated magnetic ground states at zero magnetic field, and spin-polarized scanning tunneling microscopy (SP-STM) is a powerful tool to characterize such spin structures down to the atomic scale [1-3].

Using SP-STM we have recently observed several different square or hexagonal magnetic ground states in Fe monolayers in contact with Rh and Ir layers. The details of the resulting states with magnetic periods on the order of one nanometer depend critically on the stacking of the Fe layer and the number of adjacent Rh or Ir layers [1,4-7].

[1] S. Heinze *et al.*, Nature Phys. **7**, 713 (2011).
[2] Y. Yoshida *et al.*, Phys. Rev. Lett. **108**, 087205 (2012).
[3] J. Spethmann *et al.*, Phys. Rev. Lett. **124**, 227203 (2020).
[4] K. von Bergmann *et al.*, Nano Lett. **15**, 3280 (2015).
[5] N. Romming *et al.*, Phys. Rev. Lett. **120**, 207201 (2018).
[6] A. Kubetzka *et al.*, Phys. Rev. Materials **4**, 081401(R) (2020).
[7] M. Gutzeit *et al.*, (in preparation).

MA 10.6 Wed 16:00 H5

Three- and four-spin interactions from first-principles: calculations and properties — •Sergiy Mankovsky, Svitlana Polesya, and Hubert Ebert — Dept. Chemistry, LMU Munich, Butenandtstrasse 11, D-81377 Munich, Germany

We discuss an extension of the Heisenberg Hamiltonian by accounting for the contributions of higher order interactions calculated on a first-principles level, that can play a crucial role for the stabilization of various types of non-collinear magnetic structure, as for example skyrmions. All calculations are performed by making use of the fully relativistic Korringa-Kohn-Rostoker (KKR) Green function method. We focus on the three-spin and four-spin interaction parameters concerning their calculation and properties. In particular, we discuss their controversial interpretation and the origin of the three-spin chiral interaction (TCI) represented by an expression worked out recently (Phys. Rev. B, **101**, 174401 (2020)). An interpretation of the TCI is suggested, showing explicitly its dependence on the relativistic spin-orbit coupling and on the topological orbital susceptibility (TOS). This is based on an expression for the TOS that is worked out on the same footing as the expression for the TCI. Using first-principles calculations we demonstrate in addition numerically the common topological properties of the TCI and TOS.

MA 10.7 Wed 16:15 H5

Role of higher-order exchange interactions for skyrmion stability — •Souvik Paul[1,2], Soumyajyoti Haldar[2], Stephan von Malottki[2], and Stefan Heinze[2] — [1]Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich, Germany — [2]Institute of Theoretical Physics and Astrophysics, Christian-Albrechts-Universität zu Kiel, Germany

Magnetic skyrmions have recently become a research focus as they show promise for future magnetic memory and logic devices. One key obstacle for applications is the stability of skyrmionic bits against thermal fluctuations. The importance of Heisenberg exchange interaction, Dzyaloshinskii-Moriya interaction, magnetocrystalline anisotropy and dipole-dipole interactions in skyrmion stability has been reported. However, due to their origin from a fourth-order perturbation theory, non-Heisenberg higher-order exchange interactions (HOI) – the biquadratic, the three-site-four-spin and the four-site-four-spin interaction – have so far been neglected. Using *ab-initio* parametrized atomistic spin dynamics simulations in ultrathin films, we demonstrate that the HOI play an important role for skyrmion stability. We find that the effect of the first two HOI, to a large extent, can be included in the effective Heisenberg exchange constants. However, the four-site four spin interaction behaves qualitatively in a different way and has a large contribution on the energy barrier stabilizing skyrmions and antiskyrmions against annihilation. Our study opens up a new avenue for increasing the stability of topological spin structures.

MA 11: Posters Magnetism III

Topics: Magnonics (11.1-11.16), Terahertz Spintronics (11.17-11.23), Spintronics (other effects) (11.24-11.26), Spin Transport and Orbitronics, Spin-Hall Effects (11.27-11.32), Cooperative Phenomena: Spin Structures and Magnetic Phase Transitions (11.33-11.34)

Time: Wednesday 13:30–16:30 Location: P

MA 11.1 Wed 13:30 P

Formation of magnon polarons in ferromagnetic nanogratings — •Felix Godejohann[1], Alexey Scherbakov[1,2], Serhii Kukhtaruk[1,3], Alexander Poddubny[2], Dmytro Yaremkevych[1], Mu Wang[5], Achim Nadzeyka[4], Dmitri Yakovlev[1,2], Andrew Rushforth[5], Andrey Akimov[5], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Inst., RAS, St. Petersburg, Russia — [3]Dept. of Theo. Phys., V.E. Lashkaryov Inst. of Semiconductor Phys., Kyiv, Ukraine — [4]Raith GmbH, 44263 Dortmund, Germany — [5]School of Phys. and Astronomy, Univ. of Nottingham, UK

In our time-resolved experiments with ferromagnetic nanogratings (NGs), the formation of coherent magnon polarons is confirmed by direct evidence of the avoided crossing effect, as well as by several bright indirect manifestations. The NGs have been produced by focused ion beam milling into a 105 nm-thick Fe0.81Ga0.19 film. They have a lateral period of 200 nm and consist of parallel grooves of 100 nm width and 7-21 nm depth milled along the [100]-crystallographic direction. We perform transient magneto-optical measurements in a conventional pump-probe scheme with micron spatial resolution, where the femtosecond pump pulse excites the NGs, while the probe pulse serves to detect coherent lattice and magnetic responses. Using an external magnetic field, the magnon modes can be brought into resonance with the localized phonon modes of the NG resulting in the formation of magnon polarons, where the coupling strength is determined by the spatial overlap of the interacting modes.

MA 11.2 Wed 13:30 P

Topological magnon-polaron in a two-dimensional ferromagnet — •Gyungchoon Go, Se Kwon Kim, and Kyung-Jin Lee — Department of Physics, KAIST, Daejeon 34141, Republic of Korea

We theoretically investigate the topological aspects of the magnon-phonon hybrid excitation in a simple two-dimensional (2D) square-lattice ferromagnet with perpendicular magnetic anisotropy. In our 2D model, the Berry curvature we find requires neither a special spin asymmetry such as the DM interaction nor a special lattice symmetry: Our 2D model description is applicable for general thin-film ferromagnets. We show that even without such long-range dipolar interaction, DM interaction, or special lattice symmetry, the nontrivial topology of a magnon-phonon hybrid can emerge by taking account of the well-known magnetoelastic interaction originates from the magnetocrystalline anisotropy. Because the magnetocrystalline anisotropy is ubiquitous in ferromagnetic thin-film structures, our result does not rely on specific preconditions and thus is quite generic. Furthermore, we show that the topological structures of the magnon-polaron bands can be manipulated by effective magnetic fields via topological phase transition. We uncover the origin of the nontrivial topological bands by mapping our model to the well-known two-band model for topological insulators, where the Chern numbers are read by counting the number of topological textures, called skyrmions, of a certain vector in momentum space. In this picture, the magnon-phonon hybridization induces the chiral texture of the momentum space vector. As an experimental probe for our theory, we propose the thermal Hall conductivity.

MA 11.3 Wed 13:30 P

Magnetization Dynamics in Hybrid Ferromagnetic Systems — •Misbah Yaqoob[1,2,3], Lukas Liensberger[1,2], Luis Flake[1,2], David Weffling[3], Vitaliy Vasyuchka[3], Matthias Althammer[1,2], Rudolf Gross[1,2], and Mathias Weiler[1,3] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Physik-Department, TU München, Germany — [3]Fachbereich Physik, TU Kaiserslautern, Germany

Thin film heterostructures consisting of several magnetically ordered layers are a promising platform for magnon spintronics because they can host complex magnetic textures, hybrid spin dynamics and spin torques [1,2].

We have investigated the magnetization dynamics of purely metallic ferromagnetic thin film multilayers and insulating magnet/metallic magnet thin film hybrid systems using broadband ferromagnetic resonance (FMR) and microfocused frequency-resolved magneto-optic Kerr effect (μFR-MOKE) at room temperature. With FMR, we find that the anisotropy of all-metallic systems can be tuned from $\mu_0 M_{\mathrm{eff}} \approx 300$ mT to $\mu_0 M_{\mathrm{eff}} \approx 0$ by varying the number of multilayer repeats without affecting magnetic damping. We extract the spinwave dispersion using μFR-MOKE and find μm scale spinwave propagation lengths and group velocities in the order of 10 km/s. We compare these findings to those obtained in hybrid metallic ferromagnet/insulating yttrium iron garnet thin film heterostructures.

[1] Klingler et al. Phys. Rev. Lett. 120, 127201 (2018)
[2]Flacke et al. arXiv:2102.11117 (2021)

MA 11.4 Wed 13:30 P

Amplification of Propagating Spin Waves by Rapid Cooling — •David Breitbach[1], Michael Schneider[1], Bert Lägel[1], Carsten Dubs[2], Andrei N. Slavin[3], Vasyl Tyberkevych[3], Philipp Pirro[1], Burkard Hillebrands[1], and Andrii Chumak[4] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, Kaiserslautern, Germany — [2]Innovent e.V. Technologieentwicklung, Jena, Germany — [3]Department of Physics, Oakland University, Rochester, MI, United States — [4]Faculty of Physics, University of Vienna, Vienna, Austria

Recently, the formation of a magnon Bose-Einstein Condensate (BEC) triggered by the rapid cooling of magnonic nano-structures has been reported [1]. A rapid decrease of the phonon temperature achieved after heating with an applied DC pulse in a nano-sized YIG|Pt sample leads to a non-equilibrium between the phonon and the magnon system. This results in a redistribution of magnons to the lowest frequencies of the spectrum and, finally, to the formation of a BEC. Building on this mechanism, we show the coherent amplification of externally excited, propagating spin waves in a YIG-waveguide using time-resolved BLS microscopy. This amplification is maximal when the spin-wave packet propagates through the Pt-region during the process of rapid cooling. This study shows the applicability of the rapid cooling mechanism to compensate for the intrinsic damping in spintronic devices and also gives insight into new physics, namely the interaction of a prepared coherent state with a magnon BEC. [1] M. Schneider, et. al., Nat. Nanotechnol. 15, 457-461 (2020)

MA 11.5 Wed 13:30 P

Theory of quantum entanglement and the structure of two-mode squeezed antiferromagnetic magnon vacuum — •Dennis Wuhrer, Niklas Rohling, and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

Recent investigations of the quantum properties of an antiferromagnet in the spin wave approximation have identified the eigenstates as two-mode squeezed sublattice states. The uniform squeezed vacuum and one-magnon states were shown to display a massive sublattice entanglement. Here we expand this investigation and study the squeezing properties of all sublattice Fock states throughout the magnetic Brillouin zone.

We derive the full statistics of the sublattice magnon number with wave number $\vec{k}$ in the ground state and show that magnons are created in pairs with opposite wave vectors, hence, resulting in entanglement of both modes. To quantify the degree of entanglement we apply the Duan-Giedke-Cirac-Zoller inequality and show that it can be violated for all modes. The degree of entanglement decrease towards the corners of the Brillouin zone. We relate the entanglement to measurable correlations of components of the Néel and the magnetization vectors, thus, allowing to experimentally test the quantum nature of the squeezed vacuum.

The distinct k-space structure of the probabilites shows that the squeezed vacuum has a nonuniform shape that is revealed through the $\vec{k}$-dependent correlators for the magnetization and the Néel vectors.

MA 11.6 Wed 13:30 P

Combined tr-MOKE, BLS and THZ-radiation setup for the investigation of magnetization dynamics on different time scales — •Akira Lentfert[1], Benjamin Stadtmüller[1], Martin Aeschlimann[1], Georg von Freymann[1,2], and Philipp Pirro[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern — [2]Fraunhofer Institute for Industrial Mathematics ITWM

Two separate models commonly describe spin and magnetization dynamics on different time scales. Systems in the sub-picosecond regime in ultrafast demagnetization processes are dominated by single-particle excitations. Here, a femtosecond laser pulse induces a loss of the magnetic order, which can be observed with time-resolved pump-probe spectroscopy based on the magneto-optical Kerr effect (tr-MOKE). In the nanosecond time scale, dynamics are described by collective excitations in terms of spin waves. However, due to the nature of the measurement technique mentioned above, it is impossible to detect incoherent collective dynamics. Therefore, the role of spin-waves up to the THz regime on ultrashort time scales could not be studied sufficiently. In this work, a combined setup of tr-MOKE with Brillouin-Light-Scattering spectroscopy (BLS) is presented, which allows the simultaneous investigation of magnetization dynamics on different time scales, from 1 ns down to 10 fs. Furthermore, using electromagnetic THz radiation to excite spin waves in this frequency regime resonantly gives further insight into the magneto-optical interactions. This research has been supported by DFG (TRR 173: Spin+X).

MA 11.7 Wed 13:30 P

Influence of Spatial Confinement on Spin-Wave Frequency Combs — •Christopher Heins[1], Tobias Hula[1,2], Katrin Schultheiss[1], Francisco Goncalves[1], Lukas Körber[1,3], Mauricio Bejarano[1,3], Luis Flacke[4,5], Lukas Liensberger[4,5], Aleksandr Buzdakov[1], Attila Kákay[1], Mathias Weiler[4,5,6], Jürgen Fassbender[1,3], and Helmut Schultheiss[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]TU Chemnitz, Germany — [3]TU Dresden, Germany — [4]Walther-Meißner-Institut, Garching, Germany — [5]TU München, Germany — [6]TU Kaiserslautern, Germany

Recently, it has been shown that four-magnon scattering in a stripe-shaped magnonic waveguide can be stimulated and utilized to generate spin wave frequency combs [1].

Here, we demonstrate that by restricting possible eigenstates via a two-dimensional spatial confinement the stimulated four-magnon scattering can be enhanced and a single RF excitation leads to the spontaneous formation of a frequency comb. We determine the frequency spacing of the spin wave modes in a $Co_{25}Fe_{75}$ rectangular microconduit with micromagnetic simulations and explore the formation of spin-wave frequency combs experimentally by means of micro-focused Brillouin light scattering. Further, we show that the spontaneously generated frequency comb can be resonantly amplified by a second RF excitation.

The authors acknowledge financial support from the Deutsche Forschungsgemeinschaft within program SCHU 2922/1-1.

[1] Hula et al., arXiv:2104.11491 (2021)

MA 11.8 Wed 13:30 P

Magnon condensates in magnetization landscapes — •Matthias R. Schweizer, Alexander J.E. Kreil, Georg von Freymann, Alexander A. Serga, and Burkard Hillebrands — Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, Kaiserslautern, Germany

In this study, we demonstrate the potential to control a magnon condensate by spatial modulation of the saturation magnetization.

As shown in previous studies, a magnon condensate can be created via parallel parametric pumping in a stripline-resonator. We use a 458 nm laser in combination with a phase-based wavefront modulation technique to create confined temperature patterns in an yttrium-iron-garnet film of 5 μm thickness, which result in a decrease of the local saturation magnetization and in modify the local frequency of the condensate. The magnon density is measured by means of k-vector-resolved Brillouin-light-scattering-spectroscopy. We provide evidence of strong, directed magnon accumulation by magnon supercurrents [1] and anomalous decay behavior for several distances between heated positions.

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - TRR 173 - 268565370.

[1] *D. A. Bozhko et al.*, Nat Commun **10**, 2460 (2019)

MA 11.9 Wed 13:30 P

Parametric pumping in out-of-plane magnetized ferrite films towards magnon Bose-Einstein condensation — •Andra Pirktina, Timo B. Noack, Vitaliy I. Vasyuchka, Alexander Serga, and Burkard Hillebrands — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany

The Bose–Einstein condensate (BEC) in a parametrically overpopulated gas of spin-wave quanta—magnons—manifests itself as a spontaneous formation of a coherent spin wave state at the energy minimum of the magnon spectrum. Magnon BECs, which are observed at gigahertz frequencies in tangentially magnetized yttrium iron garnet (YIG) films even at room temperature, can be used as signal sources for microwave applications and as information carriers in wave and quantum computing. However, due to the wavelength of the order of a few micrometers, the magnon BEC is detected mainly by the Brillouin light scattering spectroscopy, which is hardly applicable to real devices.

Here, we report on the spontaneous BEC formation in the out-of-plane magnetization geometry, where the magnon spectrum has a minimum at zero wavenumber, and the BEC frequency coincides with the ferromagnetic resonance frequency. In this case, the BEC was detected as a microwave electromagnetic signal by an inductive microstrip antenna. A small signal line width of 1.4 MHz was measured after the pump power exceeded the parametric instability threshold by 34 dB.

Funded by the ERC Advanced Grant 694709 SuperMagnonics and by the DFG within TRR 173 – 268565370 (project B04).

MA 11.10 Wed 13:30 P

Electric phase control of magnon currents — •Rostyslav O. Serha, Vitaliy I. Vasyuchka, Alexander A. Serga, and Burkard Hillebrands — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, Kaiserslautern, Germany

New findings of interactions between electric fields and magnons are promising for novel magnonic applications. They would allow the control of the phase of magnon currents by applying a voltage to the magnetic waveguides. In our work, we investigated the influence of a strong electric field on the phase of propagating spin waves in yttrium iron garnet (YIG) films. The experiment was performed in different spin-wave excitation geometries when volume and surface magnetostatic spin waves were excited. With the help of a vector network analyzer, the phase shift of the transmitted wave, which is sensitive to different external influences, was precisely measured. It was found that the phase shift owing to the electric field influence is relatively strong in the case of magnetostatic surface spin waves but is also observable for backward volume magnetostatic waves. By comparing results obtained for different spin-wave geometries, we discuss the physical nature of the observed phase shift, including possible contributions from the magnetoelectric effect in YIG and from the Aharonov-Casher effect. Funding by the ERC Advanced Grant 694709 SuperMagnonics is gratefully acknowledged.

MA 11.11 Wed 13:30 P

Dipolar interactions and spin dynamics in the itinerant ferromagnets Fe and Ni — •Lukas Beddrich[1,2], Steffen Säubert[3,4], Johanna K. Jochum[1], Christian Franz[1,5], and Peter Böni[2] — [1]Research Neutron Source Heinz Maier-Leibnitz (FRM II) | TU München — [2]Physics Department | TU München — [3]Chair for Topology of Correlated Systems (E51) | Physics Department | TU München — [4]Department of Physics | Colorado State University — [5]Jülich Center for Neutron Science (JCNS)

The spin wave dispersion of an isotropic ferromagnet is comprehensively described by the Holstein-Primakoff theory, which takes dipolar interactions into account. The dispersion follows a quadratic form for large q values $E_{SW} \propto q^2$, whereas for small q the dispersion shows linear behavior. This is attributed to the long-range dipolar interaction between the magnetic moments. The subtle influence of these interactions on the magnon spectrum are expressed by the dipolar wave vector q_D. The dipolar interactions are primarily probed for $q \leq q_D$. Utilizing the modern MIEZE method, a neutron resonance spin echo technique, we investigated the spin wave dispersion in iron and the paramagnetic spin fluctuations in nickel at small momentum and energy transfer with high resolution, never achieved before by neutron scattering. The results show excellent agreement with previously conducted triple-axis measurements by Collins et al. in the overlapping q regime, while extending the investigated range of the spin wave dispersion down to a momentum transfer of $q = 0.015A^{-1}$ with unprecedented energy resolution.

MA 11.12 Wed 13:30 P

Integration and characterization of micron-sized YIG structures with very low Gilbert damping on arbitrary substrates — •Philip Trempler[1], Rouven Dreyer[1], Philipp Geyer[1], Georg Woltersdorf[1], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther Universität Halle-Wittenberg 06099 Halle (Saale), Germany

We present a process that allows the transfer of monocrystalline yttrium-iron-garnet microstructures onto virtually any kind of substrate. The process is based on a recently developed method that allows the fabrication of freestanding monocrystalline YIG bridges on gadolinium-gallium-garnet. Here, the bridges' spans are detached from the substrate by a dry etching process and immersed in a watery solution. Using drop-casting, the immersed YIG platelets can be transferred onto the substrate of choice, where the structures finally can be reattached and, thus, be integrated into complex devices or experimental geometries. Using time-resolved scanning Kerr microscopy and inductively measured ferromagnetic resonance, we find a ferromagnetic resonance linewidth of 195 μT at room temperature and we were even be able to inductively measure magnon spectra on a single micrometer-sized YIG platelet at a temperature of 5 K. In the future, this approach will allow for types of spin dynamics experiments until now unthinkable.

MA 11.13 Wed 13:30 P

Local and nonlocal spin Seebeck effect in lateral Pt-Cr_2O_3-Pt devices at low temperatures — •Prasanta Muduli[1], Richard Schlitz[1], Tobias Kosub[2], René Hübner[2], Artur Erbe[2], Denys Makarov[2], and Sebastian T. B. Goennenwein[1] — [1]Institut für Festköper- und Materialphysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

We have studied thermally driven magnon spin transport (spin Seebeck effect, SSE) in heterostructures of antiferromagnetic α-Cr_2O_3 and Pt at low temperatures. Monitoring the amplitude of the local and nonlocal SSE signals as a function of temperature, we found that both decrease with increasing temperature and disappear above 100 K and 20 K, respectively. Additionally, both SSE signals show a tendency to saturate at low temperatures. The nonlocal SSE signal decays exponentially for intermediate injector-detector separation, consistent with magnon spin current transport in the relaxation regime. We estimate the magnon relaxation length of our α-Cr_2O_3 films to be around 500 nm at 3 K. This short magnon relaxation length along with the strong temperature dependence of the SSE signal indicates that temperature-dependent inelastic magnon scattering processes play an important role in the intermediate range magnon transport. Our observation is relevant to low-dissipation antiferromagnetic magnon memory and logic devices involving thermal magnon generation and transport.

MA 11.14 Wed 13:30 P

Nonlinear relaxation of quantized propagating magnons in nanodevices — •Morteza Mohseni[1], Qi Wang[2], Björn Heinz[1], Michael Schneider[1], Felix Kohl[1], Carsten Dubs[3], Andrii V. Chumak[2], and Philipp Pirro[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria — [3]INNOVENT e.V., Technologieentwicklung, Prüssingstraße 27B, 07745 Jena, Germany

The use of spin waves and their quanta, the magnons, opens many opportunities in designing novel data processing units. Relaxation of linear spin waves is well described by viscous Gilbert damping processes. However, for strong excitations, nonlinear damping processes such as the decay via magnon-magnon interactions emerge and trigger additional relaxation channels. Such nonlinear dynamics are essential for the generation of magnon Bose-Einstein condensates, although their characteristics are not well investigated in magnonic nanostructures. We investigate the nonlinear relaxation of strongly generated spin waves in yttrium iron garnet nanodevices. We show that the nonlinear magnon relaxation in this highly quantized system possesses intermodal features, i.e., magnons scatter to other quantized modes through a cascade of scattering events. A further discussion of the phenomenon in the regime of its fundamental limitations is given.

MA 11.15 Wed 13:30 P

Mode selective excitation of spin waves — •Takuya Taniguchi and Christian Back — Technische Universität München

In a magnetic stripe, spin waves have eigenmodes which are energetically separated due to the geometry of the device. However, it has been difficult to selectively excite one eigenmode of spin wave. In this work, we performed micromagnetic simulation to study spin wave propagation in a T-shaped device and found that the spin wave mode in the device is controllable by varying the resonant frequency and the device structure.

MA 11.16 Wed 13:30 P

Spin-wave frequency combs — •Tobias Hula[1,2], Katrin Schultheiss[1], Francisco Goncalves[1], Lukas Körber[1,3], Mauricio Bejarano[1,3], Matthew Copus[4], Luis Flacke[5,6], Lukas Liensberger[5,6], Aleksandr Buzdakov[1], Attila Kakay[1], Mathias Weiler[5,6,7], Robert Camley[5], Jürgen Fassbender[1,3], and Helmut Schultheiss[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]TU Chemnitz, Chemnitz, Germany — [3]TU Dresden, Dresden, Germany — [4]Center for Magnetism and Magnetic Nanostructures, University of Colorado, USA — [5]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Germany — [6]TU München, Munich, Germany — [7]TU Kaiserslautern, Kaiserslautern, Germany

We present experimental observations on the generation of a spin wave frequency comb in a low damping Co25Fe75 conduit measured using Brillouin light scattering microscopy. By driving the magnetization to large precession angles, nonlinear interactions such as four magnon scattering can be observed. When applying two RF signals with tunable frequencies and amplitudes to our microstructure, we can actively control the final states populated by these scattering processes. Our results show the generation of a frequency comb, consisting of several spin wave modes with adjustable frequency spacing and amplitude. Our observations are in qualitative agreement with micromagnetic simulations. We acknowledge financial support from the DFG within programs SCHU 2922/1-1, WE5386/4-1 and WE5386/5-1. K. S. acknowledges funding within the Helmholtz Postdoc Programme.

MA 11.17 Wed 13:30 P

Identification and characterization of plastics using THz-spectroscopy — •Tobias Kleinke, Finn-Frederik Stiewe, Ulrike Martens, Jakob Walowski, and Markus Münzenberg — Institute of Physics, University Greifswald, Germany

THz-spectroscopy is an attractive tool for scientific research, especially in life science, offering non-destructive interaction with matter due to its low photon energies [1]. Current research investigates the impact of plastic nanoparticles on cell tissue in several aspects, because those particles are highly abundant in the environment and also enter the human body potentially causing harmful interactions [2]. THz spectroscopy offers the opportunity to discover and study the influence of microplastics in living human cells.

Our project aims to identify and characterize different types of plastics in the human body or even in cells. Therefore it is necessary to set up a database with THz-spectra of the most abundant polymers. We analyze transmission spectra of several plastics with a commercial THz spectrometer (bandwidth from 0.1 to 6 THz) and identified specific absorption peaks for the individual studied materials. Furthermore, by determining the refractive index and the absorption coefficient, specific polymers can be characterized and identified.

Funding by BMBF: MetaZik PlasMark-T (FKZ:03Z22C511) is acknowledged.

[1] W. Shi et al., Journal of Biophysics, Vol. 14, 2021 [2] A. Ragusa et al., Environment International, Vol. 146, 2021

MA 11.18 Wed 13:30 P

THz-2D Scanning Spectroscopy — •Finn-Frederik Stiewe, Tobias Kleinke, Tristan Winkel, Ulrike Martens, Jakob Walowski, Christian Denker, and Markus Münzenberg — Institute of Physics, University Greifswald, Germany

THz-spectroscopy offers attractive imaging capabilities for scientific research, especially in life science. Its low photon energies lead to non-destructive interaction with matter [1,2]. However, wavelengths above 100 μm principally limit its spatial resolution by diffraction. Near-field-imaging using spintronic emitters offers the most feasible approach to overcome this restriction. In our study, we investigate THz-pulses generated by fs-laser-excitations in CoFeB/Pt heterostructures, based on spin currents together with a LT-GaAs Auston switch as detector. The spatial resolution is tested by applying a 2D scanning technique with motorized stages allowing scanning steps in the sub-micrometer range. For this purpose, the spintronic emitter is directly evaporated on a gold-test pattern separated by a several hundred nanometer thick insulating spacer layer. Moving these structures with respect to the THz wave generation spot allows for resolution determination using the knife-edge method. We observe a THz beam FWHM of 4.86 *0.37 μm at 1 THz by using near-field imaging, which are in the dimension of the laser spot. Due to its simplicity, our technical approach offers a large potential for wide-ranging applications.

Funding by: MetaZIK PlasMark-T (FKZ:03Z22C511), BMBF

[1] A. G. Davies et al., Materials Today, Vol. 11 (2008) 18. [2] A. Y. Pawar et al., Drug Invention Today, Vol. 5 (2013).

MA 11.19 Wed 13:30 P

Spin-Hall-Angle measurements on magnetic heterostructures using THz-spectroscopy — •Tristan Winkel, Finn-Frederik Stiewe, Tobias Kleinke, Ulrike Martens, Jakob Walowski, and Markus Münzenberg — Institute of Physics, University Greifswald, Germany

Spin Hall angle measurements are important for spin device design. The data is used to build optimized spin Hall nano-oscillators for the fabrication of a neuromorphic computer chip [1]. THz spectroscopy provides effective means to measure spin Hall angles. In our study, we investigate THz pulses generated by fs laser excitations in magnetic heterostructures based on spin currents, together with an LT-GaAs Auston switch as a detector. The magnetic heterostructures consist of a CoFeB layer and a heavy metal layer. From the THz measurement, we can extrapolate the spin Hall angle of the heavy metal. Our technical approach offers great potential for wide-ranging applications due to its simplicity.

[1] M. Zahedinejad et al., Appl. Phys. Lett. 112, 132404 (2018)

Funding by: EU Horizon 2020, Spinage

MA 11.20 Wed 13:30 P

Microstructured spintronic terahertz emitters — •Rieke von Seggern[1], Christopher Rathje[1], Leon Gräper[1], Nina Meyer[2], Markus Münzenberg[2], and Sascha Schäfer[1] — [1]Institute of Physics, University of Oldenburg, Germany — [2]2Institute of Physics, University of Greifswald, Germany

In recent years, spintronic terahertz (THz) emitters have become a well-established source for strong single-cycle THz pulses [1]. In those metallic multilayer systems, an optically induced spin-polarized current pulse is converted into a transverse charge current, resulting in a broadband emission of THz radiation. In this work, we investigate different strategies for coupling the transverse current to micro-resonators on, or in close proximity, to the THz emitter surface and their influence on the detected THz spectrum. Various designs of resonator arrays were fabricated by electron beam lithography with expected resonance frequencies in the range of 0.5-4 THz. The resonances are visible as a decreased spectral THz amplitude at the corresponding resonance frequencies. A transition from a field- to a current-coupled regime is identified for decreasing distance between the resonator and the emitter, and compared to numerical modelling based on finite-element simulations.

[1] Seifert et al., Nat. Photonics 10, 483-488 (2016)

MA 11.21 Wed 13:30 P

Nutation resonance in antiferromagnets — •Ritwik Mondal[1,2], Levente Rózsa[3], Sebastian Grossenbach[3], and Ulrich Nowak[3] — [1]Institute of Physics of the Czech Academy of Sciences, Prague 6, Czech Republic — [2]Department of Physics and Astronomy, Uppsala University, Sweden — [3]Fachbereich Physik, Universität Konstanz, DE-78457 Konstanz, Germany

At ultrafast timescales, an additional spin torque term has to be supplemented within Landau-Lifshitz-Gilbert spin dynamics, to account for magnetic inertial dynamics causing spin nutation [1]. The experimental observation of the nutation resonance has only been achieved very recently [2]. In this work, we compare the effect of spin nutation in ferromagnets, antiferromagnets and ferrimagnets using linear response theory [3]. We identify the precession and nutation resonance peaks, and demonstrate that the precession resonance frequencies are reduced by the spin nutation, while the lifetime of the excitations is enhanced. We find the interplay between precession and nutation resonances to be more prominent in antiferromagnets compared to the ferromagnets, where the timescale of the exchange-driven sublattice dynamics is comparable to inertial relaxation times. Consequently, antiferromagnetic resonance techniques should be better suited for the search for intrinsic inertial spin dynamics on ultrafast timescales than ferromagnetic resonance [3].

[1] M.-C. Ciornei, J. M. Rubí, and J.-E. Wegrowe, Phys. Rev. B **83**, 020410(R) (2011) [2] K. Neeraj *et al.*, Nature Phys. **17**, 245 (2021) [3] R. Mondal *et al.* Phys. Rev. B **103**, 104404 (2021)

MA 11.22 Wed 13:30 P

Spintronic THz emitters tuned with Ta and modified interface qualities — •Laura Scheuer[1], Dominik Sokoluk[2], Garik Torosyan[3], René Beigang[1], Marco Rahm[2], and Evangelos Papaioannou[4] — [1]Fachbereich Physik and Landesforschungszentrum Optimas, TUK, Kaiserslautern, Germany — [2]Fachbereich Elektrotechnik, TUK, Kaiserslautern, Germany — [3]Photonic Center Kaiserslautern, Kaiserslautern, Germany — [4]Institut of Physics, MLU, Halle-Wittenberg, Germany

THz emission from metallic thin film multilayers interlinked the field of ultrafast spintronics and the field of THz optics, raising new fascinating research subjects. In principle, the THz pulse is generated by a spin current. This spin current is excited in a ferromagnetic layer by a fs laser pulse and diffuses into the adjacent layers. Usually their material is chosen to have a high spin-orbit coupling to provide a strong spin-to-charge conversion via the spin-Hall effect, resulting in a transient charge current. These accelerated electrons emit a radiation in the THz range.

Our recent experiments concentrate on materials different from our well-studied Fe/Pt-bilayers: Firstly, as Ta is a material with high spin-orbit coupling and a spin-Hall angle opposite to Pt's, we did not only replace Pt in bilayers but also added Ta as a second non-magnetic layer. Additionally we extended our investigations regarding the role of the interface to interfaces 'dusted' with Au and Cu, meaning they are grown thin enough not to form a whole monolayer.

MA 11.23 Wed 13:30 P

Modulation of Terahertz radiation by current confinement in patterned Ferromagnetic Emitters — •Bikash Das Mohapatra[1], Evangelos Th. Papaioannou[1], Reza Rouzegar[3], Tobias Kampfrath[3], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120 Halle, Germany — [2]Interdisziplinäres Zentrum für Meterialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Straße 4, D-06120 Halle, Germany — [3]Department of Physical Chemistry, Fritz Haber Institute, Faradayweg 4-6, 14195 Berlin, Germany

Spintronic Ferromagnetic Emitters are novel sources for generation of THz radiation. Various studies have shown the generation of ultrafast transverse charge current from spin current by the Inverse Spin Hall Effect resulting in THz electromagnetic pulses. We have fabricated THz emitters into arrays of geometrical structures using Sputter deposition and e-beam lithography. The structures were micron or sub-micron sized squares and rectangles. Upon fs laser irradiation these emitters show an emission spectrum which is different than for large area reference emitters. We suggest that the confinement[1] results in local charge accumulation that creates additional currents that counteract the initial inverse spin Hall effect.

[1] Z. Jin et al., "Terahertz Radiation Modulated by Confinement of Picosecond Current Based on Patterned Ferromagnetic Heterostructures ", Phys. Stat. Sol. 13, 1900057 (2019).

MA 11.24 Wed 13:30 P

Strain effect in the anomalous Hall effect of SrRuO3 thin films : a first principles study — •Kartik Samanta[1], Marjana Ležaić[2], Stefan Blügel[2], and Yuriy Mokrousov[2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Peter Grunberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We investigate the effect of strain-induced oxygen octahedral distortion in the electronic structure and anomalous Hall response of the ferromagnetic SrRuO3(SRO) ultra-thin films by virtue of density functional theory calculations. We find a strong deformation of the oxygen octahedra (RuO6) with an increasing amount of substrate induced compressive strain. Our Berry curvature calculations predict a positive value of the anomalous Hall conductivity of +76 S/cm at -1.7% strain, whereas it is found to be negative (-156 S/cm) at -0.47% strain. We attribute the observed behavior of the anomalous Hall effect to the nodal point dynamics in the electronic structure arising in response to tailoring the oxygen octahedral distortion driven by the substrate induced strain. Our calculation of the strain-mediated anomalous Hall conductivity as a function of reduced magnetization obtained by scaling down the magnitude of the exchange field inside Ru atoms, shows a good qualitative agreement with experimental observations, which indicates a strong impact of longitudinal thermal fluctuations of Ru spin moments on the anomalous Hall effect in this system.

MA 11.25 Wed 13:30 P

Anisotropy of $4f$ states in $3d$-$4f$ single molecular magnets — Andreas Rauguth[1], Ahmed Alhassanat[1], Hebatalla Elnaggar[3], Angeliki A. Athanasopoulou[1], Chen Luo[2], Hanjo Ryll[2], Florin Radu[2], Torge Mashoff[1], Frank M.F. de Groot[3], Eva Rentschler[1], and •Hans-Joachim Elmers[1] — [1]Johannes Gutenberg-Universität Mainz, Mainz, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]University Utrecht, Utrecht, Netherlands

Using X-ray magnetic circular dichroism, we determined element-specific magnetic moments in $3d$-$4f$ metallacrown single molecular magnets at low temperature (7 K) and large field (7 Tesla). The magnetic moment of the molecule is dominated by the rare earth moment revealing a large contribution of orbital moment. Angular-dependent spectra on oriented molecules in single crystals allow to disentangle magnetic and orbital anisotropies. X-ray natural linear dichroism reveals the anisotropic charge distribution of the rare earth $4f$ state in the tetragonal crystal field despite the small $4f$ crystal field splitting. The angular dependence of the spin and orbital magnetic moments are compared to theory using multiplet calculations. We determined magnetic anisotropies from the angular dependence of the orbital magnetic moment.

MA 11.26 Wed 13:30 P

Numerical dynamic study of two coupled vortex-based spin transfer oscillator — •Abbass Hamadeh[1], Milan Ender[1], Vitally Lomakin[2], and Philipp Pirro[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, Kaiserslautern, Germany — [2]Center for Magnetic Research, University of California at San Diego, La Jolla, CA, USA.

The magnetic vortex state in nano-magnetic structures is a subject of intensive research since it offers many applications. To gain key insight into engineering and manipulating the vortex core (VC) orientation reversal, it is crucial to fully understand their coupled dynamics. For this purpose, we have studied micromagnetically the auto-oscillating modes in a spin-transfer vortex oscillator with vortices in two coupled thin and thick layers for different applied magnetic fields and currents. We find that for the anti-parallel vortex polarity configurations, a region with downward/upward magnetization appears at the inner side of the vortex core resembling a deformation of the vortex profile. This deformation, induced by the vortex core's accelerating motion, breaks the lateral magnetization symmetry between the two layers of the oscillator. Our results reveal the origin of the signal measured experimentally [N. Locatelli et al., Appl. Phys. Lett. 98, 062501 (2011)] for a system based on two coupled vortices and provide key insights into engineering the vortex core orientation using DC currents.

MA 11.27 Wed 13:30 P

First principles design of Ohmic spin diodes based on quaternary Heusler compounds — •Thorsten Aull, Ersoy Sasioglu, and Ingrid Mertig — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale) Germany

The Ohmic spin diode is a new concept in spintronics whose operation principle relies on the transport properties of spin-gapless semiconductors (SGSs) and half-metallic magnets (HMMs). [1] Due to the spin-dependent filtering of electrons Ohmic spin diodes exhibit linear current-voltage characteristics in the on-state and zero threshold voltage due to the absence of an energy barrier at the interface between the SGS and HMM electrode. Quaternary Heusler compounds offer a platform to design SGSs and HMMs within the same family and these materials possess high Curie temperatures which makes them favorable for room temperature applications. By applying first-principles DFT calculations combined with the non-equilibriums Green's function method we design four different OSDs using quaternary Heusler compounds. [2] We demonstrate that these diodes exhibit zero threshold voltage and possess linear current-voltage characteristics. Moreover, we reveal that the small leakage currents can be attributed to the overlap of the conduction and valance band edges in opposite spin channels at the Fermi energy in the SGS material.

[1] E. Şaşıoğlu *et al.*, Phys. Rev. Appl. **14**, 014082 (2020)
[2] T. Aull *et al.*, Appl. Phys. Lett. **118**, 052405 (2021)

MA 11.28 Wed 13:30 P

Bipolar Spin Hall Nano-Oscillators — •Toni Hache[1], Yancheng Li[2], Tillmann Weinhold[3], Bernd Scheumann[1], Francisco T. J. Goncalves[1], Olav Hellwig[1,4], Jürgen Fassbender[1,3], and Helmut Schultheiss[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Johns Hopkins University, United States — [3]Technical University Dresden, Germany — [4]Technical University Chemnitz, Germany

Spin Hall nano-oscillators (SHNO) convert dc currents in microwave oscillations of the magnetization. The frequency can be tuned by external magnetic fields, the applied dc current magnitude or by injection locking if an additional microwave magnetic field is applied to the SHNO. Here, we demonstrate another approach to extend the frequency range of an SHNO by adding a second ferromagnetic layer. An SHNO with a layer stack NiFe/Pt/CoFeB is used. By applying a charge current a pure spin current is generated by the spin Hall effect in the Pt. It has opposite spin polarization at both interfaces being in contact with the ferromagnetic layers. Therefore, only in one of both the Gilbert damping can be compensated by the spin-orbit torque to achieve auto-oscillations. By switching the charge current polarity the spin current polarizations switch as well and the second ferromagnetic material shows auto-oscillations. In this way two frequency ranges can be accessed by switching the applied charge current. The authors acknowledge financial support from the Deutsche Forschungsgemeinschaft within programme SCHU 2922/1-1.

MA 11.29 Wed 13:30 P

Asymmetric modification of the magnetic proximity effect in Pt/Co/Pt trilayers — •Ankan Mukhopadhyay[1], Sarathlal Koyiloth Vayalil[1], Dominik Graulich[2], Imran Ahamed[3], Sonia Francoual[4], Arti Kashyap[3], Timo Kuschel[2], and Anil Kumar P S[1] — [1]Indian Institute of Science, Bangalore, India — [2]Center for Spinelectronic Materials and Devices, Bielefeld University, Germany — [3]Indian Institute of Technology, Mandi, India — [4]Deutsches Elektronen-Synchrotron, Hamburg, Germany

Interfacial spin-orbit coupling in ferromagnet/nonmagnet systems promotes remarkable spin-related phenomena and interactions which simultaneously provide the electrical manipulation of the magnetic moments up to the point of magnetization switching by current-driven domain wall motion. The phenomenon of a nominally paramagnetic material getting spin-polarized in presence of an adjacent ferromagnetic material by the exchange interaction is known as the magnetic proximity effect (MPE). The MPE in the top and bottom Pt layers induced by Co in Ta/Pt/Co/Pt and Ta/Pt/Co/Cu/Pt multilayers has been studied by interface sensitive, element-specific x-ray resonant magnetic reflectivity at the Pt L_3 absorption edge with an in-plane magnetic field. It has been observed that the Ta buffer layer with increasing thickness modifies the bottom Pt growth which in turn reduces the induced magnetic moment in the bottom Pt layer in Ta/Pt/Co/Pt[1], while it decreases in the top Pt layer in Ta/Pt/Co/Cu/Pt if the thickness of the Cu spacer is increased.

[1]A. Mukhopadhyay et al., Phys. Rev. B **102**, 144435 (2020).

MA 11.30 Wed 13:30 P

Magnon transport in YIG/Pt nanostructures with reduced effective magnetization — •Janine Gückelhorn[1,2], Tobias Wimmer[1,2], Manuel Müller[1,2], Stephan Geprägs[1], Hans Hübl[1,2,3], Rudolf Gross[1,2,3], and Matthias Althammer[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), München, Germany

The transport of information via spin waves (magnons) in magnetically ordered insulators provides novel paths for information processing. For applications based on pure magnonic spin currents damping effects resulting in a decrease of the corresponding conductivity, have to be minimized. Here, we investigate the magnon transport through an yttrium iron garnet (YIG) thin film with strongly reduced effective magnetization. Utilizing three-terminal Pt strip devices allow us to manipulate the magnon transport between the two outer strips via an additional charge current applied to the center electrode. Most importantly, above a certain threshold current, where damping compensation via spin torque is reached, the effective magnon conductivity can be enhanced by a factor of up to six. Another major observation is the linear dependence of the threshold current on the applied magnetic field. We attribute these observations to the reduced effective magnetization and the associated nearly circular mangetization precession.

Financial support by the DFG via project AL2110/2-1 and Germany's Excellence Strategy – EXC-2111 – 390814868 is acknowledged.

MA 11.31 Wed 13:30 P

Agility of spin Hall nano-oscillators — •Francisco Gonçalves[1], Toni Hache[1], Mauricio Bejarano[1,2], Tobias Hula[1,3], Olav Hellwig[1,3], Jürgen Fassbender[1,2], and Helmut Schultheiss[1,2] — [1]HZDR, Institute of Ion Beam Physics and Materials Research, Germany — [2]Technische Universität Dresden, Germany — [3]Institut für Physik, Technische Universität Chemnitz, Germany

Spin Hall nano-oscillators (SHNOs) have the ability to convert a direct current input to magnetisation auto-oscillations (AOs) in the gigahertz regime, by means of spin Hall effect and spin orbit torque [1-2]. We report the temporal response of nano-constriction SHNOs driven by voltage pulses, measured using time-resolved Brillouin light scattering microscopy. The SHNOs consist of a double-disk constriction of NiFe(5 nm)/Pt(7 nm). First, we show how few-nanosecond voltage pulses can efficiently induce AOs. Then, we show how the AOs synchronise to external microwave pulses by means of injection-locking [3]. Our findings suggest that the operation time of processes such as synchronisation and logic using SHNOs can be reduced to the nanosecond timescale and that multi-level microwave outputs can be achieved by combination of voltage and RF pulses. Financial support by the Deutsche Forschungsgemeinschaft is gratefully acknowledged within program SCHU2922/1-1.

[1] A. Manchon et al., Rev. Mod. Phys., vol. 91, p. 035004, Sep 2019. [2] T. Hache et al., Applied Physics Letters, vol. 116, no. 19, p. 192405, May 2020. [3] T. Hache et al., Applied Physics Letters, vol. 114, no. 10, p. 102403, Mar 2019.

MA 11.32 Wed 13:30 P

Monte Carlo simulation of ultrafast nonequilibrium spin and charge transport in iron — •Johan Briones, Hans Christian Schneider, and Bärbel Rethfeld — Department of Physics and Optimas Research Center, TU Kaiserslautern, Germany

Spin transport and spin dynamics after femtosecond laser pulse irradiation of iron (Fe) are studied using a kinetic Monte Carlo model. This model simulates spin dependent dynamics by taking into account elastic electron-lattice scattering, where only the direction of the excited electrons changes, and inelastic electron - electron scattering, where secondary electrons are generated. An analysis of the particle kinetics inside the material shows that a smaller elastic scattering time affects the spin dynamics by leading to a larger spatial spread of electrons in the material, whereas generation of secondary electrons affects the spin transport by increasing the propagation length of homogeneous spin polarization.

MA 11.33 Wed 13:30 P

Magnetic Transitions in Synthetic Antlerite, $Cu_3SO_4(OH)_4$ — •Darren C. Peets[1], Anton A. Kulbakov[1], Quirin Stahl[1], Pavlo Portnichenko[1], Maxim Avdeev[2], Sebastian Gass[3], Laura Teresa Corredor Bohorquez[3], Anja U. B. Wolter[3,4], Manuel Feig[5], Hagen Poddig[6], Inés Puente-Orench[7,8], Jochen Geck[1,4], and Dmytro S. Inosov[1,4] — [1]IFMP, TU Dresden, 01069 Dresden, Germany — [2]ANSTO, Lucas Heights, NSW 2234, Australia — [3]IFW-Dresden, 01069 Dresden, Germany — [4]ct.qmat, TU Dresden, 01069 Dresden, Germany — [5]IEP, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [6]Anorganische Chemie II, TU Dresden, 01069 Dresden, Germany — [7]INMA, CSIC-Universidad de Zaragoza, Zaragoza 50009, Spain — [8]ILL, 38042 Grenoble, France

In frustrated magnetic systems, geometric constraints or the competition amongst interactions introduce extremely high degeneracy and prevent the system from readily selecting a low-temperature ground state. In the mineral antlerite, $Cu_3SO_4(OH)_4$, Cu^{2+} ($S = \frac{1}{2}$) quantum spins populate triangular-lattice three-leg ladders in a novel highly-frustrated quasi-one-dimensional structural motif. We demonstrate that this mineral hosts four distinct magnetically-ordered phases in zero field alone, including an incommensurate phase and a multiple-**q** phase. Multiple-**q** phases are extremely uncommon in centrosymmetric compounds of 3d and lighter elements, and the discovery of such a phase in antlerite opens a new route to finding new materials platforms for exotic magnetic order.

MA 11.34 Wed 13:30 P

Unconventional magnetism in the $RE_3Fe_3Sb_7$ spin system — •Sabrina Palazzese[1,2], Falk Pabst[3], Sumanta Chattopadhyay[1], Shingo Yamamoto[1], Thomas Herrmannsdörfer[1], Denis Gorbunov[1], Eugen Weschke[4], Oleksandr Prokhnenko[4], Hiroyuki Nojiri[5], Thomas Doert[3], Bella Lake[4,6], Joachim Wosnitza[1,2], and Michael Ruck[3] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Fakultät für Chemie und Lebensmittelchemie, TU Dresden, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Berlin, Germany — [5]Institute for Materials Research, Tohoku University, Sendai, Japan — [6]Institut für Festkörperphysik, TU Berlin, Germany

Here we present a detailed magnetization and electrical-transport study of novel $RE_3Fe_3Sb_7$ compounds. We find a number of spontaneous magnetic phase transitions in a wide temperature range and a pronounced magnetic anisotropy. $RE_3Fe_3Sb_7$ shows an emergent spontaneous magnetization in zero field and a kink in the temperature-dependent resistivity at the spin-reorientation transition SRT. In the ground state, $RE_3Fe_3Sb_7$ displays a large uniaxial magnetic anisotropy that changes to planar at SRT. Our neutron scattering results reveal an unusual antiparallel alignment of Pr and Fe magnetic moments. In addition, XMCD measurements in pulsed magnetic fields up to 28 T indicate a continuous rotation of the Nd moment towards the Fe moment.

MA 12: INNOMAG e.V. Dissertationspreis / Ph.D. Thesis Prize (2021)

The Working Group Magnetism (Arbeitsgemeinschaft Magnetismus der DPG) awards a dissertation prize whose aim is to recognise outstanding research done within the framework of a doctorate and communication of this research in an excellent way, both verbally and in writing. The prize is kindly supported by INNOMAG e.V. In this finalists session, pre-selected nominees will present and defend their dissertation. Afterwards, the prize committee decides on the winner of the INNOMAG e.V. Dissertation Prize 2021 and the award of 1000 EURO.

Time: Wednesday 14:30–16:15 Location: H2

MA 12.1 Wed 14:30 H2

Emergent electrodynamics in non-collinear spin textures: skyrmions and beyond — •Börge Göbel — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

Magnetic skyrmions have attracted an enormous research interest since their discovery a decade ago. Especially the non-trivial real-space topology of these nano-whirls leads to fundamentally interesting and technologically relevant consequences like an enormous stability and the emergence of a topological Hall effect [1]. One issue, which is hindering the realization of spintronic applications, is the so-called skyrmion Hall effect: A skyrmion does not move parallel to an applied spin-polarized current. Instead, the skyrmion is pushed towards the edge of the sample where it annihilates. In this talk, I will present several ways, how this effect can be suppressed. Therefore, I will give an overview about observed or proposed alternative magnetic quasiparticles [1]. The stabilization, as well as the emergent electrodynamic effects will be discussed for the antiferromagnetic skyrmion [2], the bimeron [3] and the antiskyrmions. For the latter object I will present the observed coexistence with conventional skyrmions [4] which allows to suggest an advanced, less susceptible version of the racetrack data storage device.

[1] B. Göbel et al. Physics Reports 895, 1 (2021), [2] B. Göbel et al. PRB 96, 060406 (2017), [3] B. Göbel et al. PRB 99, 060407 (2019), [4] J. Jena, B. Göbel et al. Nature Communications 11, 1115 and Science Advances 6, eabc0723 (2020)

MA 12.2 Wed 14:55 H2

Complex magnetism of nanostructures on surfaces: from orbital magnetism to spin excitations — •Sascha Brinker — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Jülich, Germany — Department of Physics, RWTH Aachen University, Aachen, Germany

Magnetic nanostructures deposited on surfaces not only offer a promising route towards the miniaturization of future information technology devices, but also serve as ideal prototypes to explore fundamental physics at the nanoscale. In this theoretical thesis, I explore a wide range of fundamental magnetic properties in this class of materials ranging from a new component to the orbital degrees of freedom, and a new chiral interaction, which is the biquadratic equivalent of the well-known Dzyaloshinskii-Moriya interaction, to the complex dependence of the so-called Gilbert damping, which can be observed for example in the spin excitation spectrum, on the non-collinear magnetic structure. The fundamental theoretical studies are complemented by fruitful collaborations with experimental colleagues using scanning tunneling microscopy. Theoretical methods were developed and applied to describe the magnetic stability of coupled nanostructures and the emergence of boundary states in magnetic chains proximity-coupled to a superconducting substrate.

This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (ERC Consolidator Grant No. 681405 DYNASORE).

MA 12.3 Wed 15:20 H2

Robustness and Variation of Low-Dimensional Signal Transmission in Topological Phases — •Maik Malki and Götz Uhrig — Lehrstuhl Theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany

The signal transmission based on topological materials represents an important issue for the future. To this end, we investigate the variation of signal transmission in topological phases as well as their robustness in one- and two-dimensional systems by pursuing different approaches. By modifying the boundaries we show the possibilities to control the speed of signal transmission in various topological systems. Furthermore, the triplon excitations in $BiCu_2PO_6$ provide a non-trivial Zak phase while no localized edge states are present. Thus the bulk-boundary correspondence is put into perspective. Finally, present ferromagnetic Shastry-Sutherland model in order to realize topological magnon excitations.

Short break followed by bestowal of INNOMAG e.V. Dissertationspreis / Ph.D. Thesis Prize (2021)

MA 13: PhD Focus Session: Symposium on Strange Bedfellows - Magnetism Meets Superconductivity" (joint session MA/AKjDPG) (joint session MA/TT)

At first sight, it seems that the phenomena of magnetism and superconductivity do not go along, as indicated by the Meissner effect, when a magnetic field is completely expelled from the interior of a conventional superconductor. However, the synergy of these two manifestations of nature in condensed matter does occur and can be rather interesting! Theoretical works have predicted the existence of exotic states at the interface between a superconductor and a magnet, such as the sought-after Majorana fermions and spin-triplet superconductivity. The first have been predicted to route an efficient way to implement quantum computers (currently a European scientific flagship), while the latter allows the creation of spin-polarized supercurrents, opening up fundamentally new possibilities for spintronics. Therefore, our symposium aims at putting together experts to provide a fundamental and practical understanding of the subject to discuss most recent developments from the theoretical and experimental sides, and to show perspectives for applications.

Organizers: Annika Stellhorn, Flaviano José dos Santos, Markus Hoffmann (Forschungszentrum Jülich and Peter Grünberg Institut)

Time: Thursday 10:00–12:45 Location: H5

Invited Talk MA 13.1 Thu 10:00 H5

Magnetism and superconductivity: new physics one atom at a time — •Alexander Balatsky — NORDITA — UCONN

In this tutorial I will review the effects of magnetism and electronic defect in conventional and unconventional superconductors. The extreme case of quantum engineering where one builds magnetic and electronic features one atom at a time has proved to be a versatile approach. Impurities and defects are pair breakers in superconductors. I will discuss how defects can also enable new features in superconductors like intragap resonances, topological Majorana modes and seed new superconducting phases. Looking forward I will discuss how we might induce novel physics in superconductors with precise quantum impurity band engineering

MA 13.2 Thu 10:30 H5

Magnetic exchange interactions at proximity of a superconductor — •Uriel Aceves[1,2], Sascha Brinker[1], Filipe Guimaraes[3], and Samir Lounis[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany — [3]Jülich Supercomputing Centre, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

The coupling of magnetic impurities to superconductors prompts the arise of exciting physics such as sub-gap states like Yu-Shiba-Rusinov states and Majorana zero modes, which constitute key mechanisms on the road towards a topological quantum computer. The interplay of spin-orbit coupling and (non-collinear) magnetism enriches the complexity and topological nature of the in-gap states hosted in proximity-induced superconductors. However, little is known about the impact of superconductivity on the different contributions to the magnetic exchange interactions, like the bilinear isotropic exchange and the Dzyaloshinskii-Moriya interaction — and in turn the impact on the magnetic textures. In this work, we propose a method for the extraction of the tensor of exchange interactions in the superconducting regime as described by the Bogoliubov-de Gennes equations. Finally, with our multi-orbital tight-binding code TITAN, we investigate a Mn (110) monolayer deposited on the Nb (110) surface and analyze the magnetic interactions of the superconducting and metallic phases.

–Work funded by Horizon 2020–ERC (CoG 681405–DYNASORE).

Invited Talk MA 13.3 Thu 10:45 H5

Magnetic adatom chains on superconducting $NbSe_2$ — Eva Liebhaber[1], Lisa M. Rütten[1], Gael Reecht[1], Jacob F. Steiner[2], Sebastian Rohlf[3], Kai Rossnagel[3], Felix von Oppen[2], and •Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Germany — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, Germany — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany

Magnetic adatom chains on superconducting substrates constitute a fascinating platform to study the interplay of quantum magnetism and superconductivity. Here, we investigate magnetic adatom chains in the dilute limit. This means that the atoms are sufficiently far spaced that direct hybridization of their d orbitals is negligible, but close enough for sizeable substrate-mediated interactions. We build these chains from individual Fe atoms on a 2H-$NbSe_2$ substrate. Using scanning tunneling microscopy and spectroscopy we first characterize the exchange coupling between the magnetic adatoms and the superconductor by detecting their Yu-Shiba-Rusinov states within the superconducting energy gap. We then use the tip of the STM to assemble dimers, trimers and chains of these Fe atoms. In each step, we track the evolution of the Yu-Shiba-Rusinov states and identify magnetic interactions, hybridization and band formation.

MA 13.4 Thu 11:15 H5

Tuning the interaction between spins coupled to a superconductor on the atomic level — •Felix Küster[1], Ana M. Montero[2], Filipe S. M. Guimarães[2], Sascha Brinker[2], Samir Lounis[2], Stuart S. P. Parkin[1], and Paolo Sessi[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Jülich, Germany

Magnetic impurities coupled to superconducting condensates induce sharp in-gap resonances, the so-called Yu-Shiba- Rusinov (YSR) states. By reducing the distance between impurities, YSR quasiparticles can interact, hybridize, and eventually form bands. Here, we scrutinize the behavior of 3d atoms coupled to niobium by scanning tunneling microscopy and spectroscopy. We demonstrate how the coupling between spins and a superconducting condensate hosting an anisotropic Fermi surface can be tuned by varying the direction and distance between the impurities. We verify the existence of long range coupling as well as the crossing through a quantum phase transition, providing a promising platform for the emergence of topological superconductivity.

Invited Talk MA 13.5 Thu 11:30 H5

Yu-Shiba-Rusinov states and ordering of magnetic Impurities near the boundary — •Jelena Klinovaja — University of Basel, Basel, Switzerland

In my talk, I will discuss properties of one and two magnetic impurities near the boundary of a one-dimensional nanowire in proximity to a conventional s-wave superconductor. We showed that the energies of the subgap states, supported by the magnetic impurities, are strongly affected by the boundary for distances less than the superconducting coherence length. When the impurity is moved towards the boundary, multiple quantum phase transitions periodically occur in which the parity of the superconducting condensate oscillates between even and odd. The magnetic ground-state configuration of two magnetic impurities depends not only on the distance between them, but also explicitly on their distance away from the boundary of the nanowire. As a consequence, the magnetic ground state can switch from ferromagnetic to antiferromagnetic while keeping the interimpurity distance unaltered by simultaneously moving both impurities away from the boundary.

[1] O. Deb, S. Hoffman, D. Loss, and J. Klinovaja, Phys. Rev. B 103, 165403 (2021). [2] H. Ding, Y. Hu, M. T. Randeria, S. Hoffman, O. Deb, J. Klinovaja, D. Loss, and A. Yazdani, Proc. Natl. Acad. Sci. USA 118, 14 (2021). [3] S. Hoffman, J. Klinovaja, T. Meng, and D. Loss, .Phys. Rev. B 92, 125422 (2015). [4] T. Meng, J. Klinovaja, S. Hoffman, P. Simon, and D. Loss, Phys. Rev. B 92, 064503 (2015).

MA 13.6 Thu 12:00 H5

Temperature-Dependent Spin Transport and Current- Induced Torques in Superconductor-Ferromagnet Heterostructures — •Manuel Müller[1,2], Lukas Liensberger[1,2], Luis Flacke[1,2], Hans Huebl[1,2,3], Akashdeep Kamra[4], Wolfgang Belzig[5], Rudolf Gross[1,2,3], Mathias Weiler[1,2,6], and Matthias Althammer[1,2] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik- Department, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), München, Germany — [4]Norwegian University of Science and Technology, Trondheim, Norway — [5]Physik-Department, Universität Konstanz, Konstanz, Germany — [6]Fachbereich Physik, TU Kaiserslautern, Kaiserslautern, Germany

Proximity effects at superconductor(SC)/ferromagnet(FM) interfaces provide novel functionality in superconducting spintronics. We investigate the injection of spin currents in NbN/permalloy (Py) heterostructures with and without a Pt spin sink layer. Spin currents are excited by broadband ferromagnetic resonance in the Py-layer coupled inductively to a coplanar waveguide and quantitative information on the spin current physics is obtained by measuring the complex microwave transmission as a function of temperature. Our findings, reveal the symmetry and strength of spin-to-charge current conversion in SC/FM heterostructures and provide guidance for future superconducting spintronics devices. Our results are published in Phys. Rev. Lett. **126**, 087201 (2021). We acknowledge financial support by the DFG.

Invited Talk MA 13.7 Thu 12:15 H5

Resonance from antiferromagnetic spin fluctuations for spin-triplet superconductivity in UTe2 — •Pengcheng Dai — Rice University

Superconductivity has its universal origin in the formation of bound (Cooper) pairs of electrons that can move through the lattice without resistance below the superconducting transition temperature Tc. While electron Cooper pairs in most superconductors form anti-parallel spin-singlets with total spin S = 0, they can also form parallel spin-triplet Cooper pairs with S = 1 and an odd parity wavefunction. Spin-triplet pairing is important because it can host topological states and Majorana fermions relevant for fault tolerant quantum computation. However, spin-triplet pairing is rare and has not been unambiguously identified in any solid state systems. Since spin-triplet pairing is usually mediated by ferromagnetic (FM) spin fluctuations, uranium based heavy-fermion UTe2, which has a Tc * 1.6 K, has been identified as a strong candidate for chiral spin-triplet topological superconductor near a FM instability. Here we use inelastic neutron scattering (INS) to show that superconductivity in UTe2 is coupled with a sharp magnetic excitation at the Brillouin zone (BZ) boundary near AF order, analogous to the resonance seen in other exotic superconductors. We find that the resonance in UTe2 occurs below Tc at an energy Er = 7.9kBTc. Since the resonance has only been found in spin-singlet superconductors near an AF instability, its discovery in UTe2 suggests that AF spin fluctuations can also induce spin-triplet pairing for superconductivity.

MA 14: Focus Session: Higher-Order Magnetic Interactions - Implications in 2D and 3D Magnetism II

Materials in which the magnetic moments order or cooperate in unusual ways underpin a plethora of physical phenomena, from strong magnetoelectric effects to topological quasiparticles, thus holding great promise for future spintronic and quantum computing applications. Magnetic interactions are the fundamental quantities that explain the complex magnetic phase diagrams and exotic excitation spectra of these intriguing materials. Recent theoretical and experimental developments have led to a realization of a pivotal role played by higher-order magnetic interactions in stabilizing intricate magnetic structures. The 4-spin 3-site interaction stabilizes an up-up-down-down state, which can become chiral. Theoretically, novel 4-spin chiral interactions and even 6-spin (chiral-chiral) couplings might explain the emergence of complex short-period 3D magnetic structures, and could open a path to the discovery of materials hosting 3D topological magnetization textures, such as magnetic hopfions. Experimentally, 4-spin interactions are conjectured to play a central role in skyrmions lattice formation in frustrated centrosymmetric materials. This area of research will make a strong impact in the field of magnetism in the upcoming years.

Organizers: Samir Lounis (University of Duisburg-Essen and Forschungszentrum Jülich), Manuel dos Santos Dias and Stefan Blügel (Forschungszentrum Jülich), Jonathan White (Paul Scherrer Institut)

Time: Thursday 13:30–15:15 Location: H5

Invited Talk MA 14.1 Thu 13:30 H5

The role of itinerant electrons and higher order magnetic interactions among fluctuating local moments in metallic magnets — •Julie Staunton — University of Warwick, Coventry CV4 7AL, U.K.

When external stimuli or varying temperature alter its magnetic properties, a metal's complex electronic fluid, with its emergent magnetic 'local moments', transforms. The itinerant electrons, coupled to these more localised spin degrees of freedom, have a profound effect on structure, electronic transport, and so on. The ab initio Density Functional Theory-based Disordered Local Moment method successfully describes this physics. It can locate and characterise magnetic phase transitions and calculate temperature and field-dependent magnetic properties. It will be shown how the theory provides a Gibbs free energy function of local moment order parameters with two central objects - local moment correlation functions in the paramagnetic state and local internal magnetic fields as functions of magnetic order. The potentially most stable magnetic phases and dominant 'exchange' interactions between pairs of local moments or effective 'spins' are identifiable from the first. Higher order magnetic interactions are extracted from the second and depend on how the electronic structure evolves with the state and extent of magnetic order. The approach will be illustrated by applications to the magnetic order and its link to the Fermi surfaces of rare earth metals and their compounds, permanent magnetic properties and the rich magnetic-strain phase diagrams and associated caloric effects of some transition metal antiferromagnets.

MA 14.2 Thu 14:00 H5

Short period magnetization texture of B20-MnGe explained by thermally fluctuating local moments — •Eduardo Mendive Tapia[1,2], Manuel dos Santos Dias[1], Sergii Grytsiuk[1], Julie Staunton[3], Stefan Blügel[1], and Samir Lounis[1] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany — [3]University of Warwick, CV4 7AL, Conventry, UK

B20-type compounds, such as MnSi and FeGe, host helimagnetic and skyrmion phases at the mesoscale, which are canonically explained by the combination of ferromagnetic isotropic interactions with weaker chiral Dzyaloshinskii-Moriya ones. Mysteriously, MnGe evades this paradigm as it displays a noncollinear magnetic state at a much shorter nanometer scale [1]. Using a Disordered Local Moment theory within the KKR method [2,3], here we show that the length scale and volume-dependent magnetic properties of MnGe stem from purely isotropic exchange interactions generally obtained in the paramagnetic state. Our approach is validated by comparing MnGe with the canonical B20-helimagnet FeGe. The free energy of MnGe is calculated, from which we show how triple-q magnetic states can stabilize by adding higher-order interactions. –Work funded by the DAAD and EU Horizon 2020 via ERC-consolidator Grant No. 681405-DYNASORE.

[1] Fujishiro et al., Nat. Commun. **10**, 1059 (2019)
[2] Gyorffy et al., J. of Phys. F: Metal Phys. **15**, 1337 (1985)
[3] Jülich KKR codes (https://jukkr.fz-juelich.de)

MA 14.3 Thu 14:15 H5

Symmetry analysis of multi-spin interactions — •Levente Rózsa — University of Konstanz, Konstanz, Germany

Two-spin interactions including the isotropic exchange and Dzyaloshinsky-Moriya (DM) interactions or the magnetocrystalline anisotropy play a fundamental role in the formation of non-collinear spin structures. Going beyond the two-spin approximation enables the stabilization of, e.g., the zero-field nanoskyrmion lattice attributed to four-spin isotropic interactions [1]. A four-spin generalization of the DM interaction has also been proposed recently [2,3,4].

Multi-spin interactions are conventionally derived based on a perturbative expansion [2,4], which becomes cumbersome if many spins or higher orders of the spin-orbit coupling are involved. Here we present a systematic way of constructing multi-spin interaction terms based on a symmetry analysis. In the case of four spins, besides the isotropic and DM interactions, we identify symmetric second-order and fourth-order anisotropies, as well as a DM-like asymmetric anisotropy term. It is discussed how these coupling terms transform under point group operations, analogously to the Moriya rules; how they can be fitted based on the energies of specific spin configurations; and which types of non-collinear structures emerge based on these interactions.

[1] S. Heinze et al., Nat. Phys. 7, 713 (2011).
[2] S. Brinker et al., New J. Phys. 21, 083015 (2019).
[3] A. Lászlóffy, L. Rózsa et al., Phys. Rev. B 99, 184430 (2019).
[4] S. Grytsiuk et al., Nat. Commun. 11, 511 (2020).

MA 14.4 Thu 14:30 H5

Spontaneous atomic-scale hexagonal spin lattices driven by higher-order exchange interactions — •Mara Gutzeit[1], André Kubetzka[2], Soumyajyoti Haldar[1], Henning Pralow[1], Roland Wiesendanger[2], Stefan Heinze[1], and Kirsten von Bergmann[2] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstraße 15, 24098 Kiel, Germany — [2]Department of Physics, University of Hamburg, 20355 Hamburg, Germany

Higher-order exchange interactions (HOI) beyond the pair-wise Heisenberg exchange can be the origin of a variety of complex magnetic structures such as conical spin spirals [1], multi-Q states [2,3], or nanoskyrmion lattices [4]. Here, using spin-polarized scanning tunneling microscopy we explore uniaxial spin states as well as two-dimensionally modulated spin structures in ultrathin Fe/Rh films on the Ir(111) surface. Density functional theory calculations elucidate how HOI stabilize spontaneous atomic-scale hexagonal spin lattices exhibiting only a small deviation from collinearity in these systems which are characterized by a weak Dzyaloshinskii-Moriya interaction. We demonstrate that a subtle interplay of HOI is responsible for the transition between different magnetic ground states.

[1] Yoshida *et al.* PRL **108**, 087205 (2012)
[2] Krönlein *et al.* PRL **120**, 207202 (2018)
[3] Spethmann *et al.* PRL **124**, 227203 (2020)
[4] Heinze *et al.* Nat. Phys. **7**, 713 (2011)

MA 14.5 Thu 14:45 H5

Dzyaloshinskii-Moriya Interaction revisited — •Hiroshi Katsumoto and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In recent years, the Dzyaloshinskii-Moriya interaction (DMI) has received enormous attention. New materials, new physical issues, and new measurement methods have led to new questions. *E.g.*, recent theoretical studies have proposed higher-order interaction terms for this DMI [1]. Introduced by Dzyaloshinskii [2] on the basis of phenomenological and group-theoretical arguments in combination with classical axial vectors and substantiated by Moriya [3] for the first time microscopically based on the quantum mechanical spin-orbit interaction, in systems where the inversion symmetry is locally broken, the DMI affects the magnetic properties. We reiterate the cause of weak ferromagnetism in centrosymmetric materials and investigate the relationship between the Lifshitz invariant associated with macroscopic chiral symmetry breaking and microscopic DMI. We will discuss how to uniquely write down the interaction term in the spin Hamiltonian from the irreducible representation depending on the size of the spin.

We acknowledge funding from the DARPA TEE program through grant MIPR (#HR0011831554) from DOI, and Deutsche Forschungsgemeinschaft (DFG) through SPP-2137 and SFB-1238 (project C1).

[1] S. Brinker, *et al.*, New J. Phys. **21**, 083015 (2019).
[2] I.E. Dzialoshinskii, Sov. Phys. JETP **5**, 1259 (1957).
[3] T. Moriya, Phys. Rev. **120**, 91 (1960).

MA 14.6 Thu 15:00 H5

Chiral multi-site interactions in prototypical magnetic systems — •Sascha Brinker[1], Manuel dos Santos Dias[1], and Samir Lounis[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany

Atomistic spin models can successfully explain the properties of magnetic materials once the relevant magnetic interactions are identified. Recently, new types of chiral interactions that generalize the Dzyaloshinskii-Moriya interaction have been proposed [1,2,3,4]. Here, we present a systematic construction of a generalized spin model containing isotropic and chiral multi-site interactions, motivated by a microscopic model, and their symmetry properties are established. We show that the chiral interactions arise solely from the spin-orbit interaction and that the multi-site interactions do not have to follow Moriya's rules, unlike the Dzyaloshinskii-Moriya interaction [1,4]. We then report on density functional theory calculations for prototypical magnetic systems, finite magnetic nanostructures on heavy metal substrates and two-dimensional systems with inversion symmetry.

[1] S. Brinker, M. dos Santos Dias and S. Lounis, New J Phys **21**, 083015 (2019)
[2] A. Lászlóffy *et al.*, Phys Rev B **99**, 184430 (2019)
[3] S. Grytsiuk *et al.*, Nat Commun **11**, 511 (2020)
[4] S. Brinker, M. dos Santos Dias and S. Lounis, Phys Rev Research **2**, 033240 (2020)

Work funded by Horizon 2020–ERC (CoG 681405–DYNASORE).

MA 15: Posters Magnetism IV

Topics: Ultrafast Magnetization Effects (15.1-15.15), Caloric Effects in Ferromagnetic Materials (15.16-15.22), Spin Calorics (general) (15.23), Functional Antiferromagnetism (15.24-15.25), Magnetic Heuslers (15.26-15.31), Complex magnetic oxides (15.32), Bulk Materials: Soft and Hard Permanent Magnets (15.33-15.35), Disordered Magnetic Materials (15.36-15.39), Multiferroics and Magnetoelectric Coupling (15.40-15.44), Magnetic Domain Walls (non-skyrmionic)(15.45-15.47)

Time: Thursday 13:30–16:30 Location: P

MA 15.1 Thu 13:30 P

Coherent all-optical switching of an antiferromagnet — •Tobias Dannegger[1], Marco Berritta[2], Karel Carva[3], Severin Selzer[1], Ulrike Ritzmann[2,4], Peter M. Oppeneer[2], and Ulrich Nowak[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden — [3]Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Ke Karlovu 5, CZ-121 16 Prague, Czech Republic — [4]Dahlem Center of Complex Quantum Systems and Department of Physics, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

The physics of ultrafast magnetisation switching holds great potential for future magnetic storage applications. Much research has been conducted on ferro- and ferrimagnetic switching but more recent progress in spintronics has begun to utilise the advantages of antiferromagnets, such as robustness against external magnetic fields and high-frequency spin dynamics. Based on density functional theory calculations and atomistic spin dynamics simulations, we show, using the example of the easy-plane antiferromagnet CrPt, that the properties of antiferromagnets allow for a coherently induced ultrafast all-optical switching process that does not require the thermally induced demagnetisation of the material. This process is facilitated by the inverse Faraday effect, which, as our calculations reveal, induces staggered magnetic moments in the material. This can be used to achieve controllable switching between two perpendicular magnetisation states.

MA 15.2 Thu 13:30 P

Spin Dynamics in Magnetic Nanojunctions — •Rudolf Smorka[1], Martin Žonda[2], and Michael Thoss[1] — [1]Institute of Physics, Albert-Ludwigs-Universität Freiburg, Germany — [2]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University Prague, Czech Republic

Recent experimental advances of atomic and nanoscale magnetism motivate the study of spin dynamics on ultrafast time scales. In this contribution, we use a quantum-classical hybrid approach to study current-driven magnetization dynamics in systems consisting of tight-binding electrons and localized classical spins. Using this approach, we show that both the electronic structure of the central system and the self-consistent feedback of spin and electron dynamics play a significant role in the dynamical properties of magnetic nano-junctions with applied dc voltage. Specifically, relaxation dynamics can be enhanced by tuning the dc voltage in resonance with electronic levels of the central system. We analyze this characteristic in nano-junctions containing a single classical Kondo impurity. Furthermore, we investigate current-induced spin-transfer-torques (STT) in a ferromagnetic spin valve far away from equilibrium and show that electronic levels in the bias window lead to an enhancement of the STT.

MA 15.3 Thu 13:30 P

Tuning all-optical magnetization switching efficiency by laser pulse wavelength variation — •Marcel Kohlmann[1], Krystina Hvorakova[1], Jakob Walowski[1], Robin John[1], Cai Müller[2], Marco Berrita[3], Deninse Hinzke[4], Pablo Nieves[5], Oksana Chubykalo-Fesenko[5], Tiffany Santos[6], Henning Ulrichs[7], Ritwik Mondal[3,4], Peter M Oppeneer[3], Ulrich Nowak[4], Jeffrey McCord[2], and Markus Münzenberg[1] — [1]Greifswald University — [2]Kiel University — [3]Uppsala University — [4]Konstanz University — [5]CISC Madrid — [6]HGST Western Digital — [7]Göttingen University

The annual growth of created, transferred and stored data demands the development of new storage media with higher data storage density. Heat-assisted magnetic storage devices (HAMR) present a promising candidate for this application. Hence investigation of magnetization manipulation remains a topic of interest for research and development. We therefore study all-optical-helicity-dependent switching of FePt granular media which is a prominent candidate material for the development of HAMR devices. We calculated the switching rates for individual FePt nanoparticles in ab-initio calculations of inverse Faraday effect and magnetic dichroism induced heating which provided us with a model to describe the switching as a stochastic process. With this theoretical description we optimize the number of laser shots, fluence and wavelengths to all-optically switch FePt grains. First experiments show, that tuning wavelengths requires simultaneous fluence adjustment due to the increased photon absorption for larger wavelengths.

MA 15.4 Thu 13:30 P

Investigation of ultrafast laser-induced toggle-switching and domain wall motion in GdF — •Rahil Hosseinifar[1], Ivar Kumberg[1], Evangelos Golias[1], Sangeeta Thakur[1], Karl Frischmuth[1], Florian Kronast[2], Mario Fix[3], Manfred Albrecht[3], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [3]Institut für Physik, Universität Augsburg, Universitätsstraße 1, Building R, Level 4, 86159 Augsburg, Germany

Using purely optical means to manipulate the magnetization direction is an exciting way to introduce new potential applications in spintronic devices. We study 15 nm thin films of ferrimagnetic $Gd_{26}Fe_{74}$ with out-of-plane easy axis of magnetization by x-ray magnetic circular dichroism photoelectron emission microscopy. Individual linearly polarized laser pulses of 800 nm wavelength above a specific threshold fluence reverse the sample magnetization, independent of the magnetization direction, the so-called toggle switching. Local deviations from this deterministic behavior close to magnetic domain walls are studied. Reasons for nondeterministic toggle switching are related to extrinsic effects caused by pulse-to-pulse variations of the exciting laser system and intrinsic effects related to the magnetic domain structure of the sample. We point out intrinsic effects such as laser-induced domain-wall motion in the toggle switching and magnetic domain-wall elasticity, which cause local deviations from purely deterministic toggle switching.

MA 15.5 Thu 13:30 P

Ultrafast demagnetization dynamics including spin-, charge- and heat-transport. — •Sanjay Ashok, Sebastian T. Weber, Christopher Seibel, Johan Briones, and Bärbel Rethfeld — Fachbereich Physik and OPTIMAS Research Center, TU Kaiser- slautern, Kaiserslautern, Germany

Ultrafast Demagnetization of metallic ferromagnets induced by femtosecond laser is usually studied in homogeneously heated thick films. In such cases, due to absence of temperature and density gradients within the material, there are no heat- or charge-currents. For thicker magnetic metals, the heating is not uniform and spin-, charge- and heat-transport contribute to ultrafast de- and re- magnetization. Here we study the role of spin-resolved charge and heat transport in ultrafast demagnetization of thick magnetic metal using the thermodynamic μT-model [1] and obtain spatial and temporal evolution of magnetization. We also study the role of transport for the relation between quenching and quenching time. Further, we analyze the different transport mechanisms and their contributions to measureable quantities.

[1] B. Y. Mueller and B. Rethfeld, Phys. Rev. B 90, 144420 (2014).

MA 15.6 Thu 13:30 P

Electron-magnon scattering dynamics in a two-band Stoner model — •Felix Dusabirane, Marius Weber, and Hans Christian Schneider — TU Kaiserslautern, Kaiserslautern, Germany

We theoretically study electronic scattering dynamics in a Stoner model with two spin-split bands. We include electron-magnon scattering together with Coulomb electron-electron scattering in order to describe incoherent hot-electron dynamics at sub-picosecond and picosecond timescales after ultrashort-pulse excitation in an itinerant ferromagnet. The optical excitation process is assumed to be instantaneous and the electronic dynamics is described at the level of equations of motion for momentum-dependent distribution functions together with time-dependent Fermi's Golden rule scattering rates. The magnons are treated as a bosonic bath.

We analyze the effect on the electronic spin-polarization dynamics of phase-space filling at different excitation conditions, as well as the magnitude of the Stoner splitting.

MA 15.7 Thu 13:30 P

Wavelength dependency in ultrafast magnetization dynamics of Nickel — •Martin Stiehl, Marius Weber, Christopher Seibel, Jonas Hoefer, Bärbel Rethfeld, Hans Schneider, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Kaiserslautern, Germany

We revisit the problem of the influence of optical excitation conditions on ultrafast magnetization dynamics. In this contribution, we combined a theoretical analysis of the excitation and electron dynamics with time-resolved magneto-optical Kerr effect (tr-MOKE) studies to uncover the role played by the different pump-photon energies for ultrafast demagnetization in thin Ni films (10nm) on the insulating substrate MgO. We use a time-dependent Fermis Golden Rule approach to model the absorption and the temperature-based μ-T model for the subsequent incoherent electron dynamics. For a fixed absorbed energy one obtains rather different minority and majority carrier distributions for pump photon energies in the range from 0.5eV to 2.5eV. In contrast, we find identical tr-MOKE dynamics for all corresponding pump photon energies. The shape and fluence dependence of these photon energy dependent traces can be described well by our theoretical model. Our observations suggest a negligible influence of the details of the excited hot carrier distributions on the ultrafast demagnetization. Rather, the photon energy dependence of ultrafast demagnetization of Ni seems to be dominated by the deposited energy and quasi-thermal behavior of the electron system.

MA 15.8 Thu 13:30 P

Disentangling the Ultrafast Magnetization Dynamics in Magnet/Non-Magnet Bilayer Systems — •Jonas Hoefer, Martin Stiehl, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Kaiserslautern, Germany

In the last 20 years, different all-optical techniques based on the magneto-optical Kerr effect (MOKE) were employed to study the ultrafast magnetization dynamics of magnetic thin films, alloys and multilayer structures. While conventional time-resolved (tr) MOKE studies provided the insights into the microscopic mechanisms governing the loss of magnetic order in simple materials, tr-MOKE experiments with fs-XUV radiation provided an understanding of the element specific magnetization dynamics of composite materials. The most recent progress in tr-MOKE experiments is the implementation of the so-called C-MOKE approach. It utilizes the complex nature of the material specific Kerr response (KR) to disentangle the magnetization dynamics of magnetic/non-magnetic multilayer structures. A crucial ingredient for the separation of the magnetization dynamics of all layers is, however, the precise value of the KR of the transiently spin-polarized non-magnetic layers that is often only available from theory.

Here we present a new strategy to experimentally determine the KR of a transiently magnetized gold layer in a Permalloy (Py)/gold (Au) heterostructure after optical excitation. This allows us to disentangle the layer specific magnetization dynamics of both materials and thus to discuss the spin transport across the Py/Au interface.

MA 15.9 Thu 13:30 P

Efficient spin excitation via ultrafast damping torques in antiferromagnets
— •Christian Tzschaschel[1,2], Takuya Satoh[3], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Department of Chemistry and Chemical Biology, Harvard University, USA — [3]Department of Physics, Tokyo Institute of Technology, Japan

Damping effects form the core of many emerging concepts for high-speed spintronic applications. Important characteristics such as device switching times and magnetic domain-wall velocities depend critically on the damping rate. While the implications of spin damping for relaxation processes are intensively studied, damping effects during impulsive spin excitations are assumed to be negligible because of the shortness of the excitation process. Here we show that, unlike in ferromagnets, ultrafast damping plays a crucial role in antiferromagnets because of their strongly elliptical spin precession. In time-resolved measurements, we find that ultrafast damping results in an immediate spin canting along the short precession axis. The interplay between antiferromagnetic exchange and magnetic anisotropy amplifies this canting by several orders of magnitude towards large-amplitude modulations of the antiferromagnetic order parameter. Exemplarily, we consider optical spin excitations in antiferromagnetic hexagonal $R\mathrm{MnO}_3$ via the inverse Faraday effect. We find that a so far overlooked damping torque can even provide the dominant excitation mechanism. We thus disclose a highly efficient route towards the ultrafast manipulation of magnetism in antiferromagnetic spintronics.

MA 15.10 Thu 13:30 P

Dispersion relation of nutation surface spin waves in ferromagnets —
•Mikhail Cherkasskii[1], Michael Farle[1,2], and Anna Semisalova[1] — [1]Faculty of Physics, University of Duisburg-Essen, Duisburg, 47057, Germany — [2]Kirensky Institute of Physics, Federal Research Center KSC SB RAS, Russia

Recently, it has been theoretically and experimentally demonstrated that the effects of inertia of magnetization should be considered in the full description of spin dynamics at pico- and femtosecond timescales [1-4]. The nutation motion of magnetization is a manifestation of inertia of the magnetic moments. A rigorous derivation including inertia in the Landau-Lifshitz-Gilbert equation was carried out by Mondal et al. in the Dirac-Kohn-Sham framework [3]. In this presentation, we show that inertia effect in magnetization dynamics results in a new type of spin waves, i.e. nutation surface spin waves, which propagate at terahertz frequencies in in-plane magnetized ferromagnetic thin films. Considering the magnetostatic limit, i.e. neglecting exchange coupling, we calculate dispersion relation and group velocity, which we find to be slower than the velocity of conventional (precession) spin waves. In addition, we find that the nutation surface spin waves are backward spin waves [1].

[1]*M. Cherkasskii, M. Farle, and A. Semisalova, Phys. Rev. B 103, 174435 (2021). [2]*M. Cherkasskii, M. Farle, and A. Semisalova, Phys. Rev. B 102, 184432 (2020). [3]*R. Mondal, M. Berritta, A. K. Nandy, and P. M. Oppeneer, Phys. Rev. B 96, 024425 (2017). [4]*K. Neeraj et al, Nat. Phys. 17, 245 (2021).

MA 15.11 Thu 13:30 P

Imprinting chirality in an antiferromagnetic spin chain with ultrafast laser —
•Sumit Ghosh[1,2], Frank Freimuth[1,2], Olena Gomonay[2], Stefan Blügel[1], and Yuriy Mokrousov[1,2] — [1]PGI-1 and IAS-1, Forschungszentrum Jülich, Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg-University Mainz, Germany

Recent experimental generation of skyrmions with ultrafast laser pulses [1] has opened new horizons in ultrafast generation of chiral magnetic order. However, the theoretical understanding of the underlying physics is still under mist which poses a hurdle in further manipulation of laser induced chirality. We present here a complete picture of the laser induces chirality generation by combining the classical magnetisation dynamics with quantum evolution of states which reveals the pertinent features of fast electron dynamics as well as slow magnetisation dynamics leading to the formation of a chiral structure [2]. We have successfully identified the emergent electronic interactions resulting the formation of the chiral structure which can survive for nanoseconds. We demonstrate the distinction between the dynamics initiated by a thermal re-population, and the laser excited dynamics and also show how to manipulate the end states by tuning the laser parameter. Our findings are fairly robust against thermal fluctuation which makes them feasible for experimental realisation and thus open new ways to explore the intertwined optical and magnetisation dynamics.

[1] F. Büttner et al. Nat. Mater. 20, 30-37 (2021).

[2] S. Ghosh, F. Freimuth, O. Gomonay, S. Blügel, Y. Mokrousov, arXiv:2011.01670.

MA 15.12 Thu 13:30 P

Ultrafast light-induced torques and Hall effects driven by laser pulses in thin films —
•Hanan Hamamera[1,2], Filipe Souza Mendes Guimaraes[3], Mnauel dos Santos Dias[1], and Samir Lounis[1,4] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Department of Physics, RWTH Aachen University, 52056 Aachen, Germany — [3]Jülich Supercomputing Centre, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [4]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany

Effective control of the magnetization at ultrafast timescale using lasers have the capacity to revolutionize future technology devices. Based on realistic time-dependent electronic structure simulations [1], we have shown that the polarization of laser pulses are determinant to switch the magnetization via the inverse-Faraday like effect [1]. Even the magnetization of an elementary magnet such as bulk Ni can be reversed due to ultrafast light-induced torques. We extended this work to Co films on Pt(001), where various ultrafast Hall effects in conjunction with the inverse-Faraday effect dictate the observed complex magnetization dynamics. We discuss these phenomena in the light of the unveiled mechanisms and proceed to a systematic comparison with previous works.

— Work funded by the Palestinian-German Science Bridge (BMBF–01DH16027) and Horizon 2020–ERC (CoG 681405–DYNASORE).

[1] H. Hamamera *et al.*, arXiv:2104.13850 (2021).

MA 15.13 Thu 13:30 P

Nutational switching in ferromagnets and antiferromagnets —
•Lucas Winter, Levente Rózsa, Sebastian Grossenbach, and Ulrich Nowak — University of Konstanz , Konstanz, Germany

For magnetic memory devices, precessional switching is a promising new way of writing data. However, on ultra-short timescales, recent research[1] indicates that the magnetization does not only exhibit precession but also nutation. Here, we investigate how nutation can contribute to spin switching. We use analytic theory and atomistic spin simulations to discuss the behavior of ferromagnets and antiferromagnets in high-frequency magnetic fields. In ferromagnets, linearly polarised fields align the magnetization perpendicular to the external field, enabling 90° switching. For circularly polarized fields in the xy plane, the magnetization tilts to the z direction. During this tilting, it rotates around the z axis, allowing 180° switching. In antiferromagnets, external fields with frequencies higher than the nutation frequency align the order parameter parallel to the magnetic field direction, while for lower frequencies it is oriented perpendicular to the field.

The switching frequency increases with higher magnetic field strengths, but it deviates from the Larmor frequency characteristic for precessional switching. High field strengths are required to outpace precessional switching. Furthermore, nutational switching requires low temperatures to be observable.

[1] K. Neeraj et al., Nat. Phys. 17, 245 (2021).

MA 15.14 Thu 13:30 P

Spectroscopic Analysis of the Ultrafast Non-Equilibrium Dynamics in Nickel at the European X-Ray Free-Electron Laser —
•T. Lojewski[1], N. Rothenbach[1], Y. Kvashnin[2], L. Le Guyader[3], B. Van Kuiken[3], R. Carley[3], J. Schlappa[3], R. Gort[3], G. Mercurio[3], A. Yaroslavtsev[3], N. Gerasimova[3], M. Teichmann[3], L. Mercadier[3], R. Y. Engel[4], P. Miedema[4], L. Spieker[1], F. Döring[5], B. Rösner[5], F. De Groot[6], P. Thunström[2], O. Granäs[2], J. Jönsson[2], C. Lambert[7], I. Pronin[8], J. Rezvani[9], M. Pace[10], C. Boeglin[10], C. Stamm[7,11], M. Beye[4], C. David[5], O. Eriksson[2], A. Scherz[3], U. Bovensiepen[1], H. Wende[1], K. Ollefs[1], and A. Eschenlohr[1] — [1]Univ. Duisburg-Essen and CENIDE — [2]Uppsala Univ. — [3]European XFEL — [4]DESY — [5]PSI — [6]Utrecht Univ. — [7]ETH Zürich — [8]ITMO Univ. — [9]INFN — [10]Univ. of Strasbourg — [11]FHNW

X-ray absorption spectroscopy has become a valuable technique to study non-equilibrium dynamics due to its sensitivity to electronic and lattice dynamics combined with its element-specificity. The SCS instrument of the European X-ray free-electron laser offers unprecedented energy resolution and dynamic range in X-ray absorption spectra and their pump-induced changes. We report the time-resolved, spectroscopic analysis at the $\mathrm{L}_{2,3}$-edges of nickel-metal obtained in transmission geometry. This spectroscopic analysis was combined with *ab initio* DFT calculations. We find redshifts and reduced peak intensities of the pumped spectra, which can be related to a reduction of the magnetic moment and an electronic redistribution, respectively.

MA 15.15 Thu 13:30 P

Wavelength-dependent magnetization dynamics in Ni|Au bilayers —
•Christopher Seibel, Marius Weber, Martin Stiehl, Sebastian T. Weber, Martin Aeschlimann, Benjamin Stadtmüller, Hans Christian Schneider, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany

Existing experimental and theoretical studies of ultrafast demagnetization in ferromagnets rely mostly on only one fixed wavelength to excite the sample. However, recent experiments indicate that the dynamics of the demagnetization and remagnetization process depend on the wavelength of the exciting laser pulse [V. Cardin et al., Phys. Rev. B **101**, 054430 (2020); U. Bierbrauer et al., JOP: Cond. Mat. **29**, 244002 (2017)].

We extend the temperature-based μT-model to describe the ultrafast magnetization dynamics of magnetic/non-magnetic bilayer systems. Our theoretical model relies on realistic densities of states of both materials. It includes energy and spin transfer at the interface as well as the layer and wavelength dependent absorption of the pump pulses.

For the exemplary case of a thin nickel layer on a gold substrate, we find a faster and larger loss of the magnetic order of Ni when increasing the wavelength from 360 nm to 800 nm. Our theoretical predictions are confirmed by time-resolved MOKE experiments. This allows us to discuss the influence of energy and spin transfer processes for the photon energy dependent magnetization dynamics of magnetic bi- and multilayer structures.

MA 15.16 Thu 13:30 P

The local magnetic moment and vibrational properties of Sn in NiMnSn-Heusler alloys during magnetostructural phase transition — •Benedikt Eggert[1], Benedikt Beckmann[2], Johanna Lill[1], Tobias Lojewski[1], Simon Rauls[1], Franziska Scheibel[2], Andreas Taubel[2], Olga Miroshkina[1], Katharina Ollefs[1], Richard Brand[1], Michael Hu[3], Markus Gruner[1], Oliver Gutfleisch[2], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]Functional Materials, TU Darmstadt — [3]Argonne National Laboratory, USA

Materials with first-order magnetostructural phase transition exhibit a large magnetocaloric effect and may lead to environmentally friendly and more energy efficient alternative to conventional vapor compression refrigeration. The investigated NiMnSn Heusler alloy exhibits a first order phase transition from low temperature ferrimagnetic martensite to high temperature ferromagnetic austenite phase. We performed ^{119}Sn nuclear resonant inelastic X-ray scattering (NRIXS) and ^{119}Sn Mössbauer spectroscopy along the phase transition to track the evolution of lattice dynamics and the local magnetic moment, respectively, during this transition. Sn-NRIXS indicates variations in the phonon density of states that lead to a reduction of the Sn-selective vibrational entropy and a softening of the lattice in the austenite phase. On the other side, Sn-Mössbauer spectroscopy indicates an increase of the induced Sn-moment, showing that the magnetic structure changes. We acknowledge the financial support through the DFG (CRC/TRR270) and the U.S. DOE.

MA 15.17 Thu 13:30 P

Ferromagnetic to paramagnetic transition of $SrRuO_3$ under pressure — •Anh Tong[1], Pau Jorba[1], Marc Seifert[1], Stefan Kunkemöller[2], Kevin Jenni[2], Markus Braden[2], James S. Schilling[1], and Christian Pfleiderer[1] — [1]Technische Universität München, James-Franck-Str.1, D-85748 Garching — [2]Universität zu Köln, Zülpicher Str.77, D-50937 Köln

In the Ruddlesden-Popper perovskite series, $Sr_{n+1}Ru_nO_{3n+1}$, intense experimental and theoretical efforts have been dedicated to unravel the nature of unconventional superconductivity in single-layer Sr_2RuO_4 ($n = 1$) as well as a putative electronic nematic phase masking the quantum critical end-point in the double-layer itinerant metamagnet $Sr_3Ru_2O_7$ ($n = 2$). We report an experimental study of the zero temperature ferromagnetic to paramagnetic transition under pressures up to 20 GPa in high quality single crystals of the infinite layer itinerant ferromagnet SrRuO3 ($n = \infty$). Our study aims to reconcile the properties of $Sr_3Ru_2O_7$ and Sr_2RuO_4 with the generic temperature-pressure-magnetic field phase diagram of itinerant ferromagnets.

MA 15.18 Thu 13:30 P

Microstructural aspects of multicaloric cooling using magnetic fields and uniaxial stress in Ni-Mn-In Heusler compounds — •Lukas Pfeuffer[1], Adrià Gràcia-Condal[2], Tino Gottschall[3], David Koch[1], Enrico Bruder[1], Jonas Lemke[1], Andreas Taubel[1], Franziska Scheibel[1], Konstantin Skokov[2], Lluís Mañosa[2], Antoni Planes[1], and Oliver Gutfleisch[1] — [1]Technical University of Darmstadt, 64287 Darmstadt, Germany — [2]Universitat de Barcelona, 08028 Barcelona, Catalonia, Spain — [3]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Ni-Mn-based Heusler compounds exhibit giant magneto- and elastocaloric effects, but suffer from irreversibilities during cyclic operation due to their large thermal hysteresis. A promising way to improve cyclic performance is the sequential combination of magnetic field and uniaxial stress in an "exploiting-hysteresis cycle" which utilizes thermal hysteresis rather than avoiding it.

We have studied the influence of microstructure on the caloric response to magnetic fields, uniaxial stress and their combination in an exploiting-hysteresis cycle for Ni-Mn-In. By correlating XRD, EBSD and stress-strain data, a significant effect of grain orientation on the stress-induced martensitic transformation is revealed. Strain measurements in pulsed magnetic fields exhibit a substantial impact of grain size on the magnetic-field-induced transformation dynamics. We show that for an optimized microstructure, the maximum cyclic effect in magnetic fields of 1.9 T can be increased by more than 200 % to -4.1 K when a moderate sequential stress of 55 MPa is applied.

MA 15.19 Thu 13:30 P

Functional Properties of Ni-Mn-based Heusler alloys — •Olga Miroshkina[1,2], Markus Ernst Gruner[1], Vasiliy Buchelnikov[2], and Vladimir Sokolovskiy[2] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Condensed Matter Physics Department, Chelyabinsk State University, 454001 Chelyabinsk, Russia

Multifunctional materials exhibiting the magnetocaloric effect (MCE) at first-order phase transitions are subject to intense fundamental and applied research as a more efficient and ecologically friendly alternative to conventional compressor devices. The combination of density functional theory and empirical models has proven as a useful tool in the theory-guided search for optimized MCE materials with large entropy and temperature change together with low temperature hysteresis. In this work, we consider a statistical model based on the theory of diffuse phase transitions, the Bean-Rodbell model of first-order phase transitions, and the molecular mean-field approach. The proposed model is applied to Ni-Mn-(Ga,In) Heusler alloys demonstrating different sequences of the magnetic and structural phase transitions. We modeled the temperature dependence of magnetization and magnetic entropy change under externally applied magnetic field and pressure and perform the comparison with available experimental data.

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MA 15.20 Thu 13:30 P

Non-hysteretic first-order ferromagnetic transitions by itinerant electron feedback and Fermi surface topology change — •Eduardo Mendive Tapia[1,2], Durga Paudyal[3], Leon Petit[4], and Julie Staunton[2] — [1]Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany — [2]University of Warwick, CV4 7AL, Coventry, UK — [3]The Ames Laboratory, U.S. Dept of Energy, Iowa State University, USA — [4]Daresbury Laboratory, Warrington, UK

Refrigeration and air conditioning are crucial in modern life and in adapting to climate change. Discontinuous magnetic phase transitions have great promise for new, energy efficient and environmentally friendly solid-state cooling technology. Huge exploitable entropy and temperature changes typically result from the coupling between a material's spin polarized interacting electrons and the crystal structure. Such magnetostructurally driven cooling, however, is nearly always degraded by hysteresis. We present an *ab-initio* theory which can find mechanisms for first-order magnetic phase transitions that are purely electronic in origin [1], thus avoiding the need for magnetostructural effects. We show that this electronic mechanism arises from an itinerant electron feedback to magnetic order. In particular, it is demonstrated that a topological change of the Fermi surface explains the hysteresis free giant cooling properties recently measured in Eu_2In [2]. This work is funded by the EPSRC (UK) and the U.S. Dept of Energy, and forms part of the PRETAMAG project (University of Warwick).

[1] E Mendive-Tapia and J Staunton, PRB **101**, 174437 (2020)
[2] F Guillou et al., Nat. Comm. **9**, 2925 (2018)

MA 15.21 Thu 13:30 P

Large magnetic entropy change in Nd2In near the boiling temperature of natural gas — •Wei Liu[1], Franziska Scheibel[1], Tino Gottschall[2], Eduard Bykov[2], Imants Dirba[1], Konstantin Skokov[1], and Oliver Gutfleisch[1] — [1]Funktionale Materialien, Technische Universität, TU Darmstadt, Germany — [2]Hochfeld- Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, Germany

In the great transformation from fossil fuels to CO2-neutral renewable energies, the woldwide comsumption of liquid natural gas (LNG) is rising to facilitate the transition. Here we report a new firtst-order magnetocaloric material Nd2In with a negligible thermal hysteresis for magnetocaloric natural gas liquefaction. Nd2In shows a maximum magnetic entropy change of 7.42 J/kg K in fields of 2 T at 109 K with a fully reversible adiabatic temperature change of 1.13 K under a magnetic field change of 1.95 T. Studying thermal expansion and magnetostriction, a two-stage magnetic transition with a negligible volume change is observed. The longitudinal strain increases with magnetic fields and then decreases. This phenomenon may be a result of a pure electromic mechanism which may be the reason for the negligible thermal hysteresis. These interesting properties are useful for the practical design of a magnetocaloric natural gas liquefaction system. [1]

The work is supported by the Helmholtz-RSF joint research group (Project No. HRSF-0045) and DFG (Project No. 405553726-TRR 270, Germany).

[1] W. Liu et al., Appl. Phys. Lett. 119, 022408 (2021)

MA 15.22 Thu 13:30 P

Magnetocaloric effect in the $Ho_{1-x}Dy_xAl_2$ family in high magnetic fields — •Eduard Bykov[1,2], Wei Liu[3], Konstantin Skokov[3], Franziska Scheibel[3], Oliver Gutfleisch[3], Sergey Taskaev[4], Catalina Salazar Mejia[1], Joachim Wosnitza[1,2], and Tino Gottschall[1] — [1]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, Germany — [3]Funktionale Materialien, Technische Universität, TU Darmstadt, Germany — [4]Chelyabinsk State University, Russia

Hydrogen has the largest gravimetric energy density among all chemical fuels. At the same time, the density of gaseous H_2 is extremely low. For storage and transportation reasons it can be liquified. But it requires energy-intensive cooling down to 20 K. Magnetocaloric materials have the great potential to revolutionize gas liquefaction in order to make liquid hydrogen more competitive as fuel. We investigated a series of Laves-phase materials regarding their structural, magnetic, and magnetocaloric properties in high magnetic fields. The three compounds $HoAl_2$, $Ho_{0.5}Dy_{0.5}Al_2$, and $DyAl_2$ are suited for building a stack for cooling from liquid-nitrogen temperature (77 K) down to the boiling point of hydrogen at 20 K. This is evident from our direct measurements of the adiabatic temperature change in pulsed magnetic fields, which we compare with calorimetric data measured in static field. With this methodology, we are now able to study the suitability of magnetocaloric materials down to low temperatures up to the highest magnetic fields.

MA 15.23 Thu 13:30 P

Role of NiO in the nonlocal spin transport through thin NiO films on $Y_3Fe_5O_{12}$ — Geert R. Hoogeboom[1], Geert-Jan N. Sint Nicolaas[1], Andreas Alexander[2], Olga Kuschel[2], Joachim Wollschläger[2], Inga Ennen[3], Bart J. van Wees[1], and •Timo Kuschel[3] — [1]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [2]Osnabrück University, Germany — [3]Bielefeld University, Germany

In spin-transport experiments with spin currents propagating through an antiferromagnetic (AFM) material, the AFM is mainly treated as a passive spin conductor not generating nor adding any spin current to the system. To study the role of AFMs in local and nonlocal spin-transport experiments, we have sent spin currents through NiO of various thicknesses placed on $Y_3Fe_5O_{12}$. The spin currents are injected either electrically or by thermal gradients and measured at a wide range of temperatures and magnetic field strengths [1].

The transmissive role of NiO is reflected in the sign change of the local electrically injected spin transport and the reduction of all other signals by lowering the temperature. The thermally generated response, however, shows an additional upturn below 100 K that is unaffected by an increased NiO thickness. The temperature and magnetic field dependencies are similar to those for bulk NiO [2], indicating that NiO itself contributes to thermally induced spin currents.

[1] G. R. Hoogeboom et al., Phys. Rev. B 103, 144406 (2021)
[2] G. R. Hoogeboom et al., Phys. Rev. B 102, 214415 (2020)

MA 15.24 Thu 13:30 P

High quality antiferromagnetic Mn2Au (001) thin films for spintronics — •S. P. Bommanaboyena[1], T. Bergfeldt[2], R. Heller[3], M. Kläui[1], and M. Jourdan[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, D-55099 Mainz, Germany — [2]Institut für Angewandte Materialien, Karlsruher Institut für Technologie, 76344 Eggenstein-Leopoldshafen, Germany — [3]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

The recent experimental demomonstration of Néel order manipulation via current induced Néel spin-orbit torques in antiferromagnetic Mn2Au [1] has sparked a huge interest in this compound. We report the preparation of high-quality epitaxial Mn2Au(001) thin films using molecular beam epitaxy and compare them with magnetron sputtered films [2]. Mn and Au were co-evaporated in ultra-high vacuum onto a heated epitaxial Ta(001) buffer layer deposited on an Al2O3 substrate. Structural and morphological characterization of the thin films was carried out using in-situ reflective high energy electron diffraction, X-ray diffraction, X-ray reflectometry and temperature dependent resistance measurements. The films were found to be highly crystalline and smooth with a low defect concentration which is desirable for reduced domain wall pinning and will be useful for next generation antiferromagnetic spintronics devices which require smooth interfaces between the various active layers. [1] S. Yu. Bodnar et al, Nat. Commun. 9, 348 (2018). [2] S. P. Bommanaboyena et al, J. Appl. Phys. 127, 243901 (2020).

MA 15.25 Thu 13:30 P

Large exchange coupling of Mn2Au/Ni81Fe19 for antiferromagnetic spintronics — •S. P. Bommanaboyena[1], D. Backes[2], L. Ishibe Veiga[2], S. S. Dhesi[2], Y. R. Niu[3], B. Sarpi[3], T. Denneulin[4], A. Kovacs[4], T. Mashoff[1], O. Gomonoy[1], J. Sinova[1], K. Everschor-Sitte[1], D. Schönke[1], R. M. Reeve[1], M. Kläui[1], H.-J. Elmers[1], and M. Jourdan[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, D-55099 Mainz, Germany — [2]Diamond Light Source, Chilton, Didcot, Oxfordshire, OX11 0DE, United Kingdom — [3]MAX IV Laboratory, Fotongatan 8, 22484 Lund, Sweden — [4]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, FZ Jülich, D-52425 Jülich, Germany

Mn2Au is a prominent antiferromagnet (AFM) which possesses the requisite crystallographic symmetry to exhibit a current induced Néel spin-orbit torque [1]. We demonstrate an exceptionally strong exchange coupling of Mn2Au films with very thin Permalloy (Py) overlayers [2]. The AFM Mn2Au domain pattern is perfectly imprinted on the Py, which is attributed to a specific atomic termination of the Mn2Au(001) thin film. Ferromagnetic hysteresis loops of exchange coupled 2nm Py overlayers reveal a large coercive field of 0.5 T. This is associated with a coupled rotation of both the Py magnetization and the Néel order of the underlying Mn2Au. Our results unlock novel possibilities for the readout of next generation antiferromagnetic spintronics devices. [1] S. Yu. Bodnar et al, Nat. Commun. 9, 348 (2018). [2] S.P. Bommanaboyena et al, arXiv:2106.02333 (2021).

MA 15.26 Thu 13:30 P

A quantum-mechanical study of pressure-induced changes in magnetism of austenitic stoichiometric Ni_2MnSn with point defects — •Martin Friák[1], Martina Mazalová[1,2], and Mojmír Šob[2,1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We have performed a quantum-mechanical study of a series of stoichiometric Ni_2MnSn structures focusing on pressure-induced changes in their magnetic properties. Our study concentrated on the role of point defects, in particular Mn-Ni, Mn-Sn and Ni-Sn swaps. For most defect types we also compared states with both ferromagnetic (FM) and anti-ferromagnetic (AFM) coupling between (i) the swapped atoms and (ii) those on the original sublattice. Our calculations show that the swapped Mn atoms can lead to magnetic moments nearly twice smaller than those in the defect-free Ni_2MnSn. Further, the defect-containing states exhibit pressure-induced changes up to three times larger (but also smaller) than those in the defect-free Ni_2MnSn. Importantly, we find both qualitative and quantitative differences in the pressure-induced changes of magnetic moments of individual atoms even for the same global magnetic state. Lastly, despite of the fact that the FM-coupled and AFM-coupled states have often very similar formation energies (the differences only amount to a few meV per atom), their structural and magnetic properties can be very different. For details see M. Friák *et al.*, Materials 14 (2021) 523, doi:10.3390/ma14030523.

MA 15.27 Thu 13:30 P

Magnetisation dynamics and transport properties of epitaxial Co_2MnSi Heusler thin films — Claudia de Melo[1,2], •Anna M. Friedel[1,3], Charles Guillemard[1,4], Victor Palin[1,4], Philipp Pirro[3], Sébastien Petit-Watelot[1], and Stéphane Andrieu[1] — [1]Institut Jean Lamour, UMR CNRS 7198, Université de Lorraine, Nancy, France — [2]Chair in Photonics, LMOPS EA 4423 Laboratory, CentraleSupélec, Université de Lorraine, Metz, France — [3]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, Kaiserslautern, Germany — [4]Synchrotron SOLEIL-CNRS, L'Orme des Merisiers, Gif-sur-Yvette, France

Co_2Mn-based Heusler compounds form a family of promising candidates for spintronic and magnonic applications combining desirable properties such as a high saturation magnetisation, low Gilbert damping and high Curie temperatures. Epitaxial half-metallic Co_2MnSi thin films are of particular interest since they have been shown to exhibit a 100% spin polarisation at the Fermi level and an associated ultralow Gilbert damping in the 10^{-4} range [1]. Yet, downscaling towards ultrathin films or microstructures is a critical necessity for applications known to impact the properties of magnetic materials. In this contribution, we report on the magnetisation dynamics and transport properties of epitaxially grown Co_2MnSi thin films [2] with thicknesses in the range of 4-44 nm, where ultralow Gilbert damping was maintained down to a film thickness of 8 nm.

[1] C. Guillemard, *et al.*, Phys. Rev. Applied **11**, 064009 (2019)
[2] C. Guillemard, *et al.*, J. Appl. Phys. **128**, 241102 (2020)

MA 15.28 Thu 13:30 P

Exploration of the magnetic structure of the shape-memory Heusler alloy Mn2NiGa — •Alistair Cameron[1], Sanjay Singh[2], Robert Cubitt[3], and Dmytro Inosov[1] — [1]Institut fuer Festkoerper- und Materialphysik, Technische Universitaet Dresden, D-01069 Dresden, Germany — [2]IIT, Banaras Hindu University, Varanasi, India — [3]Institut Laue-Langevin, 71 avenue des Martyrs, CS 20156, F-38042 Grenoble Cedex 9, France

The material Mn2NiGa is an example of one of the shape-memory Heusler alloys which have been predicted to show a skyrmion lattice. The Mn2YZ Heusler compounds undergo a cubic to tetragonal phase transition with decreasing temperature, and while most of these compounds possess a centrosymmetric low-temperature phase, this phase in Mn2NiGa is noncentrosymmetric. This opens up the possibility of the presence of the anisotropic Dzyaloshinskii-Moriya interaction, which can lead to the formation of skyrmion lattices. Both simulations and AC susceptibility measurements predicted the presence of a skyrmion lattice in this system, and so we performed small-angle neutron scattering measurements in order to search for this. The lattice was predicted to emerge below the Martensitic transition, and in a field of up to 1 T. However, while we saw a clear redistribution of spectral weight, we did not see any sign of a skyrmion lattice across a large range in temperature, field and scattering vector beyond those predicted for this lattice. We conclude that other magnetic behaviour dominates this material within the noncentrosymmetric tetragonal phase.

MA 15.29 Thu 13:30 P

Structural and magnetic properties of Co(Fe)-Ni-Al(Ga) Heusler alloys — •Olga Miroshkina[1,2], Markus Ernst Gruner[1], Vasiliy Buchelnikov[2], and Vladimir Sokolovskiy[2] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Condensed Matter Physics Department, Chelyabinsk State University, 454001 Chelyabinsk, Russia

Ferromagnetic shape memory alloys (FSMA) are promising candidates for application as actuators, sensors, magnetomechanical devices, harvesters, and magnetic cooling systems. In their low-temperature, low-symmetry phases they may also posses a considerable magnetocrystalline anisotropy, which is necessary for the FSMA but may make them useful as low-cost permanent magnets. Co(Fe)-Ni-Al(Ga) alloys are an interesting subgroup, as these materials are ductile, cheap, and easily synthesized, while possessing a high Curie and martensitic transformation temperature. In this work, we report on a systematic first-principles study of the structural and magnetic properties of Co-Ni-Al, Fe-Ni-Al, and Fe-Ni-Ga Heusler alloys. We compared ground state energy and magnetic properties for different structural motives and degree of order and predict the structural stability at zero and finite temperatures.

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MA 15.30 Thu 13:30 P

Quadratic magnetooptic Kerr effect spectroscopy on partially ordered Co_2MnSi Heusler compounds — •Robin Silber[1], Daniel Král[2], Ondřej Stejskal[2], Lukáš Beran[1], Jaromír Pištora[2], Martin Veis[3], Timo Kuschel[2], and Jaroslav Hamrle[2] — [1]IT4Innovations,VŠB - Technical University of Ostrava, Czech Republic — [2]Charles University, Prague, Czech Republic — [3]Bielefeld University, Germany

The Heusler compound Co_2MnSi provides a crystallographic transition from B2 to $L2_1$ structure with increasing annealing temperature [1]. Here, we present linear and quadratic magnetooptic Kerr effect (LinMOKE and QMOKE) spectroscopy [2] for a set of Co_2MnSi thin-film samples annealed from 300°C to 500°C. Two interesting features were observed: (i) For photon energy below 3.0 eV, the shape of QMOKE spectra has resonance features, an unusual behaviour for metallic systems. (ii) The amplitude of these peaks is proportional to the annealing temperature and thus, to the amount of $L2_1$ ordering. While this dependence has been shown for a single wavelength before (1.95 eV) [3], we present this proportionality for the whole studied spectral range. The $L2_1$ ordering affects the interband contributions of the LinMOKE and QMOKE spectra, which are compared to ab-initio calculations [4].

[1] O. Gaier et al., J. Appl. Phys. 103, 103910 (2008)
[2] R. Silber et al., Phys. Rev. B 100, 064403 (2019)
[3] G. Wolf et al., J. Appl. Phys. 110, 043904 (2011)
[4] R. Silber et al., Appl. Phys. Lett. 116, 262401 (2020)

MA 15.31 Thu 13:30 P

Shell-ferromagnetism: a revised model — •Nicolas Josten[1], Sakia Noorzayee[1], Mehmet Acet[1], Franziska Scheibel[2], Asli Çakir[3], and Michael Farle[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University Duisburg Essen, Duisburg, 47057, Germany — [2]Institute of Material Science, Technische Universität Darmstadt, Alarich-Weiss-Str. 16, 64287 Darmstadt, Germany — [3]Department of Metallurgical and Materials Engineering, Mugla University, 48000 Mugla, Turkey

Shell-ferromagnetism denotes a strong pinning of magnetic moments in off-stoichometric $Ni_{50}Mn_{45}X_{05}$ (X= Al, Ga, In, Sn, Sb) Heusler alloys after decomposition into full Heusler Ni_2MnX and antiferromagnetic $Ni_{50}Mn_{50}$ above 550K [1]. The pinning is induced through magnetic annealing during decomposition resulting in coercive fields larger than 6 Tesla. The origin of this effect has been identified as ordering of excess Ni in the Mn-sublattice of the binary alloy $Ni_{50+x}Mn_{50-x}$ [2]. While the magnetic and thermal stability of the induced unidirectional anisotropy is already extremely high, maximizing the pinned magnetization is key for any technological application.

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project-ID 405553726 - TRR 270.

[1] A. Cakir et al., Sci. Rep.6, 28931 (2016) [2] L. Pál et al., Phys. Stat. Sol. 42, 49-59 (1970).

MA 15.32 Thu 13:30 P

First Principles study of spin spirals in the multiferroic $BiFeO_3$ — •Sebastian Meyer[1], Bin Xu[2,3], Matthieu Verstraete[1], Laurent Bellaiche[2], and Bertrand Dupé[1,4] — [1]Nanomat/Q-mat/CESAM, University of Liége, Belgium — [2]Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, USA — [3]Jiangsu Key Laboratory of Thin Films, School of Physical Science and Technology, Soochow University, China — [4]Fonds de la Recherche Scientifique (FNRS), Bruxelles, Belgium

We carry out density functional theory (DFT) calculations to explore the antiferromagnetic (AFM) spin spiral in multiferroic $BiFeO_3$. We calculate the spin spiral energy dispersion $E(\mathbf{q})$ along the high symmetry directions of the pseudocubic unit cell, for four different structural phases: *cubic*, $R\bar{3}c$, $R3m$ and $R3c$. In all cases, we find a large exchange frustration. The comparison provides detailed insight into how polarization and octahedral anti-phase tilting affect the different magnetic interactions and the magnetic ground state in $BiFeO_3$. For the $R3c$ structural ground state, we find an AFM spin spiral ground state with a periodicity of ~80 nm in good agreement with experiments and previous findings. This spin spiral is driven by a Dzyaloshinskii-Moriya (DM) interaction stemming from the Fe–Bi ferroelectric displacement. The spiral appears to be stable because the anisotropy energy in $R3c$ $BiFeO_3$ is too small to enforce the collinear order. For all the four phases, we discuss the magnetic ground state and identify its stabilization mechanisms [Xu, B., *et al.*, Phys. Rev. B **103**, 214423 (2021)].

MA 15.33 Thu 13:30 P

Progress in Additive Manufacturing of (Pr,Nd)-Fe-Cu-B Permanent Magnets — •Jianing Liu[1], Lukas Schäfer[1], Konstantin Skokov[1], Holger Merschroth[2], Jana Harbig[2], Ying Yang[3], Matthias Weigold[2], Stefan Barcikowski[3], and Oliver Gutfleisch[1] — [1]Functional Materials, Technical University of Darmstadt, Germany — [2]Institute of Production Management, Technology and Machine Tools, Technical University of Darmstadt, Germany — [3]Technical Chemistry I, University of Duisburg-Essen, Germany

Additive Manufacturing (AM) of permanent magnets is an upcoming and challenging task in material science and engineering. The direct use of binder-free AM technique like Laser Powder Bed Fusion (L-PBF) does not easily allow obtaining a microstructure necessary for high coercivity. In order to achieve the desired microstructure and hard magnetic properties after printing, we propose here Pr-Fe-Cu-B based alloy as a useful alloy system and compare this with its Nd-based counterpart. Our studies describe the Pr-Fe-Cu-B alloys and their annealing optimization for L-PBF. In order to achieve an improved flowability and refined microstructure, the grain boundary engineering with nanoparticles shows a great potential. The nanoparticle functionalized Pr-Fe-Cu-B powder was being validate as precursor for AM. During L-PBF, the hypothesis of heterogeneous nucleation induced by NP inoculums during resolidification is explored with the goal of suppressing grain coarsening and realizing more uniaxial growth.

We acknowledge the support of the Collaborative Research Centre/Transregio 270 HoMMage.

MA 15.34 Thu 13:30 P

Qualification of rapidly quenched permanent magnet powders applied in additive manufacturing — •Tobias Braun[1], Lukas Schäfer[1], Stefan Riegg[1], Iliya Radulov[1], Imants Dirba[1], Esmaeil Adabifiroozjaei[2], Konstantin P. Skokov[1], Leopoldo Molina-Luna[2], and Oliver Gutfleisch[1] — [1]Funktionale Materialien, Material- und Geowissenschaften, Technische Universität Darmstadt, Germany — [2]Advanced Electron Microscopy, Material- und Geowissenschaften, Technische Universität Darmstadt, Germany

Additive manufacturing (AM) of permanent magnets has been an important research field in recent years due to its potential for near net shape processing of complex geometries with tailored stray field distribution and therefore better use of mostly resource-critical materials. One of the most applied materials in production of fully dense metallic magnets by LPBF is the rare-earth lean Nd-Fe-B based, atomized commercial material MQP-S by Magnequench. The powder qualifies due to spherical shape and size for the use in LPBF. The exchange-coupling mechanism induced by the two-phase nanostructure results in significant coercive fields and enhanced remanences, both however can be strongly reduced during the LPBF process.

The influence of the AM process on the magnetic properties is studied in detail by advanced magnetic and transmission electron microscopic characterization methods supported by temperature dependent x-ray diffraction and differential thermal analysis. Based on this, we review reported results on printed materials allowing a critical view on the powder material choice in AM.

MA 15.35 Thu 13:30 P

Effect of chemical disorder on the magnetic exchange couplings in $L1_0$ FeNi (tetrataenite) — •Ankit Izardar and Claude Ederer — Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zurich, Switzerland

$L1_0$ $Fe_{50}Ni_{50}$ (tetrataenite) is a promising candidate for permanent magnets with relatively high energy product containing only cheap and abundant elements. Unfortunately, the laboratory synthesis of the ordered phase is extremely challenging and several attempts have been made to achieve a high degree of chemical order in this alloy. Therefore, it is important to know how deviations from perfect chemical order affect magnetic properties.

Using first-principles-based density-functional theory calculations, we provide insights into the impact of the chemical disorder on the magnetic exchange interactions in tetrataenite. Our calculations show very strong variations in the magnetic exchange couplings (by more than 80%). Furthermore, by employing a model study, we estimate the effect of these strong variations in, e.g., the nearest neighbour couplings, compared to simply using averaged coupling constants. Our results indicate that using averaged coupling constants can lead to an overestimation of the Curie temperature of around 5%.

MA 15.36 Thu 13:30 P

Transport properties of systematically disordered Cr_2AlC films — •Joao S. Cabaco[1], Ulrich Kentsch[1], Jurgen Lindner[1], Jurgen Fassbender[1], Christoph Leyens[2,3], Rantej Bali[1], and Richard Boucher[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute for Materials Science, Technische Universität Dresden, Dresden, Germany — [3]Fraunhofer Institute for Material and Beam Technology IWS Dresden, Dresden, Germany

Nano-lamellar composite materials, known as MAX-phases, can possess a combination of ceramic and metallic properties. A prototype compound is Cr_2AlC, formed from a unit cell of Cr_2C sandwiched between atomic planes of Al. Here we observe the modifications to the structural, transport and magnetic behavior of 500 nm thick Cr_2AlC after irradiation with Co^+ ions, and Ar^+ noble gas ions as control. X-ray shows that ion-irradiation induces a suppression of the 0002 reflection, indicating a deterioration of the crystal structure. Increasing the ion fluence leads to an increase of the saturation magnetization at 1.5 K, whereby both Ar^+ and Co^+ cause an increased magnetization, respectively to 150 $kA.m^{-1}$ and 190 $kA.m^{-1}$, for the highest fluences used. At Co^+ fluences of 5×10^{13} $ions.cm^{-2}$ the magnetoresistance (MR) shows a 2 orders of magnitude increase, up to 3% (10 T) at 100 K. A similar effect also occurs for 5×10^{12} $ions.cm^{-2}$ Ar^+ irradiated films, however, with a smaller MR-increase. The disordering of MAX phase films may reveal interesting spin-related transport phenomena.

MA 15.37 Thu 13:30 P

Local structure in FeRh thin films after ion irradiation — •Johanna Lill[1], Benedikt Eggert[1], Katharina Ollefs[1], Sakura Pascarelli[2], Alexander Schmeink[3,4], Kay Potzger[3], Jürgen Lindner[3], Jürgen Fassbender[3,4], William Griggs[5], Thomas Thomson[5], Rantej Bali[3], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]ESRF, Grenoble, France — [3]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [4]Dresden University of Technology, Germany — [5]The University of Manchester, United Kingdom

Equiatomic B2 FeRh exhibits antiferromagnetic ordering at room temperature and undergoes a meta-magnetic phase transition to ferromagnetic ordering at 370K. Ferromagnetic ordering can also be induced by structural disorder caused by moderate ion irradiation [1]. Larger irradiation fluence results in a paramagnetic state. In this work we investigate FeRh thin films for different irradiation fluences of 110 keV Ne^+ by Fe K edge extended X-ray absorption fine structure spectrosopy at low temperatures. For low irradiation fluences, we find an increase of the lattice parameter and a decrease of the Debye-Waller-factor, while for higher fluences a change from the bcc to the fcc phase occurs. XRD as well as magnetometry results confirm the phase transitions, and are consistent with the EXAFS findings. From magnetometry, we see an increase of the magnetisation and a shift of the phase transition to lower temperatures with rising irradiation fluence. Financial support by DFG (WE 2623/14-2 and BA 5656/1-2) is acknowledged.

[1] W. Griggs et al. APL Mater. 8, 121103 (2020)

MA 15.38 Thu 13:30 P

Magnetic ordering/disordering in MnS and the effects of pressure on its structural landscape — •Artem Chmeruk[1] and Maribel Núñez-Valdez[1,2] — [1]Deutsches GeoForschungsZentrum GFZ, Telegrafenberg, 14473, Potsdam — [2]Goethe-Universität Frankfurt am Main, Altenhoeferallee 1 D-60438, Frankfurt a.M., Germany

We investigate magnetic ordering/disordering in MnS polymorphs and their pressure stability fields by applying density functional theory (DFT) in combination with special quasi-random structures (SQS) and occupational matrix control (OMC) algorithms to deal with the correlated Mn *d*-electrons. Departing from the experimentally known low temperature antiferromagnetic (AFM) ordering in different MnS polymorphs, we evaluate their energy stability and compare to experimental observations. Then to simulate their paramagnetic (PM) state above Néel temperature, we construct their SQS supercells of randomly distributed *up* ↑ and *down* ↓ local Mn magnetic moments. Our calculated enthalpy landscape indicates that, the RS polymorph remains the most stable phase at 0 GPa, but as pressure increases, it undergoes a structural transformation to an orthorhombic MnP-type structure at about 21 GPa. The identification of this pressure-induced phase transition sheds light onto the nature of an unknown phase previously reported at ~26 GPa from high-pressure diamond-anvil-cell experiments. In general, we show that our methodology provides accurate magnitudes of structural parameters, energy band gaps, and local magnetic moments and it could be extended to the study of other transition metal sulphides.

MA 15.39 Thu 13:30 P

Magnetostructural phase transition in $Fe_{60}V_{40}$ alloy thin films — •Md. Shadab Anwar[1,3], H. cansever[1], B. Boehm[2], R. A. Gallardo[5], R. Hübner[1], S. Zhou[1], U. Kentsch[1], B. Eggert[4], H. Wende[4], K. Potzger[1], J. Fassbender[1], K. Lenz[1], J. Lindner[1], O. Hellwig[1,2], and R. Bali[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]TU Chemnitz, Germany — [3]TU Dresden, Germany — [4]University of Duisburg-Essen, Germany — [5]Universidad Técnica Federico Santa María, Chile

Ferromagnetism can be induced in non-ferromagnetic precursors such as B2 $Fe_{60}Al_{40}$[1] and B2 $Fe_{50}Rh_{50}$[2] through lattice disordering. Here we study a magnetostructural transition in $Fe_{60}V_{40}$ thin films using ion-irradiation. We show that the as-grown films possess an M_s of 17 kA/m and irradiation with 25 keV Ne^+-ions at a fluence of ~ 5 x 10^{15}ions/cm^2 leads to an increase of M_s to ~ 750 kA/m. A structural short-range order in the as-grown films can be observed, that transforms to A2 phase (bcc) via ion-irradiation. The A2 region appears to nucleate at the film surface, and with increasing Ne^+-fluence, it propagates deeper into the film. Mössbauer spectroscopy and ferromagnetic resonance have been applied to track the variation of local magnetic ordering and dynamic behaviour respectively.

Financial support by DFG grants BA 5656/1-2 and WE 2623/14-2 is acknowledged.

[1]Ehrler, J.*et al., New J. Phys.*,22,073004(2020)
[2]Eggert, B.*et al., RSC Adv.*,10,14386(2020)

MA 15.40 Thu 13:30 P

Manipulation of multiferroic properties in h-$YMnO_3$ upon substitution at the Mn-site with non-magnetic impurities — •M. Giraldo[1], M. Lilienblum[1], E. Gradauskaite[1], H. Sim[2], J.-G. Park[2], Th. Lottermoser[1], and M. Fiebig[1] — [1]ETH Zurich — [2]Seoul National University

Chemical substitution is an effective way to tailor the properties of complex oxides. For example, pronounced effects in domain wall conductivity or mixing of magnetic groundstates in h-$RMnO_3$ have been explored by chemical substitution at the Mn-site. Here, we investigate the enhancement and suppression of electric and magnetic long-range order in h-$YMnO_3$ upon substituting Mn by Al and Ga. By combining second-harmonic spectroscopy and piezoresponse force microscopy, a complete suppression of ferroelectric order upon 20% Al substitution was found. In contrast, substitution with Ga upon 50% leads to an enhancement of the ferroelectric (FE) response. This is due to the chemical pressure induced by the distinct ionic sizes of Al, Ga & Mn. On the level of the FE domains, the suppression of the FE order manifests in a progressive size decrease upon increased Al concentration while there is no size variation upon Ga substitution. On the magnetic level, we find a progressive decrease of the ordering temperatures. This is due to the direct perturbation of the magnetic sublattices formed by the Mn^{3+} moments and the progressive dilution of the magnetic long-range order. By tracing changes in the inherent properties of these systems, we aim to broaden the understanding for new routes in the manipulation of ferroic properties in these compounds.

MA 15.41 Thu 13:30 P

Antiferromagnetic spin cycloids imaged with a Scanning Nitrogen-Vacancy Magnetometer — •Hai Zhong[1], Johanna Fischer[2], Aurore Finco[3], Vincent Jacques[3], and Vincent Garcia[2] — [1]Qnami AG, Switzerland — [2]Unité Mixte de Physique, CNRS, Thales, Université Paris Saclay, France — [3]Laboratoire Charles Coulomb, CNRS, Université de Montpellier, France

Multiferroics, such as $BiFeO_3$, in which antiferromagnetism and ferroelectricity coexist at room temperature, appear as a unique platform for spintronic and magnonic devices. The nanoscale structure of its ferroelectric domains has been widely investigated with piezoresponse force microscopy (PFM). However, the $BiFeO_3$ nanoscale magnetic textures and their potential for spin-based technology remain concealed. We present two different antiferromagnetic spin textures in $BiFeO_3$ thin films with different epitaxial strains, using a commercial scanning Nitrogen-Vacancy magnetometer (SNVM) based on a single NV defect in diamond. Two $BiFeO_3$ samples were grown on $DyScO_3$ (110) and $SmScO_3$ (110) substrates. The striped ferroelectric domains in both samples are first observed by the in-plane PFM, and SNVM confirms the existence of the spin cycloid texture. At the local scale, the combination of PFM and SNVM allows to identify the relative orientation of the ferroelectric polarization and cycloid propagation directions on both sides of a domain wall. Our results show the potential for reconfigurable nanoscale spin textures on multiferroic systems by strain engineering.

MA 15.42 Thu 13:30 P

Coupling of magnetic and electric order in hybrid improper ferroelectric $Ca_3Mn_{1.9}Ti_{0.1}O_7$ — •Yannik Zemp[1], Mads C. Weber[1], Thomas Lottermoser[1], Morgan Trassin[1], Bin Gao[2], Sang-Wook Cheong[2], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Rutgers University, New Jersey

Multiferroic hybrid improper ferroelectrics such as $Ca_3Mn_{1.9}Ti_{0.1}O_7$ (CMTO) provide a novel mechanism to couple ferroelectricity and ferromagnetism. Both ferroic orders are induced by the same structural distortions. Theoretically, these structural distortions allow an electrical control of the magnetic order. Experimental evidence of such a coupling is lacking, however, because high leakage currents prevent contact-based electrical measurements. Here we use two complementary non-contact methods, namely SQUID magnetometry and optical second harmonic generation (SHG) to scrutinize the magnetic and polar orders and their coupling in CMTO. We find clear evidence for a ferromagnetic moment below T_N = 115 K. Furthermore, we detect a massive increase in the SHG signal below the magnetic ordering temperature. Using SHG spectroscopy and domain analysis, we unveil the origin of this increase as a direct influence of the magnetic order on the ferroelectric state. This work shows that the magnetic and polar orders in multiferroic hybrid improper ferroelectrics can indeed be strongly coupled.

MA 15.43 Thu 13:30 P

Voltage control of perpendicular exchange bias — •Jonas Zehner[1,2], Daniel Wolf[2], Mantao Huang[3], Usama M. Hasan[3], David Bono[3], Kornelius Nielsch[2], Karin Leistner[1], and Geoffrey S. D. Beach[3] — [1]TU Chemnitz — [2]IFW Dresden — [3]MIT Cambridge

Ferromagnetic layers adjacent to an antiferromagnetic layer give rise to the exchange bias effect which is the basis for a variety of magnetic field sensors or magnetophoretic devices. Controlling exchange bias systems by voltage rather than by electrical current is highly desired for low power magnetic devices. So far, voltage control of exchange bias was mainly reported for systems with an in-plane unidirectional anisotropy below room temperatures. In this abstract, we present the voltage control of a NiO/Pd/Co system exhibiting perpendicular exchange bias system at room temperature. We show that the presence of a Pd interlayer (0.2 nm) is crucial for achieving perpendicular magnetic anisotropy (PMA), and thus also perpendicular exchange bias, in our system. We apply a hydrogen gating mechanism to reversibly switch between PMA and in-plane magnetic anisotropy, and thus to switch on and off perpendicular exchange bias. The observed correlation between an increased coercivity and a decreased exchange bias in the first cycle is explained with a crystallization process of the initially amorphous ferromagnetic layer. The hydrogen gating effect is further transferred to an exchange biased ferrimagnetic (GdCo) system in which we achieve a sign change of the exchange bias due to a hydrogen induced shift of the Curié temperature.

MA 15.44 Thu 13:30 P

Fast non-volatile electrical switching of the magnetoelectric domain states in the cubic spinel Co_3O_4 — •Maximilian Winkler, Somnath Ghara, Korbinian Geirhos, Lilian Prodan, Vladimir Tsurkan, Stephan Krohns, and Istvan Kezsmarki — Experimentalphysik V, Universität Augsburg, Germany

Here, we investigate the magnetoelectric effect of Co_3O_4 at temperatures below the Neel-temperature of T_N = 30K. A large magnetoelectric coefficient of up to 14ps/m is achieved if the system is cooled through T_N while magnetic and/or electric fields are applied. According to these poling procedures we provide a systematic analysis of how the magnetoelectric domain state can be controlled and even in situ switched by reversing the direction of either the electric or the magnetic field. The complete switching of the antiferromagnetic state is found to be faster than microseconds. Altogether, the control of the magnetoelectric domains and the fast switching dynamics makes the linear magnetoelectric coupling of Co_3O_4 highly interesting for spintronics.

MA 15.45 Thu 13:30 P

Domain Walls in a Row-Wise Antiferromagnetic Monolayer — Jonas Spethmann, Martin Grünebohm, Roland Wiesendanger, Kirsten von Bergmann, and •André Kubetzka — Department of Physics, University of Hamburg

We investigate magnetic domain walls in a row-wise antiferromagnetic (AFM) system, the fcc-stacked manganese monolayer on Re(0001) [1], employing spin-polarized STM, atom manipulation, and spin dynamics simulations [2]. In contrast to traditional AFM domain walls, which can be described by a coherent spin rotation, we find that the low symmetry of the row-wise AFM state facilitates a new type of domain wall which connects rotational domains by a transient 2Q state [3], a non-collinear spin texture with characteristic 90° angles in the wall center. Surprisingly, the wall width of about 2 nm is determined by a balance of Heisenberg and higher-order exchange interactions and independent of crystal anisotropy. Based on the mathematical equivalence of uniaxial anisotropy and fourth-order exchange interactions, we can establish simple formulas for domain wall width and energy. Furthermore, magnetic atom manipulation is used to image the domain wall structure with atomic spin-resolution and to modify wall positions, opening new possibilities to investigate AFM systems and prepare AFM spin configurations.

[1] J. Spethmann, *et al.*, Phys. Rev. Lett. **124**, 227203 (2020).
[2] J. Spethmann, *et al.*, Nature Commun. **12**, 3488 (2021).
[3] P. Kurz, PhD thesis, Aachen, Germany (2000).

MA 15.46 Thu 13:30 P

Surface spin flop mediated vertical magnetic textures — •Benny Boehm[1], Lorenzo Fallarino[2], and Olav Hellwig[1,2,3] — [1]Insitute of physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, D-01328 Dresden, Germany — [3]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, D-09107 Chemnitz, Germany

Antiferromagnets (AFs), and in particular synthetic antiferromagnets (SAFs), are gaining increasing interest due to their wide variety of useful properties at the micro and nanoscale. Despite of their macroscopically vanishing remanent magnetic moment and therefore high stability with respect to external magnetic field, AFs and SAFs may also provide other unique static magnetic states as well as promising characteristics for dynamic applications, such as high domain wall velocities and excitation frequencies reaching into the THz regime.

Although the static magnetic properties of atomic AFs are intrinsically predefined by their crystal structure, SAFs allow for much more freedom, due to their much larger degree of tunability. Furthermore, SAFs grant easy access to magnetic textures and even allow to manipulate them, for example via the surface spin flop (SSF), towards the desired behavior. We will report on the control of SSF mediated vertical AF domain walls, which may prove to be a promising platform for magnetization dynamics and thus are an interesting candidate for future applications, such as re-programmable spin wave guides.

MA 15.47 Thu 13:30 P

Control of stripe domain-wall magnetization in multilayers with perpendicular magnetic anisotropy — •Ruslan Salikhov[1], Fabian Samad[1], Aladin Ullrich[2], Manfred Albrecht[2], Nikolai Kiselev[3], and Olav Hellwig[1,4] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]University of Augsburg, Augsburg, Germany — [3]Forschungszentrum Jülich, Jülich, Germany — [4]Chemnitz University of Technology, Chemnitz, Germany

We report on the controlled switching of domain wall (DW) magnetization in aligned stripe and bubble domain systems, stabilized in [Co (0.44 nm)/Pt (0.7 nm)$]_X$ (X = 48, 100, 150) multilayers. We show that the remanent in-plane magnetization originates from the polarization of the Bloch-type DWs. The magnetization reversal process within the DWs does not influence the overall stripe and bubble domain morphology. Therefore our approach allows to study and control the magnetization reversal inside the DW by performing in-plane minor hysteresis loop sequences with field applied parallel to the magnetization of the DW Bloch component. The DW magnetization switching mechanisms will be discussed in detail. Our findings are relevant for DW-based magnonics and bubble skyrmion applications in magnetic multilayers.

MA 16: General Assembly of the Division of Magnetism

Time: Thursday 17:30–18:30 Location: MVMA

All members of the Division of Magnetism are invited to participate!

MA 17: Skyrmions II (joint session MA/KFM)

Time: Friday 10:00–13:15 Location: H5

Invited Talk MA 17.1 Fri 10:00 H5

Emergent electromagnetic response of nanometer-sized spin textures — •Max Hirschberger[1,2], Takashi Kurumaji[2], and Leonie Spitz[2] — [1]Quantum-Phase Electronics Center, The University of Tokyo, Bunkyo-ku 113-8656, Tokyo, Japan — [2]RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Saitama, Japan

Recently, we have worked to reduce the size of topological spin textures in bulk magnets towards the scale of several nanometers, exploiting new material platforms which are centrosymmetric and thus fundamentally different from previously explored non-centrosymmetric (chiral or polar) systems. Nanometer-sized skyrmions reported here are not stabilized by the Dzyaloshinskii-Moriya interaction, but rather by frustrated exchange or Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions. A wide array of experimental techniques in condensed matter was incorporated to establish the presence of skyrmion lattices in the new materials Gd_2PdSi_3 and $Gd_3Ru_4Al_{12}$, with Heisenberg Gd^{3+} magnetic moments.

When a conduction electron moves through such a topological spin texture, it acquires a quantum mechanical phase (Berry phase), sometimes modeled by a (virtual) emergent magnetic field B_{em} acting on the electron. Nanometric skyrmions give rise to B_{em} of order 500 Tesla, and we have recently found quantitative evidence for this giant B_{em} using electrical Hall measurements and thermoelectric properties such as the topological Nernst effect. Ongoing work is focused on the control of magnetic interactions and electromagnetic responses via chemical composition tuning.

MA 17.2 Fri 10:30 H5

Current-induced H-shaped-skyrmion creation and their dynamics in the helical phase — •Ross Knapman[1], Davi R Rodrigues[2], Jan Masell[3], and Karin Everschor-Sitte[2,4] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany — [2]Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany — [3]RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan — [4]Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47057 Duisburg, Germany

A promising application of magnetic skyrmions is in racetrack memory devices. [1] While efforts focussing on this have often been concentrated on the use of ferromagnetic racetracks, previous work has suggested that the use of helimagnets could be more effective. [2] Here, the helices provide a means to naturally confine the skyrmions to quasi-1D channels, mitigating the skyrmion Hall effect. They additionally allow for high-speed skyrmion motion. Inspired by previous works in which it is suggested that skyrmions can be created through the interplay of spin-polarized currents and magnetic impurities, [3] we propose a method of creating skyrmions in a helical background. [4]

[1] Fert, A et. al., Nat. Nanotechnol. 8(3), 152-156 (2013).
[2] Müller, J. et.al., Phys. Rev. Lett. 119(13), 137201 (2017).
[3] Everschor-Sitte, K. et. al., New J. Phys. 19(9), 092001 (2017).
[4] Knapman, R. et. al., J. Phys. D: Appl. Phys. 54(40). 404003 (2021).

MA 17.3 Fri 10:45 H5

Magnetic skyrmions probed by SP-STM: topology imprinted on the charge current and spin transfer torque — •Krisztian Palotas[1,2], Levente Rozsa[3], and Laszlo Szunyogh[2] — [1]Wigner Research Center for Physics, Budapest, Hungary — [2]Budapest University of Technology and Economics, Hungary — [3]University of Konstanz, Germany

The controlled creation/annihilation of individual magnetic skyrmions have been demonstrated by using spin-polarized scanning tunneling microscopy (SP-STM) [Science 341, 636], where the spin-polarized current exerts a torque on the spin moments of the sample. However, the detailed microscopic mechanism of this process is presently unknown. Our work contributes to this understanding by a theoretical investigation of the tunneling electron charge and spin transport probing magnetic skyrmions. The spin-polarized charge current (I) and tunneling spin transport vector quantities, the longitudinal spin current and the spin transfer torque (STT), are consistently calculated within a simple electron transport theory [PRB 94, 064434]. The electron tunneling model is extended to SP-STM in high spatial resolution, and applied to magnetic skyrmions [PRB 97, 174402; PRB 98, 094409]. Besides the vector spin transport characteristics, the relationships among conventional charge current SP-STM images [PRB 96, 024410], the magnitudes of the spin transport quantities [PRB 97, 174402], and the topology of various skyrmionic objects are analyzed [J. Magn. Magn. Mater. 519, 167440]. It is also shown that at specific SP-STM tip positions the STT efficiency (STT/I) can reach very large values ~h/e.

MA 17.4 Fri 11:00 H5

Alternative to Dzyaloshinskii-Moriya interaction for monolayer Fe_3GeTe_2 and other two-dimensional ferromagnets with trigonal prismatic symmetry — •Ivan Ado[1,2], Gulnaz Rakhmanova[3], Dmitry Zezyulin[3], Ivan Iorsh[3], and Misha Titov[1] — [1]Radboud University, Institute for Molecules and Materials, 6525 AJ Nijmegen, The Netherlands — [2]Institute for Theoretical Physics, Utrecht University, 3584 CC Utrecht, The Netherlands — [3]ITMO University, Faculty of Physics, Saint-Petersburg, Russia

Our work reveals a new potential source of noncollinear magnetic textures in a certain class of two-dimensional ferromagnets. Namely, in those that are described by the trigonal prismatic symmetry (point group D_{3h}): monolayer Fe_3GeTe_2, some transition metal dichalcogenides, and others. It is known that the Dzyaloshinskii-Moriya interaction does not contribute to the free energy density in such systems. We find that there exists a single (!) fourth order "chiral" contribution beyond the Dzyaloshinskii-Moriya interaction compatible with D_{3h} (if boundary effects are neglected). We study whether it is consistent with recent experiments on Fe_3GeTe_2. We also find that this contribution might stabilize bimerons – the in-plane analog of skyrmions. Surprisingly, we were even able to estimate the radius of such bimerons analytically.

[1] I. A. Ado, Gulnaz Rakhmanova, Dmitry A. Zezyulin, Ivan Iorsh, and M. Titov, arXiv:2105.14495

MA 17.5 Fri 11:15 H5

Skyrmions as quasiparticles: Free energy and entropy — •Daniel Schick, Markus Weissenhofer, Levente Rózsa, and Ulrich Nowak — Fachbereich Physik, Universität Konstanz, DE-78457 Konstanz, Germany

Magnetic skyrmions are quasiparticles primarily investigated due to their exceptional stability enabling data storage [1] and magnetic logic applications[2]. While at low temperatures they are robust against thermal fluctuations, they are rapidly created and annihilated at high temperatures[3]. In our paper[4], we calculated the free energy and entropy of magnetic skyrmions for a (Pt0.95Ir0.05)/Fe bilayer on Pd(111), using atomistic spin simulations at different temperatures. At low temperatures, skyrmions possess a higher entropy than the topologically trivial state, reducing the free-energy difference between skyrmions and collinear states with increasing temperature. At elevated temperatures we find the free energy of skyrmions to be lower than that of topologically trivial states, meaning that they are energetically preferred due to entropic stabilization. While this result is qualitatively in line with linear spin-wave theory, going beyond this approximation reveals deviations and even sign changes in both the energy difference and the entropy difference at increased temperatures.

[1] G. Yu et al., Nano Lett. 17, 1, 261-268, 2017
[2] S. Luo et al., Nano Lett. 18, 2, 1180-1184, 2018
[3] S. von Malottki et al., Phys. Rev. B 99, 060409(R), 2019
[4] D. Schick et al., Phys. Rev. B 103, 214417, 2021

MA 17.6 Fri 11:30 H5

Non-linear Magnetic Response of Topological Spin Textures in Helimagnetic FeGe — •Mariia Stepanova[1,2], Jan Masell[3], Erik Lysne[1,2], Peggy Schoenherr[4], Laura Köhler[5], Michael Paulsen[6], Alireza Qaiumzadeh[2], Naoya Kanazawa[7], Achim Rosch[8], Yoshinori Tokura[3,7], Arne Brataas[2], Markus Garst[5], and Dennis Meier[1,2] — [1]NTNU, Trondheim, Norway — [2]Center for Quantum Spintronics, NTNU, Trondheim, Norway — [3]RIKEN, Wako, Japan — [4]UNSW, Sydney, Australia — [5]KIT, Karlsruhe, Germany — [6]PTB, Berlin, Germany — [7]University of Tokyo, Tokyo, Japan — [8]Universität zu Köln, Köln, Germany

Chiral magnets possess a periodic layered structure which is similar to cholesteric liquid crystals, forming a wide variety of non-trivial topological defects. Using magnetic force microscopy (MFM), we resolve 1D and 2D topological defects in the near-room temperature helimagnet FeGe, including disclinations and dislocations with nonzero topological winding number, as well as three fundamental types of helimagnetic domain walls. Interestingly, in addition to their non-trivial structure, all topological defects in FeGe exhibit a pronounced non-linear magnetic response in MFM, which is not observed in regions with perfect lamellar-like order. This magnetic signature is reminiscent of the "lines of flare" that arise in cholesteric liquid crystals, suggesting local variations in magnetic susceptibility. By combining MFM and micromagnetic simulations, we investigate the origin of the magnetic signature of the topological defects and discuss possibilities to utilize the anomalous local response as read-out signal in spintronics devices.

MA 17.7 Fri 11:45 H5

Lifetimes of skyrmions and antiskyrmions in exchange frustrated films — •Moritz A. Goerzen[1], Stephan von Malottki[1,2], Sebastian Meyer[1,4], Pavel F. Bessarab[2,3], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel — [2]University of Iceland, Reykjavík, Iceland — [3]ITMO University, St. Petersburg, Russia — [4]Université de Liège, Sart Tilman, Belgium

Recently, it has been shown that isolated skyrmions can be stabilized in zero magnetic field in a Rh/Co bilayer on the Ir(111) surface due to frustration of exchange interactions [1]. Here, we predict that antiskyrmions are also metastable at zero field in this film system and can co-exist with skyrmions. Based on an atomistic spin model parametrized from density functional theory [1], we calculate the lifetime of these co-existing topological states using the geodesic nudged elastic band method as well as transition state theory in harmonic approximation [2,3]. We find significant differences between the lifetimes of skyrmions and antiskyrmions due to the effect of the Dzyaloshinskii-Moriya interaction.

[1] Meyer, Perini *et al.*, Nature Comm. **10**, 3823 (2019)
[2] Bessarab *et al.*, Sci. Rep. **8**, 3433 (2018)
[3] von Malottki *et al.*, Phys. Rev. B **99**, 060409 (2019)

MA 17.8 Fri 12:00 H5

Identification of skyrmion transition mechanisms by sub-10 nm maps of the transition rate — •Stephan von Malottki[1,2], Florian Muckel[3], Christian Holl[3], Benjamin Pestka[3], Marco Pratzer[3], Pavel F. Bessarab[1,4], Stefan Heinze[2], and Markus Morgenstern[3] — [1]Science Institute, University of Iceland — [2]ITAP, University of Kiel — [3]Institute of Physics B and JARA-FIT, RWTH Aachen University — [4]ITMO University, St. Petersburg

In addition to the conventional radial symmetric collapse of magnetic skyrmions, recent studies predicted the occurrence of skyrmion annihilation processes via the chimera skyrmion state [1-3]. Here, we demonstrate the realization of both the radial symmetric and the chimera transition mechanism in the ultra-thin film system fcc-Pd/Fe/Ir(111) [4]. Scanning tunneling microscopy is used to create transition rate maps of magnetic switching events induced by single electron events. In combination with energy density maps of the transition states obtained by atomistic spin simulations parametrized from first principles, they allow for the identification of both annihilation mechanisms. It is further shown, that a transition between both mechanisms can be achieved by the application of external in- and out-of-plane magnetic fields, yielding a sound agreement between experiment and theory.

[1] Meyer et al., Nat. Commun. **10**, 3823 (2019)
[2] Heil et al., Phys. Rev. B **100**, 134424 (2019)
[3] Desplat et al., Phys. Rev. B **99**, 174409 (2019)
[4] Muckel et al., Nat. Phys. **17**, 395-402 (2021)

MA 17.9 Fri 12:15 H5

Kinetic small-angle neutron scattering of skyrmion lattice order in chiral magnets — •Denis Mettus[1], Alfonso Chacon[1], Andreas Bauer[1], Sebastian Mühlbauer[2], Alla Bezvershenko[3], Lukas Heinen[3], Achim Rosch[3], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [3]Institute for Theoretical Physics, Universität zu Köln, D-50937 Köln, Germany

Skyrmions are topologically non-trivial spin textures that attract great interest, offering a possible avenue towards novel spintronics applications, e.g. in skyrmion-based racetrack memory. A key feature that motivates this interest is related to the exceptionally efficient coupling of skyrmion lattice order to spin currents, notably spin-polarized charge currents and magnon currents as observed in MnSi, FeGe, and Cu_2OSeO_3. This raises the question of the microscopic mechanisms that control the pinning and the elasticity modulus of the skyrmion lattice, and how they depend on the topology, electronic structure, and disorder. In the following contribution, we report kinetic studies of skyrmion lattice order by means of Time-resolved Small Angle Neutron Scattering (TISANE). We compare the unpinning processes in different systems, such as $Mn_{1-x}Fe_xSi$ where spin-transfer torques are dominated by spin-polarized charge currents and insulating material Cu_2OSeO_3 with the spin transfer torques being due to magnon currents.

MA 17.10 Fri 12:30 H5

Decoding of complex magnetic structures from Hall-effect measurements — •Juba Bouaziz[1], Hiroshi Ishida[2], Samir Lounis[1,3], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany — [2]College of Humanities and Sciences, Nihon University, Sakura-josui, Tokyo 156-8550, Japan — [3]Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany

It is generally accepted that the Hall response of complex spin-textures is given in terms of the linear superposition of the ordinary (OHE), the anomalous (AHE) and the topological Hall effect (THE). This addition is not questioned and is experimentally used to relate Hall responses to magnetic textures. Here, using a simple and transparent multiple scattering approach, we show that this relation is incomplete [1]. We introduce a missing contribution, the non-collinear Hall effect (NHE). The angular form of this term depends on the underlying crystal structure. The presence of the NHE may results in a substantial Hall response in non-collinear magnets without invoking the presence of non-coplanar spin textures or magnetic skyrmions and enables the decoding of exotic non-collinear magnetic textures that have been observed in itinerant magnets. [1] J. Bouaziz et al. PRL 126, 147203 (2021).

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MA 17.11 Fri 12:45 H5

Spin-orbit enabled all-electrical readout of chiral spin-textures — •Imara Lima Fernandes[1], Stefan Blügel[1], and Samir Lounis[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany — [2]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany

Non-collinear magnetic states are promising candidates for future information technology. However, their implementation in conventional memories is hindered by the inability of the electrical readout of their chiral nature based on current perpendicular to-plane (CPP) geometries [1,2,3]. In this work, we investigate the emergence of a rich family of new spin-mixing magnetoresistances enabling highly efficient all-electrical readout of the chirality and helicity of spin-swirling textures. Such transport effects are systematised at various non-collinear magnetic states and compared with the revealed spin-orbit-independent multi-site magnetoresistances. Owing to their simple implementation in readily available reading devices, the proposed magnetoresistances offer exciting and decisive ingredients to explore with all-electrical means the rich physics of topological and chiral magnetic objects.

– Funding is provided by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 – DYNASORE and grant 856538 – 3D MAGiC). [1] Crum et al., Nat. Commun. 6, 8541 (2015); [2] Hanneken et al., Nat. Nano. 10, 1039 (2015); [3] Fernandes et al., Nat. Commun. 11, 1602 (2020).

MA 17.12 Fri 13:00 H5

Skyrmion Dynamics at Finite Temperatures: Beyond Thiele's Equation — •Markus Weissenhofer, Levente Rózsa, and Ulrich Nowak — Fachbereich Physik, Universität Konstanz, Universitätsstraße 10, DE-78457 Konstanz, Germany

Magnetic textures are often treated as quasiparticles following Thiele's equation of motion [1]. We use atomistic spin simulations based on the stochastic Landau-Lifshitz-Gilbert equation to simulate the Brownian and current-driven motion of ferromagnetic skyrmions in a (Pt0.95Ir0.05)/Fe-bilayer on a Pd(111) surface.

Our results reveal that the existing theory based on Thiele's equation is insufficient to describe the dynamics of skyrmions at finite temperatures. We propose an extended equation of motion that goes beyond Thiele's equation by taking into account the coupling of the skyrmion to the magnonic heat bath leading to an additional dissipative term that is linear in temperature. Our results indicate that this so-far-neglected magnon-induced friction even dominates for elevated temperatures and lower Gilbert damping values, typical for thin films and multilayers [2].

[1] A. A. Thiele, Phys. Rev. Lett. 30, 230, (1973)
[2] Weißenhofer et al. , Phys. Rev. Lett., (in press 2021)

MA 18: Posters Magnetism V

Topics: Magnetic Particles / Clusters (18.1-18.8), Magnetic Instrumentation and Characterization (18.9-18.18), Magnetic Imaging Techniques (18.19-18.21), Computational Magnetism (18.22-18.27), Electron Theory of Magnetism and Correlations (18.28-18.31), Bio- and Molecular Magnetism, Biomedical Applications (18.32-18.38), Magnetic Information Technology, Recording, Sensing (18.39-18.42)

Time: Friday 10:00–13:00 Location: P

MA 18.1 Fri 10:00 P

Influence of surface water on adhesive forces in chondritic material — •Cynthia Pillich[1], Tabea Bogdan[2], Joachim Landers[1], Gerhard Wurm[2], and Heiko Wende[1] — [1]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CENIDE), Faculty of Physics, Lotharstr. 1, 47057 Duisburg, Germany — [2]University of Duisburg-Essen, Faculty of Physics, Lotharstr. 1, 47057 Duisburg, Germany

The growth of planetesimals at the so called "bouncing barrier" is still not fully understood. Evaporation of surface water on protoplanetary dust grains induced by high temperatures in the vicinity of the young star might explain improved sticking at the mm-range. As meteorites contain primordial phases representing the material in our young solar system, they offer an insight into the mechanics of planetary formation. A fragment of the iron-rich meteorite "Sayh al Uhaymir" was ground and subsequently heated in vacuum at temperatures up to 1400 K and adhesive forces were determined by Brazilian tests after cooling down to room temperature. We compare changes in adhesive forces upon exposure to high temperatures of meteoritic matter holding surface water and dried material. Compositional and concomitant structural transformations induced by tempering were investigated by ^{57}Fe-Mössbauer spectroscopy, probing the abundance of iron bearing phases.

Funding by the DFG (projects WE 2623/19-1 and WU 321/18-1) is gratefully acknowledged.

MA 18.2 Fri 10:00 P

Exploring the dynamical behaviour of spherical exchange-biased Janus particles as a new tool for microfluidic biointeraction screening — •Rico Huhnstock, Claudia Jauregui Caballero, Meike Reginka, Michael Vogel, and Arno Ehresmann — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

Janus particles (JPs) with engineered magnetic properties show significant potential for controlled motion in fluids by external dynamic magnetic fields [1]. In this work, we introduce an exchange bias (EB) thin film system on spherical non-magnetic particles as functionalized JPs and investigate their motion behaviour when being manipulated by dynamically varying artificial magnetic field landscapes above a topographically flat substrate. Due to the EB an Onion magnetization texture is stabilized within the magnetic cap of the JP [2], which is usually not accessible for micron-sized particles and allows for comparably high transport velocities. Probing the dynamics of the JPs in a microfluidic environment resulted in a superposition of controlled translational and rotational movements, emphasizing their potential use for biomolecular interaction analysis. This holds true not only for one-dimensional, but also two-dimensional translational motion. In addition, we highlight experimental possibilities to address and seperate each motion domain (translation and rotation) individually.

[1] Baraban *et al.* (2012), ACS Nano, 6(4):3383-3389.
[2] Tomita *et al.* (2021), J. Appl. Phys., 129:015305.

MA 18.3 Fri 10:00 P

Study of nanoparticle dynamics in binary solutions across phase transitions — •Juri Kopp[1], Joachim Landers[1], Samira Webers[1], Soma Salamon[1], Julian Seifert[2], Karin Koch[2], Annette M. Schmidt[2], and Heiko Wende[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — [2]Institute for Physical Chemistry, University of Cologne

In previous magnetorheological measurements of cobalt ferrite nanoparticles in aqueous polymer solutions, Webers et al. [1] studied the thermomagnetic behavior across phase transitions showing a distinct change in magnetization. To prepare pre-aligned hybrid materials, it is important to know their stability and magnetic behavior under the influence of phase transitions such as crystallization. Here, we study the dynamics of hematite nanospindles and cobalt ferrite nanoparticles in sucrose solutions of different concentration via temperature dependent Mössbauer spectroscopy and AC-susceptometry (ACS). These methods enable us to analyze the particle mobility and particle orientation across phase transitions. ACS data obtained upon decreasing temperature reveal a supercooled state and spontaneous crystallization whereas during the heating process a mixed-fluid phase is observed, which has also been shown in the Mössbauer spectroscopy results of the sample with the smallest amount of sucrose. This work is supported by the DFG, priority programme SPP1681 (WE 2623/7-3).

[1] S. Webers et al., ACS Appl. Polym. Mater. 2020, 2, 7, 2676-2685

MA 18.4 Fri 10:00 P

High throughput analysis of surface-functionalized super-paramagnetic particles in dynamic magnetic field landscapes — •Yahya Shubbak[1,2], Rico Huhnstock[1,2], Kristina Dingel[2,3], Katharina Getfert[1,2], Bernhard Sick[2,3], Arno Ehresmann[1,2], and Michael Vogel[1,2] — [1]Institute of Physics & Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, D-Kassel — [2]AIM-ED - Joint Lab Helmholtzzentrum für Materialien & Energie, D-Berlin — [3]Intelligent Embedded Systems, University of Kassel, D-Kassel

The precise manipulation of micro- and nano-particles in microfluidic environments opens new avenues for investigations of biomolecular analyte detection and interactions.[1] Motion control schemes based on a combination of static magnetic field landscapes superposed with external magnetic field pulses enable translatory motion control of magnetic particles at the nanoscale over macroscopic distances.[3] Here we demonstrate a novel method harnessing AI-enhanced fully-automated optical recognition algorithms [4] to analyze changes in the motion behavior of such particles due to liquid mediated surface to surface (particle to substrate) interaction.

[1] Lim, B. et al. J. Phys. D: Appl. Phys. 50, 33002 (2017) [2]*Lin, G. et al. Lab on a chip 17, 1884*1912 (2017) [3]*Issadore, D. et al. Lab on a chip 14, 2385*2397 (2014) [4] Dingel, K .et al. Computer Physics Communications, 262, 107859 (2021)

MA 18.5 Fri 10:00 P

Structure and magnetism of Fe/Fe3C/Carbon nanocomposites: Influence of the pyrolysis conditions — •Elisavet Papadopoulou[1], Nikolaos Tetos[1], Aram Manukyan[2], Harutyun Gyulasaryan[2], Gayane Chilingaryan[2], Michael Farle[1], and Marina Spasova[1] — [1]Faculty of Physics and Center of Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, 47057 Germany — [2]Institute for Physical Research of National Academy of Sciences (IPR-NAS), Ashtarak, 0203 Armenia

Carbon-encapsulated iron-cementite (Fe/Fe3C) magnetic nanoparticles were synthesized by an up-scalable solid-state pyrolysis method using iron phthalocyanine as metal precursor. The dependence of the magnetic, structural and morphological parameters on the pyrolysis conditions are presented. The nanocomposites contain α-Fe, cementite (Fe3C) and pure carbon with an average particle size of 12.5 * 2 nm. The saturation magnetization of Fe M=102 Am2/kg measured at room temperature increases by 30 % for higher synthesis temperature (973 K < T < 1173 K), indicating an increase in Fe content. This is in good agreement with the increasing volume fraction of iron from 0.5% to 8.6% in the same synthesis temperature range from the XRD. The effective magnetic anisotropy constant obtained from an analysis of approach to saturation magnetization (LAS) is 4.9 * 0.72 x 104 J/m3 at room temperature.

This work was supported by the EC project H2020-EU.4.b. - Twinning of research institutions no. 857502 (MaNaCa).

MA 18.6 Fri 10:00 P

Magnetic structure of Fe chains on Rh(111) substrate — •Balázs Nagyfalusi[1], László Udvardi[1,2], and László Szunyogh[1,2] — [1]Budapest University of Technology and Economics, Budapest Hungary — [2]MTA-BME Condensed Matter Research Group, Budapest, Hungary

As the size of the functional elements of spintronics devices approaches the scale of a few hundreds of atoms, the role of first principles simulations designed to model the magnetic properties of such systems becomes more pronounced. We present a method developed in the framework of the embedded cluster Green's function method aimed at minimizing the overall torque on the magnetic moments. In order to find the local minima of the energy landscape we use the gradient descent method combined with Newton-Raphson iterations where the torque and the Hessian matrix are calculated directly from first principles instead of relying on an effective spin Hamiltonian.

This procedure is applied to Fe chains deposited on Rh(111) substrate in different stacking positions. The stability of the ground state spin configurations is tested against a small vertical relaxation of the layers. The symmetry of the magnetic configurations is explained in terms of exchange interactions appearing in a suitable spin model. The comparison of the magnetic ground states obtained from ab initio and spin model calculations indicates the limits of spin models.

MA 18.7 Fri 10:00 P

Element-specific characterization of catalytic ferrite nanoparticles via Mössbauer spectroscopy — •Soma Salamon[1], Joachim Landers[1], Georg Bendt[2], Sascha Saddeler[2], Anna Rabe[2], Swen Zerebecki[3], Malte Behrens[2], Stephan Schulz[3], Stephan Barcikowski[3], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]Institute of Inorganic Chemistry and CENIDE, University of Duisburg-Essen — [3]Institute of Technical Chemistry I and CENIDE, University of Duisburg-Essen

Mössbauer spectroscopy is utilized as an element-specific, non-destructive measurement method to probe hyperfine interactions in ferrite materials, which are promising candidates for electrocatalysis applications. Evaluation of low temperature spectra recorded at high magnetic fields allows us to determine the degree of inversion in spinel systems, providing important clues on the distribution of Fe-ions on different crystallographic sites, while the isomer shift makes it possible to draw conclusions on the valency states. This enables us to correlate changes in ion distribution in the lattice with improvements in catalytic activity, which can be achieved by a number of methods. Several examples of nanoparticulate systems will be shown: The modification of particle composition during and after synthesis, as well as laser treatment of nanoparticles. In all cases, our measurement method offers valuable insights into which parameters are modified by the respective sample treatment, facilitating a more effective search for the best method to increase catalytic efficiency. Funding by the DFG via the CRC/TRR 247 (ID 388390466, Project B2) is acknowledged.

MA 18.8 Fri 10:00 P

Electronic and magnetic properties of building blocks of Mn and Fe atomic chains on Nb(110) — •András Lászlóffy[1], Krisztián Palotás[1], Levente Rózsa[2], and László Szunyogh[3] — [1]Wigner RCP, ELKH, Budapest, Hungary — [2]Department of Physics, University of Konstanz — [3]Budapest University of Technology and Economics, Budapest, Hungary

We present results for the electronic and magnetic structure of Mn and Fe clusters on Nb(110) surface, focusing on building blocks of atomic chains as possible realizations of topological superconductivity. The magnetic ground states of the atomic dimers and most of the monatomic chains are determined by the nearest-neighbor isotropic interaction. To gain physical insight, the dependence on the crystallographic direction as well as on the atomic coordination number is analyzed via an orbital decomposition of this isotropic interaction based on the spin-cluster expansion and the difference in the local density of states between ferromagnetic and antiferromagnetic configurations. A spin-spiral ground state is obtained for Fe chains along the $[1\bar{1}0]$ direction as a consequence of the frustration of the isotropic interactions. Here, a flat spin-spiral dispersion relation is identified, which can stabilize spin spirals with various wave vectors together with the magnetic anisotropy. This may lead to the observation of spin spirals of different wave vectors and chiralities in longer chains instead of a unique ground state.

MA 18.9 Fri 10:00 P

Magnetic field dependent power loss of surface acoustic waves in thin nickel layers — •Jan Philipp Kress, Sebastian Kölsch, Alfons Schuck, and Michael Huth — Physikalisches Institut, Goethe Universität, Frankfurt am Main, Germany

Though mostly applied in mobile communication devices for high-frequency filtering in the GHz regime, surface acoustic wave (SAW) technology is also a promising approach in magnonics by employing the coupling of spin degrees of freedom with time-dependent elastic deformations. We present a simple setup for ferromagnetic resonance excitation by a surface acoustic wave with a rotatable electromagnet operating at room temperature. We tested our setup with an interdigital-transducer structure made from Cr/Au by UV lithography on YZcut $LiNbO_3$ and excited a Rayleigh-type SAW at a fundamental frequency of 290 MHz and measured its attenuation for various higher harmonics after passing a polycrystalline Ni thin film. By varying the magnetic field direction within the Ni thin film plane we measured the angle-dependent attenuation which can be related to the magneto-elastic coupling coefficient of Ni.

MA 18.10 Fri 10:00 P

Analysis of the magnetization profile of 3D printed shape programmable magnetic elastomer actuators — •Kilian Schäfer, Martin Lehmann, Iliya Radulov, and Oliver Gutfleisch — Institute of Materials Science, Technical University Darmstadt, Germany

Magnetically responsive materials can be used as sensors and actuators. The advantages of magnetic actuation mechanisms are fast response, wireless operation and the possibility to operate in enclosed confined spaces. Mechanically soft sensors and actuators are beneficial when compliant and safe interaction with the human body is needed. In addition to that, they can easily adapt to changing environments and can have a simpler design, which potentially results in greater durability and lower cost.

One example of magneto responsive soft materials are composites of polymers and hard magnetic particles, like NdFeB. Recently it was shown that the shape of these composites can be controlled with a magnetic field if the material was magnetized in a specific way beforehand. The material has to be folded in the same way as the desired deformation. Here we realized a programmable magnetic elastomer actuator based on polyurethane and NdFeB particles and present a method to characterize the imprinted magnetization profile in these composites with a custom build 3D Hall Mapper. The device measures all components of the stray field with a spatial resolution of 150 μm. The detailed information will help to improve the design and magnetization strategies of magneto-active composites. Based on this, we evaluate the actuation performance of a 3D printed composite.

MA 18.11 Fri 10:00 P

Kompaktes membranbasiertes Faraday-Magnetometer für tiefe Temperaturen — •Lukas Worch, Markus Kleinhans, Marc A. Wilde und Christian Pfleiderer — Technische Universität München, Garching, Deutschland

Auf Basis von metallisierten SiN-Membranen wurde ein kompaktes, kapazitiv ausgelesenes Faradaymagnetometer konstruiert, welches in einem ^{3}He-Einsatz und einem supraleitenden 15 T Magneten betrieben wird. Mithilfe einer unabhängigen supraleitenden Gradientenspule können die Kraft- und Drehmomentbeiträge zur Kapazitätsänderung voneinander getrennt werden. Eine elektrostatische Kalibrationsroutine erlaubt die quantitative Bestimmung der Magnetisierung. Die kommerziell verfügbaren Membranen erlauben ein einfaches und schnelles Tauschen der Probe. Durch eine drehbare Probenbühne können zudem winkelabhängige Messungen durchgeführt werden. Erste Messergebnisse an Gadolinium Gallium Granat zeigen Signaturen des komplexen Phasendiagramms in der Magnetisierung.

MA 18.12 Fri 10:00 P

Quadratic and third-order magneto-optic Kerr effect in Ni(111) thin films with and without twinning — •Maik Gaerner[1], Robin Silber[2], Tobias Peters[1], Jaroslav Hamrle[3], and Timo Kuschel[1] — [1]Bielefeld University, Germany — [2]IT4Innovations, VŠB - Technical University of Ostrava, Czech Republic — [3]Charles University, Prague, Czech Republic

To separate and study the dependencies of the linear magneto-optic Kerr effect (MOKE) and quadratic MOKE on the crystallographic direction, the so-called eight-directional method can be used [1]. So far, this method or similar ones have been utilized to characterize (001)- and (011)-oriented thin films of cubic crystal structure [2,3]. Here, we apply the eight-directional method to Ni(111) thin films and report on a strong three-fold anisotropy in longitudinal MOKE (LMOKE). This anisotropy can be explained by theory as an optical interplay of elements in the permittivity tensors of first and second order in M, effectively creating cubic MOKE contributions, i.e., MOKE of third order in M. Furthermore, we observe that in a Ni(111) thin film with twinning (two structural (111) phases with 60 deg. in-plane rotation), those oscillations are substantially reduced compared to a thin film with almost no twinning. This indicates that the LMOKE anisotropy truly is of crystallographic origin in the ferromagnetic layer and is not due to other, e.g., interface effects.

[1] K. Postava et al., J. Appl. Phys. 91, 7293 (2002)
[2] R. Silber et al., Phys. Rev. B 100, 064403 (2019)
[3] J. H. Liang et al., Appl. Phys. Lett. 108, 082404 (2016)

MA 18.13 Fri 10:00 P

Exploring the phase diagram of GdTe3 using thermal expansion and magnetostriction — •Thom Ottenbros[1], Claudius Müller[1], Shiming Lei[2], Ratnadwip Shingha[2], Leslie Schoop[2], Nigel Hussey[1,3], and Steffen Wiedmann[1] — [1]HFML-EMFL, Nijmegen, Netherlands — [2]Princeton University, USA — [3]University of Bristol, UK

Thermal expansion and magnetostriction are powerful tools to explore phase transitions and ultimately determine the phase diagram of correlated electron systems.

We present the mapping of the phase diagram of GdTe3, a van der Waals layered antiferromagnetic metal with high carrier mobility [1]. At zero magnetic field, we find three magnetic transitions in the thermal expansion: a Néel transition at 12.0 K, and two others at 7.0 and 10.0 K. In magnetostriction experiments up to 30 T and at 1.3 K, another transition occurs around 20 T before the onset of quantum oscillations.

Furthermore, we give an overview of capacitive dilatometry at the HFML-EMFL in Nijmegen and discuss new high field experiments using a uniaxial stress dilatometer [2].

[1] S. Lei et al., Science Advances 6, eaay6407 (2020). [2] R. Kuechler et al., Rev. Sci. Inst. 87, 073903 (2016).

MA 18.14 Fri 10:00 P

Single-crystal growth and magnetic characterization of rare-earth-doped yttrium orthosilicate — •Tim Hofmann, Andreas Bauer, Fabian Kessler, and Christian Pfleiderer — Chair for the Topology of Correlated Systems, Department of Physics, Technical University of Munich, Germany

The monoclinic Yttrium orthosilicate Y2SiO5 doped with several ten ppm of rare-earth atoms, such as Er^{3+}, Yb^{3+}, or Nd^{3+}, is a candidate material for optical applications in quantum information technology. The amount of dopants decisively influences key properties, such as the linewidth or the coherence time, and in turn precise control on the doping levels is essential. Here, we report the preparation of poly-crystalline material using a sol–gel process, followed by single-crystal growth by means of the optical floating zone technique. The quantitative determination of doping on ppm level is challenging when using conventional characterization techniques. Instead, we infer information from magnetization measurements at low temperature for magnetic fields up to 14 T applied along the optical axes b, $D1$, and $D2$. We find paramagnetic contributions characteristic of rare-earth ions. Distinct anisotropy hints towards the importance of crystal electric field effects for both the fundamental characterization and potential applications in quantum information technology.

MA 18.15 Fri 10:00 P

2.6 Tesla Cryogen Free Mu3e System — •Dr. Roger Mitchell — Cryogenic Ltd, London, UK

Cryogenic Ltd has manufactured a large bore cryogen-free magnet system to enable investigations of the lepton-flavour violating decay of muons into an electron and two positrons. The magnet is installed at the Paul Scherrer Institute in Villigen, Switzerland. The cryostat has a 1 metre room temperature bore and houses a 2.6T magnet with a base homogeneity of <0.12% over a 1.3m central region. The NbTi magnet comprises four separately powered windings. Varying the current in the windings permits subtle changes to the field profile as well as establishing a shallow gradient field along the bore. The magnetic stray field is limited to 5mT at 1m by encasing the cryostat in a 27 tonne passive shield with overall dimensions of 2.1m diameter x 3.4m long. Access to 1m bore tube is via semicircular swing doors each weighing 0.5 tonnes. The magnet cold mass is 1.5 tonnes and is cooled to 3.5K using four 1.5W Gifford McMahon two-stage cryocoolers. The magnet operated to full field without training. To ensure safety in operation the magnet is magnetically balanced within the iron shield using a series of load cells to monitor relative displacements between the cryostat and the shield. The overall system footprint was subject to severe spatial restrictions imposed by the beamline architecture. Careful optimisation was necessary to achieve the critical specifications within the dimensional constraints. The room temperature bore will house a purpose-built detector developed at PSI which is inserted via a rail system attached to the bore wall.

MA 18.16 Fri 10:00 P

Measurement of de Haas-van Alphen effect by means of temperature modulation — •Michelle Hollricher, Marc A. Wilde, and Christian Pfleiderer — Department of Physics, Technical University of Munich, D-85748 Garching, Germany

Measurements of the quantum oscillations of the magnetization M as a function of magnetic field B, i.e. the de Haas-van Alphen effect, are a powerful tool for mapping the Fermi surfaces of metals. The most established methods for measuring $M(B)$ or other quantities utilize either the magnetic torque or inductively pick up the response to a large-amplitude modulation of B. Here we report the development and characterization of a temperature modulation technique (TMT) for measuring quantum oscillations in M, combining a thermally linked sample-heater-thermometer arrangement with an inductive pickup. Advantages of the method are the absence of dissipation due to a modulated field and the ability to separate signals arising from orbits with different effective masses. It was found that TMT may prove to be especially advantageous for detecting oscillations related to orbits with heavy effective masses. The TMT was employed on Bi single crystals at temperatures down to 1.9 K and in magnetic fields up to 9 T. Pronounced quantum oscillations well into the quantum limit of the electron pockets were observed.

MA 18.17 Fri 10:00 P

Meissner flux repulsion and trapped flux in sub-millimeter size superconductors observed with enhanced neutron depolarization — •Jorba Pau[1], Schulz Michael[2], Seifert Marc[1,2], Tsurkan Vladimir[3,4], Böni Peter[1], and Pfleiderer Christian[1] — [1]Physik-Department, Technische Universität München, Garching, Germany — [2]Heinz-Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [3]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — [4]Institute of Applied Physics, Chisinau, Republic of Moldova

Neutron depolarization is a unique probe which can quantify the level of magnetic inhomogeneity at a mesoscopic scale in the bulk of a sample. We report the construction of a focusing neutron guide module increasing the neutron flux at the focal spot by a factor of 20. This module was used to enhance ND measurements, demonstrating an increase of an order of magnitude in the signal to noise ratio while maintaining the exposure time. The construction and utilization details are addressed. Additionally, a proof of principle experiment on superconducting niobium and lead was conducted. We demonstrate that, with the enhanced ND technique, the Meissner flux repulsion and trapped magnetic flux of very small superconducting samples can be observed. This opens the possibility of using ND to investigate superconductors, ferromagnets, or even spin glasses under very high pressures.

MA 18.18 Fri 10:00 P

MIASANS at the longitudinal neutron resonant spin echo spectrometer RESEDA — •Jonathan Leiner[1,2], Christian Franz[1,2,3], Johanna Jochum[1,2], and Christian Pfleiderer[1,2] — [1]Technical University of Munich, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [3]JCNS at MLZ, FZ Jülich GmbH, Garching, Germany

The RESEDA (Resonant Spin-Echo for Diverse Applications) instrument has been optimized for neutron scattering measurements of quasi-elastic and inelastic processes over a wide parameter range. One spectrometer arm of RESEDA is configured for the MIEZE (Modulation of Intensity with Zero Effort) technique where the measured signal is an oscillation in neutron intensity over time, which is prepared by two precisely tuned radio-frequency (RF) flippers. With MIEZE, all of the spin-manipulations are performed before the beam reaches the sample, and thus the signal from sample scattering is not disrupted by any depolarizing conditions there (i.e. magnetic materials). The MIEZE spectrometer is being further optimized for the requirements of small-angle neutron scattering (MIASANS), a versatile combination of the spatial and dynamical resolving power of both techniques. We present the progress on (i) installing new superconducting solenoids as part of the RF flippers to significantly extend the dynamic range (ii) design and installation of modular options for both reflecting guides and evacuated flight paths with absorbing walls for background reduction (iii) installation of a new detector on a translation stage within a vacuum vessel for flexibility with angular coverage and resolution.

MA 18.19 Fri 10:00 P

Microfocused optical spin-wave spectroscopy with vector magnetic fields — •Yannik Kunz, Michael Schneider, Björn Heinz, Lars Niklas Hess, Philipp Pirro, Vitaliy Vasyuchka, and Mathias Weiler — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany

The field of magnonics aims to exploit spin waves for information processing purposes. Experimental techniques that allow accurate spin-wave spectroscopy in magnonic microstructures are needed to tailor magnonic devices. The microfocused frequency-resolved magneto-optic Kerr effect (FR-MOKE) can be used for spatially resolved spin-wave measurements in the frequency-domain with phase resolution, empowered by vector network analysis [1]. Here we present a FR-MOKE setup that provides 3D vector magnetic fields to study linear and nonlinear spin-wave dynamics in micropatterned magnonic conduits in all field geometries. The setup allows simultaneous integration of micro-focused Brillouin Light Scattering and time-resolved MOKE to access both coherent and incoherent spin-wave dynamics as a function of frequency and/or time. We characterize the setup performance through optical spin-wave spectroscopy measurements of metallic and insulating magnonic devices. [1] L. Liensberger et al. IEEE Magn. Lett. 10, 5503905 (2019)

MA 18.20 Fri 10:00 P

Time-Resolved Imaging of Ferromagnetic Resonances in the Oldenburg Ultrafast Transmission Electron Microscope (UTEM) — •Jonathan Weber, Nikita Porwal, Michael Winkelhofer, and Sascha Schäfer — Carl-von-Ossietzky Universität Oldenburg, Deutschland

Recent progress in the development of laser driven, high-brightness photocathodes offers a path to investigate magnetization dynamics with unparalleled resolution by employing a Lorentz imaging scheme in an ultrafast transmission electron microscope [1,2].

Aiming to extend the accessible frequency range, we develop a setup for Lorentz-imaging detected ferromagnetic resonances. Beyond the nanometer spatial resolution, inherent to transmission electron microscopy, a setup for fs-temporal resolution is presented, employing nano-localized photoemission from a Schottky-field emitter in the Oldenburg UTEM. The laser system which is used for the generation of ultrashort electron pulses is also utilized as a master clock for the synthetization of phase-locked microwave signals [3]. Making use of a custom-made sample holder we pass these signals to a microresonator which excites precessions of the magnetic moments in nanostructured Py films at GHz frequencies. With this advanced excitation scheme we aim to further establish ultrafast Lorentz microscopy as a powerful tool to characterize magnetic dynamics on the nanoscale.

[1] T. Eggebrecht et al. Phys. Rev. Lett. 118, 097203 (2017)
[2] N. R. da Silva et al. Phys. Rev. X 8, 031052 (2018)
[3] M.R. Otto et al. Struct. Dyn. 4, 051101 (2017)

MA 18.21 Fri 10:00 P

Force-detected magnetic resonance of nanometer thin films: measuring copper nuclear spins with a nanoladder sensor — •Gesa Welker[1], Martin Héritier[2], Martin de Wit[1], Tim Fuchs[1], Jaimy Plugge[1], Freek Hoekstra[1], Alexander Eichler[2], Christian Degen[2], and Tjerk Oosterkamp[1] — [1]Leiden Institute of Physics, Leiden University, The Netherlands — [2]ETH Zurich, Switzerland

Magnetic Resonance Force Microscopy (MRFM) is a non-invasive 3D imaging technique that can be used to characterize biological and solid-state samples on the nanoscale. Small ensembles of spins are detected by measuring the attonewton forces they exert on an ultrasoft cantilever. State of the art for biological samples is the imaging of a single tobacco mosaic virus with nanometer resolution (Degen, 2009), based on the detection of nuclear 1H (proton) spins. An important goal in the field is improving measurement sensitivity in order to achieve higher image resolution, the ultimate goal being single-nuclear-spin resolution. In this poster we present a new type of force sensor for MRFM, designed for increased sensitivity and operation at millikelvin temperatures to reduce thermal noise. The sensor combines a nanoladder cantilever (spring constant 16 μN/m) with a micromagnet of 1.1 μm radius. Using the new sensor, we unambiguously identified a copper nuclear resonance signal.

MA 18.22 Fri 10:00 P

Finite-element dynamic-matrix approach to calculate spin-wave dispersions in waveguides with arbitrary cross section — •Lukas Körber[1,2], Gwen Quasebarth[1,2], Andreas Otto[2], and Attila Kákay[1] — [1]Helmholtz-Zentrum Dresden - Rossendorf, Dresden Germany — [2]Technische Universität Dresden

One of the key objectives in curvilinear magnetism is the determination of the spin-wave dispersion and mode profiles in magnetic waveguides with surface curvature. Due to the geometrical complexity, dynamic micromagnetic simulations are often used to obtain quantitive predictions where only approximate analytical approaches are available. However, especially in geometries which require an accurate modeling of the sample surface, these dynamic micromagnetic simulations become computionally exhausting. To address this challenge, we present a finite-element dynamic-matrix approach to efficiently calculate the dispersion and spatial mode profiles of spin waves propagating in waveguides with arbitrary cross section where the equilibrium magnetization is invariant along the propagation direction. This is achieved by solving a linearized version of the equation of motion of the magnetization numerically only in a single cross section of the waveguide at hand. To take account of the dipolar interaction we present an extension of the well-known Fredkin-Koehler method to plane waves. As an application of our method, we present the first results on the spin-wave dispersion in nanotubes with thick shell which exhibits higher-order standing modes along the radial direction as well as an extremely strong dispersion asymmetry compared to thin-shell nanotubes.

MA 18.23 Fri 10:00 P

Automated spin-dynamics simulations with AiiDA-Spirit — •Philipp Rüssmann[1], Jordi Ribas Sobreviela[1,2], Moritz Sallermann[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]RWTH Aachen University, Aachen, Germany

The Spirit framework (spirit-code.github.io) allows to perform spin-dynamics simulations of magnetic materials based on the solution of the Landau-Lifshitz-Gilbert equation. These calculations can be used, for example, to find the magnetic ground state based on exchange coupling parameters, to calculate the Curie Temperature with a Monte Carlo method or perform geodesic nudged elastic band calculations for the minimal energy transition path between two magnetic states. We present the AiiDA-Spirit plugin (aiida-spirit.readthedocs.io) that connects the Spirit code to the AiiDA framework. AiiDA allows to perform automated calculations while keeping track of the data provenance between calculations. The AiiDA-Spirit plugin is able to use exchange coupling parameters calculated based on first-principles calculations within the AiiDA-KKR package (aiida-kkr.readthedocs.io). This facilitates multi-scale modelling, bridging the gap from the atomic scale of quantum mechanical simulations to the micrometer scale of magnetic structures and devices. — We acknowledge funding by the

Deutsche Forschungsgemeinschaft (DFG) under Germany's Excellence Strategy – Cluster of Excellence Matter and Light for Quantum Computing (ML4Q) EXC 2004/1 – 390534769.

MA 18.24 Fri 10:00 P

Energy-efficient control of magnetization reversal in bistable nanowires — •Mohammad Badarneh[1], Grzegorz Kwiatkowski[1], and Pavel Bessarab[1,2] — [1]University of Iceland, Reykjavík, Iceland — [2]ITMO University, St. Petersburg, Russia

We explore theoretical limits for the energy-efficient control of switching phenomena in bistable magnetic nanowires. We calculate optimal control paths (OCPs) for the magnetization switching as functions of the switching time, damping and various parameters of the nanowires. Following an OCP involves concerted rotation of the magnetic moments in such a way that the system's internal modes are effectively used to aid magnetization switching. OCP calculations demonstrate that short nanowires reverse their magnetization via coherent rotation which can be induced by applying uniform external magnetic field with frequency defined by a collective in-phase precession of the magnetization [1]. If the length of the wire exceeds a certain critical length, standing spin wave emerges during magnetization switching [2]. Such spin wave assisted magnetization switching has recently attracted much attention as a promising technique to reduce the switching field for magnetic recording. Our results demonstrate that optimal switching mechanisms and corresponding control stimuli can be predicted from first principles, contributing to the development of low-power technologies.

[1] G.J. Kwiatkowski et al., Phys. Rev. Lett. 126, 177206 (2021)
[2] M.H.A. Badarneh et al., Nanosyst. Phys. Chem. Math. 11(3), 294 (2020)

MA 18.25 Fri 10:00 P

Exchange interactions in hematite from first principles — •András Deák[1], Tobias Dannegger[2], Martin Evers[2], László Szunyogh[1,3], and Ulrich Nowak[2] — [1]Department of Theoretical Physics, Budapest University of Technology and Economics, Hungary — [2]Fachbereich Physik, Universität Konstanz, Germany — [3]MTA-BME Condensed Matter Research Group, Budapest University of Technology and Economics, Hungary

Antiferromagnets have lately appeared in the forefront of spintronics research, with exciting novel magnonic spin transport applications for collinear insulating antiferromagnets. We will detail our investigations of hematite (α-Fe_2O_3), a well-known collinear insulating antiferromagnet showing weak ferromagnetism.

We assess magnetic ordering in the material using the Screened Korringa–Kohn–Rostoker (SKKR) multiple scattering theory. We use a multiscale description by deriving spin model parameters from first principles and investigating the ground state spin configuration and its stability using this model. With this approach we can tackle the nature of the weak ferromagnetic distortion in this antiferromagnet, and provide spin model parameters that can be used in large-scale simulations of magnon dynamics effects.

MA 18.26 Fri 10:00 P

Quantum effects in thermally activated domain wall switching in ferromagnets — •Grzegorz J. Kwiatkowski[1] and Pavel F. Bessarab[1,2] — [1]Science Institute of the University of Iceland, Reykjavík, Iceland — [2]ITMO University, St. Petersburg, Russia

Most widely used data storage technologies are based on nanoscale magnetic structures [1]. In order to improve both memory retention and energy efficient writability one needs to increase stability of magnetic samples without a change in energy barrier which directly affects the costs or rewritning the memory. Due to this fact it is vital to optimise the preexponential factor in Arrhenius law, which requires one to properly study the effect of internal degrees of freedom on thermal switching pocesses [2,3]. We present analytic estimation of rate of escape for domain wall switching in 3D samples with focus on how results scale with internal parameters and sample size. Since for spin waves minimum excitation energy is larger then average thermal fluctuation for high frequency modes we employ Bose-Einstein statistics, which leads to nontrivial temperature dependencies of the preexponential factor opening up new possibilities for enhancing stability of magnetic structures. This work was funded by the Russian Science Foundation (Grant No. 19-72-10138) and the Icelandic Reseach Fund (Grant No. 184949-052).

[1] W. A. Challener et al. Nature Photonics volume 3, pages 220-224 (2009) [2] P. F. Bessarab, V. M. Uzdin and H. Jónsson Physical Review Letters 110.2, 020604 (2013) [3] G. Fiedler et al. Journal of Applied Physics 111, 093917 (2012)

MA 18.27 Fri 10:00 P

Energy-efficient control of magnetic states — Mohammad Badarneh[1], Grzegorz Kwiatkowski[1], Sergei Vlasov[2], Igor Lobanov[2], Valery Uzdin[2], and •Pavel Bessarab[1,2] — [1]University of Iceland, Reykjavik — [2]ITMO University, St. Petersburg, Russia

Control of magnetization switching is critical for the development of novel technologies based on magnetic materials. Transitions between magnetic states can follow various pathways which are not equivalent in terms of energy consumption and duration. In this study, we propose a general theoretical approach based on the optimal control theory to design external stimuli for efficient switching between target magnetic states. The approach involves calculation of optimal control paths (OCPs) for the desired magnetic transition. Following an OCP involves rotation of magnetic moments in such a way that the strength of the external stimulus is minimized, but the system's internal dynamics is effectively used to aid the switching. All properties of the switching pulses including temporal and spatial shape can be derived from OCPs in a systematic way. Various applications of OCP calculations are presented, including energy-efficient switching of a nanomagnet by means of external magnetic field [1] or electric current, and spin-wave assisted magnetization reversal in nanowires [2].

This work was funded by the Russian Science Foundation (Grant No. 19-72-10138), the Icelandic Reseach Fund (Grant No. 184949-052).

[1] G.J. Kwiatkowski *et al.*, Phys. Rev. Lett. **126**, 177206 (2021).
[2] M.H.A. Badarneh *et al.*, Nanosyst. Phys. Chem. Math. **11**, 294 (2020).

MA 18.28 Fri 10:00 P

Magnon topology in chiral crystals: Multifold crossings and nodal planes — •Niclas Heinsdorf, Xianxin Wu, and Andreas Schnyder — Max Planck institute for condensed matter physics

We investigate the topology of magnon excitations in magnets with chiral space groups. The presence of (magnetic) screw rotations lead to symmetry enforced Weyl points and nodal planes in the magnon band structure. In addition, there are multifold crossings pinned at high-symmetry points. We systematically analyze the band topology of these crossings and calculate their topological charges. In particular, we find that the magnon nodal planes carry a quantized topological charge similar to magnon Weyl points. Analogous to the protected spin currents on the surface of topological insulators, the topologically nontrivial magnon crossings result in protected surface modes of heat quanta. We propose several candidate materials and calculate their magnon band structures, topological invariants, and topologically protected surface modes.

MA 18.29 Fri 10:00 P

Magnetic interactions in correlated systems from first principles — •Vladislav Borisov[1], Yaroslav O. Kvashnin[1], Nikolaos Ntallis[1], Qichen Xu[2], Rebecca Clulow[1], Peter Svedlindh[1], Danny Thonig[3], Patrik Thunström[1], Manuel Pereiro[1], Anders Bergman[1], Erik Sjöqvist[1], Anna Delin[2], Lars Nordström[1], and Olle Eriksson[1,3] — [1]Uppsala University, SE-75120 Uppsala, Sweden — [2]KTH Royal Institute of Technology, SE-10691 Stockholm, Sweden — [3]Örebro University, SE-70182, Örebro, Sweden

The formation of non-trivial magnetic textures, such as skyrmions, depends on the interplay between the Heisenberg and Dzyaloshinskii-Moriya (DM) interactions. In this work, we discuss a general theoretical framework based on density functional (DFT) and dynamical mean-field theories which allows to calculate these interactions accurately from first principles including electronic correlations.

First, we demonstrate that dynamical correlations can lead to non-monotonic variations of magnetic exchange, for example, in skyrmionic B20 compounds MnSi and FeGe and low-dimensional system of Co/Pt(111) bilayer [1].

Secondly, we use the proposed theoretical approach to study the doped B20 compounds $Fe_{0.75}TM_{0.25}Si$ (TM = Co, Rh, Ir) and $Co_{0.75}TM_{0.25}Si$ (TM = Fe, Ru, Os) and predict that skyrmions can be stabilized in all these compounds and the DM interaction is enhanced in the $4d$- and $5d$-doped systems. We also report successful synthesis for (Fe,Ir)Si and (Co,Ru)Si and measurements for the later.

1. PRB 103, 174422 (2021).

MA 18.30 Fri 10:00 P

Local spin Hamiltonians from model electronic structure theory — Simon Streib[1], Vladislav Borisov[1], Manuel Pereiro[1], Anders Bergman[1], Erik Sjöqvist[1], Anna Delin[2,3], Mikhail Katsnelson[4], Olle Eriksson[1,5], and •Danny Thonig[5] — [1]Department of Physics and Astronomy, Uppsala University, Sweden — [2]Department of Applied Physics, KTH Royal Institute of Technology, Sweden — [3]Swedish e-Science Research Center (SeRC), KTH Royal Institute of Technology, Sweden — [4]Institute for Molecules and Materials, Radboud University, The Netherlands — [5]School of Science and Technology, Örebro University, Sweden

The derivation of spin Hamiltonians from ab initio calculations is an important tool for modeling effective precession fields in the dynamics of magnetic materials since a full electronic description of the dynamics is computationally very demanding. In this work, we contrast two different – "local" and "global" – approaches. The global approach aims at describing arbitrary spin configurations, whereas the local approach is only valid for small magnetic fluctuations locally around a given spin configuration. We argue that global symmetry requirements, such as time-reversal symmetry, do not necessarily restrict local spin Hamiltonians if the dependence of the effective exchange parameters on the magnetic state is taken into account. We present a general formalism to map model electronic structure theory to a local spin Hamiltonian and we check our formalism by means of numerical calculations for low-dimensional structures, like dimers and chains [1].

[1] S. Streib et al., Phys. Rev. B 103, 224413 (2021)

MA 18.31 Fri 10:00 P

An automated tool for generation of optimal Voronoi tessellation of crystal structures by the inclusion of void sites — •Roman Kováčik and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The performance of the electronic structure calculation within the Korringa-Kohn-Rostoker Green function method strongly relies on a good convergence with respect to the angular momentum expansion. This in turn depends on an as close-packed as possible definition of the atomic structure, due to the Voronoi tessellation used to partition the space. Hence, for the crystal structures with low packing density, an appropriate set of void sites has to be defined, which we address in our newly developed python tool.

The lower and upper bound of the number of void sites is estimated from the packing density, using simple geometrical arguments or assuming atomic radii of the present species. Within these bounds, a number of all distinct sets of Wyckoff positions is generated, corresponding to the space group of the input structure and yet unoccupied by present atoms. In case of a free coordinate in a particular Wyckoff position, a user defined number of random initial positions are tried. The fitness of the resulting Voronoi tessellation is examined as a function of the radius of void sites from the minimum ratio of inscribed and circumscribed sphere and the maximum ratio of circumscribed sphere and nearest neighbor distance over the Voronoi cells. Solutions are presented for several trivial and non-trivial crystal structures.

MA 18.32 Fri 10:00 P

Light-, temperature-, and x-ray-induced spin-crossover transition of molecules adsorbed on a graphite surface — •Jorge Torres[1], Lalminthang Kipgen[1], Sascha Ossinger[2], Sangeeta Thakur[1], Clara W.A. Trommer[2], Ivar Kumberg[1], Rahil Hosseinifar[1], Evangelos Golias[1], Sebastien Hadjadj[1], Jendrik Gördes[1], Chen Luo[3], Kai Chen[3], Florin Radu[3], Felix Tuczek[2], and Wolfgang Kuch[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Berlin, Germany — [2]Christian-Albrechts-Universität zu Kiel, Institut für Anorganische Chemie, Kiel, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

When iron spin-crossover molecules (SCM) are irradiated by light, their spin configuration can be excited from the ground state S_0 to an exited state S_1 and from there even to a metastable state of different multiplicity. For Fe(II) complexes this corresponds to a transition from low-spin (LS) to high-spin (HS) states. When the temperature is changed, this transition takes place in terms of thermodynamic effects. In this work we deposited different sub-, mono- and multilayer coverages of $[Fe\{(pzpy)pz\}_2]$ on highly oriented pyrolytic graphite and measured them by X-ray absorption spectroscopy. Analysis of the HS and LS fraction showed that for almost all samples the light-induced excited spin-state trapping (LIESST) effect resulted in twice the HS fraction than the thermally induced spin-state transition. The transition temperature $T_{1/2}$ (50% HS and 50% LS) is located at 300 K, opening a window for potential applications at room temperature.

MA 18.33 Fri 10:00 P

Hyperthermia setup for efficient nanoparticle heating — •Daniel Kuckla, Amirarsalan Asharion, Julia-Sarita Brand, Vinzenz Jüttner, and Cornelia Monzel — Heinrich-Heine-Universität Düsseldorf

All biological systems are temperature dependent. Of special interest is the influence of elevated temperatures on malignant tissue and how this can be exploited for medical treatments. One approach called "magnetic hyperthermia" uses bio-functionalized magnetic nanoparticles (MNPs) which heat in an alternating magnetic field. By targeting MNPs to the malignant cells, a spatially selective heating of tissue is realized. Here, we present a hyperthermia setup, which allows to image the behaviour of cells marked with MNPs on a microscope while being subjected to an alternating magnetic field. We provide a comprehensive characterization of the setup components and magnetic fields generated, as well as strategies to limit off-target power dissipation. We further quantify the heat generated by MNPs in well-defined in vitro and biomimetic environments. The efficient generation of high-frequency magnetic fields and direct observation of MNP responses will provide valuable information on the heat generation mechanism in different environments.

MA 18.34 Fri 10:00 P

Spectroscopic studies of a Fe(II) spin-crossover complex in the room temperature regime — •Lea Spieker[1], Stephan Sleziona[1], Gérald Kämmerer[1], Carolin Schmitz-Antoniak[2], Torsten Kachel[3], Soma Salamon[1], Damian Günzing[1], Tobias Lojewski[1], Nico Rothenbach[1], Andrea Eschenlohr[1], Katharina Ollefs[1], Senthil Kumar Kuppusamy[4], Mario Ruben[4,5], Uwe Bovensiepen[1], Peter Kratzer[1], Marika Schleberger[1], and Heiko Wende[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — [2]Jülich Research Center — [3]Helmholtz Center Berlin — [4]Karlsruhe Institute of Technology — [5]CNRS-University of Strasbourg

Spin-crossover complexes with a bi-stable spin-state switching in the room temperature regime, influenced by external stimuli such as light, pressure, temperature, or X-rays, are desirable for applications. With different spectroscopic methods, like Raman- and X-ray absorption spectroscopy, we investigated a Fe(II) complex showing a phase transition from a diamagnetic low-spin (S=0) to a paramagnetic high-spin (S=2) state in the room temperature regime ($T_{1/2\uparrow} = 330$ K) with a broad thermal hysteresis of $\Delta T = 50$ K. Unique changes of the molecular bondings during a temperature-induced phase transition are confirmed by Raman spectroscopy measurements combined with density functional theory calculations. In addition, X-ray absorption spectroscopy measurements reveal a thermally reversible soft X-ray induced excited spin-state trapping effect in the room temperature regime. Financially supported by CRC 1242 Project A05 (Project-ID 278162697).

MA 18.35 Fri 10:00 P

High-frequency Electron Paramagnetic Resonance studies on a pentagonal-bipyramidal V(III) complex — •Lena Spillecke, Changhyn Koo, and Rüdiger Klingeler — Kirchhoff-Institute for Physics, Heidelberg University, Germany

We present detailed high-frequency/high-field electron paramagnetic resonance (HF-EPR) studies as well as magnetic susceptibility measurements down to 400 mK on the first pentagonal-bipyramidal Vanadium(III) complex with a Schiff-base N_3O_2 pentadentate ligand. [1] By detailed measurements on loose and fixed powder samples we rationalized precisely the crystal field parameters and g-value information of this complex and also quantified small but finite intermolecular dimer-like antiferromagnetic magnetic coupling of $J = -1.1$ cm^{-1}. Especially the observation of intermolecular coupling is somehow surprising considering the isolated character and large distance between the V(III) centers. However, theoretical analysis reveals that the interaction between distant V(III) centers is mediated via π-stacking contacts between the ligands of neighboring complexes. In conclusion this work gives a deep insight into the magnetic properties of a V(III) complex and demonstrates how HF-EPR spectroscopy can act as powerful tool for the investigation of magnetic properties.

[1] *Bazhenova et al., Dalton Trans. 49, 15287-15298 (2020)*

MA 18.36 Fri 10:00 P

High-frequency EPR study on the exchange couplings in 3d-4f heterometallic complexes with diverse structures — •Changhyun Koo[1], Lena Spillecke[1], Silvia Menghi[1], Sebastian Schmidt[2], Yan Peng[2], Naushad Ahmed[3], Maheswaran Shanmugam[3], Annie K. Powell[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Institute of Inorganic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany. — [3]Department of Chemistry, Indian Institute of Technology, Mumbai, India.

3d-4f heterometallic complexes are suggested to enhance the magnetic anisotropy barrier in single molecular magnets (SMM) candidate metal organic complexes as combining benefits of 3d and 4f magnetic ions. Though the exchange coupling between 3d and 4f ions, J_{3d-4f}, is essential, its quantitative determination is still challenging. In this presentation, the precise J_{3d-4f} values in several 3d-4f heterometallic complexes with various molecular structures, i.e. Cu_2Ln with linear bonding, Fe_4Ln_2 with ring-like structure, and Fe_2Ln_2 butterfly-like structure (Ln = Tb, Dy, Ho, Yb, and Gd) are determined by means of the high-frequency electron paramagnetic resonance (HF-EPR) technique. Based on the current studies, the effect of the exchange interaction on the magnetic properties of the complexes is discussed.

MA 18.37 Fri 10:00 P

Thermal- and Light-Induced Spin-Crossover Characteristics of a Functional Iron(II) Complex at Submonolayer Coverage on HOPG — •Sangeeta Thakur[1], Evangelos Golias[1], Ivar Kumberg[1], Kuppusamy S. Kumar[2], Rahil Hosseinifar[1], Jorge Torres[1], Lalminthang Kipgen[1], Christian Lotze[1], Lucas M. Arruda[1], Florin Radu[3], Mario Ruben[2], and Wolfgang Kuch[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Berlin, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

The role of molecule-substrate interactions on the thermal- and light-induced spin-state switching characteristics of 0.4 monolayer of a functional spin-crossover(SCO)-complex $[Fe(H_2B(pz)_2)_2COOC_{12}H_{25}\text{-bipy}]$ on a highly oriented pyrolytic graphite (HOPG) substrate was studied using x-ray absorption spectroscopy [1]. A spin-state coexistence of 42% low-spin (LS) and 58% high-spin (HS) is observed for the complex at 40 K, in contrast to the complete spin-state switching observed in the bulk and in SiOx-bound 10 nm thick films [2], highlighting the role of molecule-substrate interactions. The 100% HS state obtained after light irradiation at 10 K indicates the occurrence of efficient on-surface light-induced spin switching, encouraging the development of light-addressable molecular devices based on SCO complexes.

[1] S. Thakur et al. J. Phys. Chem. C 125, 25, (2021).
[2] K. S. Kumar et al., Adv. Mater. 30, 1705416, (2018).

MA 18.38 Fri 10:00 P

Modeling spin-phonon relaxation in organic semi-conductors from first-principles — •Uday Chopra, Erik R. McNellis, and Jairo Sinova — Johannes Gutenberg University, Staudingerweg 7, Mainz 55128

Spin-orbit coupling (SOC) is one of the major causes of spin-relaxation in organic semiconductors. It generally works in conjunction with other factors, for example a hopping driven spin-flip mechanism [1,2]. In this work, we explore spin-relaxation caused due to molecular vibrations. We present a model to estimate the spin-phonon couplings using finite-differences within harmonic approximation from a first-principles approach. Using these couplings we are able to derive the spin-relaxation times (T1) between the Zeeman energy levels for Raman-like processes using the Fermi's Golden rule. Our model assumes a relaxation mediated via two phonons via an intermediate state. This enables us to evaluate and predict the temperature dependence of T1 and analyse the contribution of relevant phonon-modes that dominate the relaxation. We present our findings using organic-semiconductors and single-molecule magnets to demonstrate transferability across different systems. [1] Chopra et al. Phys. Rev. B 100, 134410 (2019) [2] Chopra et al. J. Phys. Chem. C 123, 19112, (2019)

MA 18.39 Fri 10:00 P

Optical control of 4f orbital state in rare-earth metals — N. Thielemann-Kühn[1], •T. Amrhein[1], W. Bronsch[1], S. Jana[2], N. Pontius[2], R. Engel[3], P. Miedema[3], D. Legut[4], K. Carva[5], U. Atxitia[1], B. Van Kuiken[6], M. Teichmann[6], R. Carley[6], L. Mercadier[6], A. Yaroslavtsev[6,7], G. Mercurio[6], L. Le Guyader[6], N. Agarwal[6], R. Gort[6], A. Scherz[6], M. Beye[3], P. Oppeneer[7], M. Weinelt[1], and C. Schüssler-Langeheine[2] — [1]Freie Universität Berlin — [2]HZB — [3]DESY — [4]IT4Innovations — [5]Charles University — [6]European XFEL — [7]Uppsala University

High density magnetic storage devices base on materials with large magneto crystalline anisotropy (MCA) that needs to be overcome by laser heating above the Curie temperature to enable bit writing [1]. In a time-resolved X-ray absorption experiment at the European XFEL we found that the MCA itself can be manipulated on fs time scales by an optical stimulus [2]. In 4f rare-earth metals the magnetic moment and high MCA stems from the 4f system that is not directly accessible with optical wavelengths. We show, however, that the direct excitation of 5d electrons drives 4f-5d inelastic electron scattering and 4f-5d electron transfer, initiating orbital excitations in the 4f shell that change the MCA tremendously. Besides the technological relevance of such handle on MCA, 4f electronic excitations directly alter exchange and electron-phonon coupling and thus contribute to a more fundamental understanding of non-equilibrium dynamics.

[1] W. Challener et al. Nature Photon 3, 220-224 (2009).
[2] arXiv:2106.09999

MA 18.40 Fri 10:00 P

Characterization of superconducting niobium lumped-element-resonators for strong magnon-photon coupling to yttrium-iron-garnet (YIG) structures — •Philipp Geyer[1], Karl Heimrich[1], Philip Trempler[1], Frank Heyroth[2], Sandra Gottwals[1], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Nanotechnikum Weinberg, 06120 Halle (Saale), Germany

In the past years the field of hybrid quantum magnonics appears a promising candidate for quantum information processing. Here, magnons can be an important mediator for coupling between different quantum states [1]. We investigate superconducting Nb lumped-element-resonators grown on annealed sapphire (0001) substrates. The resonators are fabricated by optical lithography, Nb sputtering and lift-off. The deposition of niobium was done by argon ion sputtering at room-temperature and the niobium was not covered by a protecting layer. Nevertheless, we observe for 50 nm thin films superconducting transition temperatures above 7 K and sufficiently high critical B-fields. Our work is focused on resonators which excite preferably high localized magnetic fields. YIG particles will be transferred from high quality free standing YIG microstructures to achieve strong coupling between microwave photons and magnons [3]. [1] D. Lachange-Quirion et.Al. Science, Vol. 367, Issue 6476, pp. 425-428 (2020) [2] P. Trempler et. Al. Appl. Phys. Lett. 117, 232401 (2020)

MA 18.41 Fri 10:00 P

Mapping the Stray Fields of a Micromagnet Using Spin Centers in SiC — •Mauricio Bejarano[1,2], Francisco Jose Trindade Goncalves[1], Michael Hollenbach[1,2], Toni Hache[1,3], Tobias Hula[1,3], Yonder Berencén[1], Jürgen Fassbender[1], Manfred Helm[1], Georgy V. Astakhov[1], and Helmut Schultheiss[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Technische Universität Chemnitz, 09107 Chemnitz, Germany

We report on utilizing an ensemble of V_{Si} centers as a room-temperature sensor of static stray fields generated by magnetic microstructures patterned on top of a SiC substrate. We use optically-detected magnetic resonance (ODMR) to measure the impact of the stray fields on the intrinsic V_{Si} resonance frequencies. The spin resonance at the spin centers is driven by a micrometer-sized microwave antenna patterned next to the magnetic element. The antenna pattern is made to ensure that the driving microwave fields are delivered locally and more efficiently compared to conventional millimeter-sized circuits. We observe a spatially dependent frequency shift of the V_{Si} resonances which enables us to determine the field contribution from the magnetic element in its close vicinity. Our results are a first step toward developing magnon-quantum applications by deploying local microwave fields and stray fields at the micrometer length scale. This work was supported in part by the German Research Foundation under Grants SCHU 2922/4-1 and AS 310/5-1.

MA 18.42 Fri 10:00 P

Optical read-out of the Néel vector in metallic antiferromagnet Mn_2Au — •V. Grigorev[1], M. Filianina[1], S. Yu. Bodnar[1], S. Sobolev[1], N. Bhattacharjee[1], S. Bommanaboyena[1], Y. Lytvynenko[1], Y. Skourski[2], D. Fuchs[3], M. Klaeui[1], M. Jourdan[1], and J. Demsar[1] — [1]Institute of Physics, Uni Mainz, 55128 Mainz, Germany — [2]HLD-EMFL, HZDR, 01328 Dresden, Germany — [3]IQMT, KIT, 76344 Eggenstein-Leopoldshafen, Germany

Metallic antiferromagnets with broken inversion symmetry on the two sublattices, strong spin-orbit coupling and high Néel temperatures offer new opportunities for applications in spintronics. Especially Mn_2Au, with high Néel temperature and conductivity, is particularly interesting for real-world applications. The read-out of the staggered magnetization, *i.e.* the Néel vector is limited to studies of anisotropic magnetoresistance or X-ray magnetic linear dichroism. Here, we report on the in-plane reflectivity anisotropy of Mn_2Au (001) films, which were Néel vector aligned in pulsed magnetic field. In the near-infrared, the anisotropy is ≈ 0.6%, with higher reflectivity for the light polarized along the Néel vector. The observed magnetic linear dichroism is about four times larger than the anisotropic magnetoresistance, suggesting the dichroism in Mn_2Au is a result of the strong spin-orbit interactions giving rise to anisotropy of interband optical transitions, in-line with recent studies of electronic band-structure. The considerable magnetic linear dichroism in the near-infrared could be used for ultrafast optical read-out of the Néel vector in Mn_2Au.

MA 19: PhD Focus Session: Symposium on "Magnetism - A Potential Platform for Big Data?" (joint session MA/O/AKjDPG)

As pointed out in a recent Nature editorial article titled "Big data needs a hardware revolution", new technologies and hardware architectures are necessary in order to cope with the ever increasing amount of information. Google's AlphaGo's success apprised of the potential of parallel computing, yet energy efficiency remained as a major challenge. Hardware developers came up with mimicking the human brain as the most efficient processor, leading to the field of neuromorphic computing. An immense amount of research is deployed in different fields to screen for fast, low energy consuming and scalable solutions. In this focus session we elucidate on the potential role of magnetism in the development of non-Von Neumann hardware platforms to fulfill the current needs of AI and Big Data. An introduction to neuromorphic computing is followed by implementations of magnetic devices for processing and data storage in the information age. We finalise with a panel conversation with the speakers, where we aim to discuss the potential of magnetic-based devices in helping solve current challenges in the field of brain-inspired computing.

Organizers: Mauricio Bejarano and Tobias Hula (Helmholtz-Zentrum Dresden Rossendorf), Luis Flacke (Walther-Meissner Institute and TU Munich)

Time: Friday 13:30–16:30 Location: H5

Invited Talk MA 19.1 Fri 13:30 H5

"Neuromorphic Computing": A Productive Contradiction in Terms — •Herbert Jaeger — Rijksuniversiteit Groningen (NL) Faculty of Science and Engineering - CogniGron

The term "computing" has a specific, firm, powerful, traditional meaning – condensed in the paradigm of Turing computability (TC). A core aspect of TC is the perfectly reliable composition of perfectly identifiable symbolic tokens into complex, hierarchical symbolic structures. But all which is novel and promising and original in "neuromorphic" information processing leads away from such perfect symbolic compositionality. Apparently new formal conceptions of "computing" would be most welcome (and a new term for it, too). In my talk I will carve out a number of concrete aspects that separate neuromorphic information processing from symbolic computing - some of them being classical topics in the philosophy of AI, others having more recently emerged from technological progress in non-digital hardware.

Invited Talk MA 19.2 Fri 14:00 H5

Neuromorphic computing with radiofrequency spintronic devices — •Alice Mizrahi[1], Nathan Leroux[1], Danijela Markovic[1], Dedalo Sanz Hernandez[1], Juan Trastoy[1], Paolo Bortolotti[1], Leandro Martins[2], Alex Jenkins[2], Ricardo Ferreira[2], and Julie Grollier[1] — [1]Unité Mixte de Physique CNRS, Thales, Université Paris-Saclay, 91767 Palaiseau, France — [2]International Iberian Nanotechnology Laboratory (INL), 4715-31 Braga, Portugal

The need for energy efficient artificial intelligence has motivated research on the implementation of neural networks in hardware, using emerging technology. In particular, spintronic nano-oscillators have emerged as promising candidates to emulate neurons due to their non-linear behavior. However, in order to scale such systems to deep neural network capable of performing state of the art artificial intelligence tasks, it is necessary to have physical synapses – which weights can be tuned –connecting the neurons. Here we propose a scalable architecture for neural networks using spintronic RF oscillators as neurons and spintronic RF resonators as synapses. First, we show how individual spintronic resonators, and in particular magnetic tunnel junctions, can multiply RF signals by a tunable weight, thus emulating synapses. Then, we show how to assemble these devices into chains performing the multiply and accumulate function, which is at the core of neural network. Finally, we show how to assemble a full neural network and perform classification tasks. These results open the path for compact and energy efficient deep neural networks.

10 min. break.

Invited Talk MA 19.3 Fri 14:40 H5

Data Storage and Processing in the Cognitive Era — •Giovanni Cherubini — IBM Research - Zurich

In this talk, I will present the emerging vision of cognitive data systems. A data system comprises physical devices that provide means to acquire, store and modify data for analytics and communications tasks, with the goal of obtaining high-value information. With the need to deal with exponentially growing amounts of data, however, the system size and complexity present major challenges for data storage and processing. In addition, with the approaching end of Moore's law, there is a dire need to significantly improve the energy efficiency of data systems. To address these challenges, cognitive data systems will require novel learning algorithms and computing paradigms. The talk will be divided into two parts, focusing on data storage and processing aspects. First, I will present advanced technologies for big data storage systems, with focus on magnetic tape drives of future generations, targeting areal densities of several hundred gigabits per square inch on a flexible medium. Next, I will introduce novel in-memory computing techniques and devices that are based on non-von Neumann architectures and aim at achieving the efficiency of the human brain.

Invited Talk MA 19.4 Fri 15:10 H5

Brain-inspired approaches and ultrafast magnetism for Green ICT — •Theo Rasing — Radboud University, Institute for Molecules and Materials, Heijendaalseweg 135, 6525AJ Nijmegen, the Netherlands

The explosive growth of digital data use and storage has led to an enormous rise in global energy consumption of Information and Communication Technology (ICT), which already stands at 7% of the world electricity consumption. New ICT technologies, such as Artificial Intelligence push this exponentially increasing energy requirement even more, though the underlying hardware paradigm is utterly inefficient: tasks like pattern recognition can be performed by the human brain with only 20W, while conventional (super)computers require 10 MW. Therefore, the development of radically new physical principles that combine energy-efficiency with high speeds and high densities is crucial for a sustainable future. One of those is the use of non-thermodynamic routes that promises orders of magnitude faster and more energy efficient manipulation of bits. Another one is neuromorphic computing, that is inspired by the notion that our brain uses a million times less energy than a supercomputer while, at least for some tasks, it even outperforms the latter. In this talk, I will discuss the state of the art in ultrafast manipulation of magnetic bits and present some first results to implement brain-inspired computing concepts in magnetic materials that operate close to these ultimate limits.

10 min. break.

Discussion MA 19.5 Fri 15:50 H5

Panel discussion PhD Focus Session — •Tobias Hula[1], Mauricio Bejarano[1], and Luis Flacke[2] — [1]Helmholtz-Zentrum Dresden Rossendorf — [2]Walther-Meissner Institute and TU Munich

Panel discussion for PhD Focus Session:"Magnetism - A Potential Platform for Big Data?"

Metal and Material Physics Division
Fachverband Metall- und Materialphysik (MM)

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On this conference the Metals and Materials Division sets a topical focus on interface-dominated phenomena: segregation, nucleation and phase transformations.

The overall properties of modern nano-structured metals and alloys are to a large extent determined by the mechanical and kinetic behavior of the interfaces in their microstructure. Therefore, a precise characterization and understanding of the processes at interfaces is a key to effective alloy development. In this symposium, we want to review the state of the art in theoretical and experimental analysis, as well as in modeling of interface structure and evolution as a response to annealing, segregation, irradiation, and mechanical deformation, as well as the coupling between these processes. In particular, we focus on contributions on atomistic, micro- and multiscale simulations of interface dominated microstructures, on the experimental characterization and mechanical testing of such structures, as well as on the development of thermodynamic and micromechanical models of interfacial effects.

Overview of Invited Talks and Sessions

(Lecture halls H2 and H8; Poster P)

Invited Talks

MM 1.1	Mon	10:00–10:30	H8	**Using mobile interfaces to rapidly move atoms and create sharp chemical boundaries in Fe-C-Mn alloys** — •Sybrand van der Zwaag
MM 4.1	Mon	15:15–15:45	H2	**Investigation of the early stage of reactive interdiffusion in the Cu-Al system by in-situ transmission electron microscopy** — Florent Moisy, •Xavier Sauvage, Eric Hug
MM 6.1	Wed	10:00–10:30	H8	**CALPHAD-informed density-based grain boundary thermodynamics** — •Reza Darvishi Kamachali, Lei Wang, Linlin Li, Anna Manzoni, Birgit Skrotzki, Gregory Thompson
MM 7.1	Wed	11:15–11:45	H8	**Computational methods for grain boundary segregation in metallic alloys** — •Lorenz Romaner, Daniel Scheiber, Vsevolod Razumovskiy, Oleg Peil, Christoph Dösinger, Alexander Reichmann

Plenary Talk

PV VIII	Tue	16:30–17:15	Audimax 1	**The Structural Origins of Wood Cell Wall Toughness** — •Cynthia Volkert

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium Potentials for NVs sensing magnetic phases, textures and excitations (SYNV)

See SYNV for the full program of the symposium.

SYNV 1.1	Mon	13:30–14:00	Audimax 2	**Harnessing Nitrogen Vacancy Centers in Diamond for Next-Generation Quantum Science and Technology** — •Chunhui Du
SYNV 1.2	Mon	14:00–14:30	Audimax 2	**Nanoscale imaging of spin textures with single spins in diamond** — •Patrick Maletinsky
SYNV 1.3	Mon	14:30–15:00	Audimax 2	**Spin-based microscopy of 2D magnetic systems** — •Jörg Wrachtrup
SYNV 1.4	Mon	15:15–15:45	Audimax 2	**Exploring antiferromagnetic order at the nanoscale with a single spin microscope** — •Vincent Jacques
SYNV 1.5	Mon	15:45–16:15	Audimax 2	**Nanoscale magnetic resonance spectroscopy with NV-diamond quantum sensors** — •Dominik Bucher

Invited talks of the joint symposium Amorphous materials: structure, dynamics, properties (SYAM)

See SYAM for the full program of the symposium.

SYAM 1.1	Tue	13:30–14:00	Audimax 1	**Glassy dynamics of vitrimers** — •Liesbeth Janssen
SYAM 1.2	Tue	14:00–14:30	Audimax 1	**Liquid-Liquid Phase Transition in Thin Vapor-Deposited Glass Films** — •Zahra Fakhraai
SYAM 1.3	Tue	14:30–15:00	Audimax 1	**Connection between structural properties and atomic motion in ultraviscous metallic liquids close to the dynamical arrest** — •Beatrice Ruta, Nico Neuber, Isabella Gallino, Ralf Busch
SYAM 1.4	Tue	15:15–15:45	Audimax 1	**Signatures of the spatial extent of plastic events in the yielding transition in amorphous solids** — •Celine Ruscher, Daniel Korchinski, Joerg Rottler
SYAM 1.5	Tue	15:45–16:15	Audimax 1	**Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment** — •Olfa D'Angelo, W. Till Kranz

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Diversity on the Device Scale (SYHN)

See SYHN for the full program of the symposium.

SYHN 1.1	Thu	10:00–10:30	Audimax 1	**Scaling behavior of stiffness and strength of hierarchical network nanomaterials** — •Shan Shi
SYHN 1.2	Thu	10:30–11:00	Audimax 1	**Functional and programmable DNA nanotechnology** — •Laura Na Liu
SYHN 1.3	Thu	11:15–11:45	Audimax 1	**Multivalent nanoparticles for targeted binding** — •Stefano Angioletti-Uberti
SYHN 1.4	Thu	11:45–12:15	Audimax 1	**Programming Nanoscale Self-Assembly** — •Oleg Gang
SYHN 1.5	Thu	12:15–12:45	Audimax 1	**Achieving Global Tunability via Local Programming of a Structure's Composition** — •Jochen Mueller

Invited talks of the joint symposium The Rise of Photonic Quantum Technologies – Practical and Fundamental Aspects (SYPQ)

See SYPQ for the full program of the symposium.

SYPQ 1.1	Fri	10:00–10:30	Audimax 2	**Quantum dots operating at telecom wavelengths for photonic quantum technology** — •Simone Luca Portalupi
SYPQ 1.2	Fri	10:30–11:00	Audimax 2	**Photonic graph states for quantum communication and quantum computing** — •Stefanie Barz
SYPQ 1.3	Fri	11:00–11:30	Audimax 2	**Rare-earth ion doped solids at sub-Kelvins: practical and fundamental aspects** — •Pavel Bushev
SYPQ 1.4	Fri	11:45–12:15	Audimax 2	**Quantum Light and Strongly Correlated Electronic States in a Moiré Heterostructure** — •Brian Gerardot
SYPQ 1.5	Fri	12:15–12:45	Audimax 2	**Quantum communication in fibers and free-space** — •Rupert Ursin

Sessions

MM 1.1–1.3	Mon	10:00–11:00	H8	**Topical Session Interface-Dominated Phenomena - Moving Interfaces**
MM 2.1–2.6	Mon	11:15–12:45	H8	**Topical Session Interface-Dominated Phemomena - Moving Interfaces / Functional Properties**
MM 3.1–3.6	Mon	13:30–15:00	H2	**Topical Session Interface-Dominated Phenomena - Defect Structures and Mechanical Properties**
MM 4.1–4.3	Mon	15:15–16:15	H2	**Topical Session Interface-Dominated Phenomena - Diffusion**
MM 5.1–5.13	Tue	10:00–12:45	P	**Topical Session Interface Dominated Phenomena - Poster**
MM 6.1–6.3	Wed	10:00–11:00	H8	**Topical Session Interface-Dominated Phenomena - Thermodynamics**
MM 7.1–7.5	Wed	11:15–12:45	H8	**Topical Session Interface-Dominated Phenomena - Segregation and Embrittlement**
MM 8	Wed	18:00–19:00	MVMM	**Annual General Meeting**

Annual General Meeting of the Metal and Material Physics Division

Wednesday 18:00–19:00 Online Session (session link will be announced in time)

Sessions

– Invited Talks, Contributed Talks, and Posters –

MM 1: Topical Session Interface-Dominated Phenomena - Moving Interfaces

Time: Monday 10:00–11:00 Location: H8

Invited Talk MM 1.1 Mon 10:00 H8

Using mobile interfaces to rapidly move atoms and create sharp chemical boundaries in Fe-C-Mn alloys — •Sybrand van der Zwaag — TU Delft, Delft, the Netherlands

In this presentation we will show how cyclic partial phase transformations in Fe-X alloys and low alloyed steels can be used to rapidly displace substitutional solute atoms and to leave behind ridges of solute atoms upon reversal of the interface migration. These enriched regions locally retard the passing interfaces during a subsequent transformation and this causes a macroscopically detectable halting of the rate of transformation and/or a change in resulting microstructure.

The concept works not only for diffusional and bainitic phase transformations but can (under well-selected conditions) also be used to manipulate the austenite to martensite transformation and to create nano-structured medium Mn steels with exceptional mechanical properties such as a strength above 2 GPa and a uniform elongation in excess of 20%.

The experimental observations are linked to 1D and 3D transformation models and in-situ TEM observations of the moving interface.

MM 1.2 Mon 10:30 H8

Abnormal grain growth in nanocrystalline PdAu: The Case of the Fractal Fingerprint — Raphael A. Zeller[1], Christian Braun[2], Markus Fischer[1], Jörg Schmauch[2], Christian Kübel[3], Rainer Birringer[2], and •Carl E. Krill III[1] — [1]Institute of Functional Nanosystems, Ulm University, Ulm, Germany — [2]Department of Experimental Physics, Saarland University, Saarbrücken, Germany — [3]Karlsruhe Nano Micro Facility, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

In most polycrystalline materials, coarsening tends to be a civilized affair, with adjacent grains taking pains to exchange atoms so as to maintain a smooth boundary. The grains that grow in nanocrystalline PdAu, however, behave like uncouth neighbors crashing a fancy dinner party: once they get revved up, all hell breaks loose! Before you know it, a few nanometer-sized grains have grown four orders of magnitude in diameter, and the resulting interfaces are so convoluted that they resemble fractal objects. Our usual notion of curvature-driven grain boundary migration fails to explain the persistence of these interfacial fluctuations, but recent experiments find the onset of fractality to depend on the Au concentration as well as on a characteristic length scale. We consider this evidence to be a kind of "fractal fingerprint" that, ultimately, incriminates a specific mechanism as being responsible for the system's abnormal grain growth.

MM 1.3 Mon 10:45 H8

Dislocation path and long-range strain associated with interface migration — •Jin-yu Zhang, Zhi-peng Sun, Fu-zhi Dai, and Wen-zheng Zhang — School of Materials Science and Engineering, Tsinghua University, Beijing

Major interphase interfaces generated from phase transformations in steels or Ti alloys are semicoherent. The knowledge of dislocation motion and long-range strain accompanying the interface migration is fundamental to the understanding of phase transformations. In this study, we performed a molecular dynamics simulation on the migration of various α/β interfaces in pure Ti. The simulation results explicitly demonstrated that the interfacial dislocation path can deviate significantly from the slip planes of individual dislocations due to the dislocation interaction when the interface contains multiple sets of dislocations. For these complex situations, previous theories based on conventional slip planes would lead to either non-atom-conservation or slip-sequence-dependent results. We developed a new geometric model, which is capable to generate self-consistent descriptions on the dislocation path and the shear displacement during migration of a general semicoherent interface, in the condition that atoms are conserved during interface migration. This model is validated by the simulations and it covers the simple cases applicable by previous theories. The present study offers new insight into the dislocation path during interface migration and provides a general framework for evaluating the long-range strain caused by interface migration during a phase transformation process, such as precipitation and martensite transformation.

MM 2: Topical Session Interface-Dominated Phemomena - Moving Interfaces / Functional Properties

Time: Monday 11:15–12:45 Location: H8

MM 2.1 Mon 11:15 H8

Theory and modeling of the austenite-martensite interface structure and glissile transformation in steels — •Francesco Maresca[1] and William Curtin[2] — [1]University of Groningen, Groningen, Netherlands — [2]EPFL, Lausanne, Switzerland

The austenite-martensite (fcc-bcc) transformation controls the formation of microstructures in a wide range of high strength steels. Recent progress in the physical metallurgy of steels has shown that nanolaminate austenite/martensite microstructures contribute to high material toughness and resistance to hydrogen-embrittlement. Despite its relevance for applications, there is no established theory for the transformation capable to predict the contribution of the austenite-martensite phase transformation to ductility. To clarify the mechanism of transformation, we have performed atomistic simulations of the interface reproducing the major experimental TEM and HRTEM observations in Fe alloys. The atomistic model reveals for the first time the structure and motion of the athermal and glissile fcc austenite/bcc martensite interface in steels. The interface structure consists of [-101](111)fcc screws, as envisioned by previous theories, and [1-11](-101)bcc screws with kinks, which was not envisioned before. The atomistic findings have guided the formulation of a new, parameter-free double-shear predictive theory of martensite crystallography. Theory predictions show that the fcc/bcc lattice parameter ratio is the key factor controlling the shape deformation (i.e. the in-situ transformation strain), which can achieve more than 90%, namely three times the existing experimental estimates. The theory can be used to guide design of tougher AHSS.

MM 2.2 Mon 11:30 H8

Atomistic simulation of grain boundary phases and transitions in fcc metals — •Tobias Brink and Gerhard Dehm — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Grain boundaries (GBs) can be treated as interface phases (also called "complexions") with different thermodynamic excess properties. Congruent phase transitions in pure metals—where the macroscopic GB parameters remain constant—are hard to observe experimentally, but GB phases with distinct atomic structures could recently be identified in a copper tilt GB (Meiners et al., Nature 579, 2020). It remains an open question if such phases are specific to this copper GB or a more general feature of fcc metals. Using molecular dynamics computer simulations, we investigated both Cu and Al ⟨111⟩ tilt GBs with different misorientations to verify if the copper GB phases can indeed be generalized. We furthermore used simulations with Lennard-Jones pair potentials to determine how much materials physics needs to be included in the model to recover the phases of the more realistic potentials. Recurring structural motifs appeared in all of these systems, but we found that the actual material strongly influences which phases occur and their stability. This probably excludes the possibility of deriving simple rules for the atomic structure of GB phases.

Acknowledgment: This result is part of a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 787446; GB-CORRELATE).

MM 2.3 Mon 11:45 H8

Simulations of a fs laser induced A7 to sc transition in antimony — •Bernd Bauerhenne[1,2], Felipe Valencia[3], and Martin E. Garcia[1,2] — [1]Theoretische Physik - Universität Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany — [2]Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), Heinrich-Plett-Strasse 40, D-34132 Kassel, Germany — [3]Physics Department, Universidad Nacional de Colombia, Edificio 404, Ciudad Universitaria, Bogota, Colombia

We simulated the fs laser excitation of a 50 nm thick free standing antimony film using more than 4 million atoms. In our simulations, we condidered the laser-induced changes of the potential energy surface and the effects of the incoherent electron-phonon collisions - the electron-phonon coupling - into account. To do so, we derived an electronic temperature (Te) dependent interatomic potential for antimony. For this, we fitted forces and energies obtained from ab-initio MD simulations of a thin antimony film at increased Te. Furthermore, we calculated the Te-depend electron-phonon coupling constant for antimony ab-initio. In our large-scale MD simulations, we observed a laser induced A7 to sc like transition at moderate intensities. If the excitation intensity is further reduced, the transition starts at the surface and moves to the center of the film. In addtion, we analyzed the influeces of the laser-induced changes of the potential energy surface and of the electron-phonon coupling on the transition.

MM 2.4 Mon 12:00 H8

Nanoscale Friction Under Active Control in Systems With Tailored Degrees of Freedom — •Niklas A. Weber[1], Miru Lee[2], Richard L.C. Vink[1], Matthias Krüger[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

In this project, we use lateral force microscopy to investigate how friction of manganite films can be controlled by the properties of the surrounding materials. Specifically, we use phase transformations [1,2] and superlattice thin film samples [3] to actively control the film properties while keeping the surfaces unchanged.

We observed an increase in friction during resistive switching of a $La_{0.55}Ca_{0.45}MnO_3$ film [1] and during heating of a $La_xSr_{1-x}MnO_3$ thin film through the metal-insulator phase transformation [2]. Careful consideration of the different contributions and comparison with literature lead to the conclusion that the electronic contributions are not sufficient to account for our observations and make phononic contributions a promising candidate.

To test our hypothesis, we have started to perform measurements on $LaMnO_3/SrMnO_3$ superlattice systems in which the propagation of phonons can be actively manipulated by the layer spacing [3], while the morphology of the surface layer remains unchanged.

[1] H. Schmidt et.al., Phys. Rev. Mater. 2020, 4, 113610.
[2] N. A. Weber et.al., Adv. Sci. 2021, 2003524.
[3] D. Meyer et al., arXiv:2009.14532v3.

MM 2.5 Mon 12:15 H8

Interplay of domain structure and phase transitions in ferroelectric $BaTiO_3$ — Madhura Marathe, Ruben Khachaturyan, Yijing Yang, and •Anna Grünebohm — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Domain walls and phase boundaries are fundamental ingredients of ferroelectrics and strongly influence their functional properties. Although both interfaces have been studied for decades, often only a phenomenological macroscopic understanding has been established and it is now timely to revisit nucleation and the coupling of domains and phase transitions on an atomistic level [1]. We study domain walls in $BaTiO_3$ by means of molecular dynamics simulations based on the effective Hamiltonian approach [2]. We show that domain walls may promote the tetragonal to orthorhombic phase transition [3] and can act as nucleation centers.

[1] A. Grünebohm et al., Interplay of domain structure and phase transitions: theory, experiments and functionality, (2021).
[2] Nishimatsu et al., Phys. Rev. B 78, 104104 (2008).
[3] A. Grünebohm and M. Marathe, Phys. Rev. Mater. 4, 114417 (2020).

MM 2.6 Mon 12:30 H8

Optical properties of 3D nanosponge models created by phase-field simulations — •Malte Grunert[1], Sebastian Bohm[1], Hauke Lars Honig[1], Dong Wang[1], Jinhui Zhong[2], Peter Schaaf[1], Christoph Lienau[2], and Erich Runge[1] — [1]Technische Universität Ilmenau, Germany — [2]University of Oldenburg, Germany

We present an efficient method for the numerical creation of three-dimensional nanoporous sponge models with specified geometric properties. Such nanoporous structures can be manufactured with different geometric properties and exhibit fascinating optical properties [1,2]. We show how phase-field simulations can be used to obtain nanoporous structures with predefined optical and structural characteristics. The sponge geometries generated in this way show excellent similarity to experimentally produced sponges and the averaged geometric properties are comparable. In addition, the optical properties such as the absorption and scattering cross sections are similar. The computer-generated sponges also exhibit experimentally confirmed optical properties such as strong spatial localization of fields and the associated strong local field enhancement.

[1] G. Hergert, J. Vogelsang, F. Schwarz, D.Wang, H. Kollmann, P. Groß, C. Lienau, E. Runge and P. Schaaf, *Long-lived electron emission reveals localized plasmon modes in disordered nanosponge antennas*, Light: Science & Applications **6**, e17075 (2017).
[2] J. Zhong et al., *Nonlinear plasmon-exciton coupling enhances sum-frequency generation from a hybrid metal/semiconductor nanostructure*, Nature Communications **11**, 1464 (2020)

MM 3: Topical Session Interface-Dominated Phenomena - Defect Structures and Mechanical Properties

Time: Monday 13:30–15:00 Location: H2

MM 3.1 Mon 13:30 H2

Imaging the Deformation-Induced Accumulation of Defects in Nanoporous Gold — •Maowen Liu[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Hereon

Nanoporous gold (NPG) provides a model material for studying small-scale deformation and the mechanical behavior of network solids. While studies of nanopillars indicate dislocation starvation, the strain hardening of NPG suggests dislocation accumulation. Yet, the approach to confirm that latter process by direct experimental observation, namely transmission electron microscopy (TEM), is impaired by the need to distinguish native defects in the microstructure from artifacts due to sample slicing or thinning. Here, we report a TEM study of the defect structure in electron-transparent NPG leaf deformed by rolling. The results confirm that plastic deformation significantly enhances the defect density. Specifically, twins are formed on several crystallographic planes, and their interaction forms Lomer-Cottrell locks. This inhibits dislocation escaping from NPG, thus avoiding the dislocation starvation scenario that is often considered in the "smaller is stronger" context of small-scale plasticity. Instead, strain-hardening is apparently linked to accumulation and interaction of twins.

MM 3.2 Mon 13:45 H2

How the interface type manipulates the thermomechanical response of nanostructured metals: A case study on nickel — •Oliver Renk[1], Verena Maier-Kiener[2], Christian Motz[3], Daniel Kiener[2], Jürgen Eckert[1], and Reinhard Pippan[1] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria — [2]Montanuniversität Leoben — [3]Saarland University, Germany

The presence of interfaces with nanoscale spacing significantly enhances the strength of materials, but also changes the rate controlling processes of plastic flow. Due to the confined grain volumes, intragranular dislocation-dislocation interactions are replaced by emission and absorption of dislocations from and at the interfaces. Both processes not only depend on the interfacial spacing, but also on the interface structure. The present study attempts to rationalize this effect by investigating the thermomechanical behavior of samples consisting of three different interfaces. Nickel samples with predominant fractions of low- and high-angle as well as twin boundaries with a similar average spacing of 150 nm are investigated using high temperature nanoindentation strain rate jump tests. Depending on the interface structure, hardness, strain rate sensitivity and apparent activation volumes evolve different with temperature. While in case of high-angle boundaries for all quantities a pronounced thermal dependence is found, the other two interface types behave almost athermal. These differences can be rationalized based on the different interfacial diffusivity, affecting the predominant process of interfacial stress relaxation.

MM 3.3 Mon 14:00 H2

Atomistic simulation study of grain boundary migration for different complexions in copper — •Swetha Pemma[1], Rebecca Janisch[2], Gerhard Dehm[1], and Tobias Brink[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Interdisciplinary Centre of Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, 44780 Bochum, Germany

Grain boundary (GB) migration is significant to study the microstructural evolution which determines the properties of polycrystalline materials. Previous studies showed that the coupling between applied shear and GB migration differed for different complexions on the same GB. In this work, shear coupled grain boundary migration (SCGBM) of two complexions ("pearl" and "domino") observed experimentally in $\Sigma 19b$ $\langle 111 \rangle$ tilt GBs in copper was investigated by molecular dynamics simulations. Effects of these complexions on the shear-coupling factor, critical shear stress for GB motion, and elementary GB migration mechanism were analysed. The coupling factors of the complexions were observed to be of same magnitude and sign for several temperatures and shear velocities.

However, the critical shear stress differs by 31 % between pearl and domino, indicating a difference in activation barriers. Additionally, the precise atomistic mechanisms of SCGBM were examined using nudged elastic band calculations.

Acknowledgment: This result is part of a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 787446; GB-CORRELATE).

MM 3.4 Mon 14:15 H2

Prismatic slip in pure Magnesium with a Neural Network Potential — •Markus Stricker[1] and William A. Curtin[2] — [1]ICAMS, Ruhr-Universität Bochum, Germany — [2]LAMMM, EPFL, Lausanne, Switzerland

Studying fundamental mechanisms of deformation in metals and alloys requires dependable interatomic potentials because dislocations and cracks are above scales accessible with first-principles calculations. While classical potential forms like the modified embedded atom method (MEAM) have been successfully employed in many cases, non-fcc metals and almost all alloys are not modeled sufficiently quantitative. As a first step towards Mg-alloys we present a broadly applicable machine learned potential for pure Magnesium in the Behler-Parrinello neural-network framework trained on first-principles density-functional theory. We show that the potential predicts dislocation and crack structures very well and subsequently apply it to cross-slip of prismatic screw dislocations, which is not accessible to first-principles approaches. Prismatic slip is achieved by double-cross-slip of stable basal dislocations in steps of c/2 driven by a shear stress on the prismatic plane. The geometry of the observed process compares very well with the process deduced from experiments, the enthalpy barrier not. This mimics the stress-driven double-kink nucleation in bcc elements: the geometry of the mechanism is predicted well, but stress and activation barriers are overestimated by first-principles predictions.

MM 3.5 Mon 14:30 H2

Ab-initio study of the Mo/SiC interfacial adhesion — •David Sebastian Kasdorf and Karsten Albe — Fachgebiet Materialmodellierung, Institut für Materialwissenschaft, TU Darmstadt, Otto-Berndt-Str. 3, Darmstadt, Germany

Mo-Si-based alloys are a potential alternative to commercially available Ni-based superalloys for high-temperature applications. While the optimization of corrosion, oxidation and creep behavior of Mo-Si-based alloys are the object of current research efforts, also materials that could act as a thermal barrier coating (and possibly bond coats) need to be identified in order to maximize the temperature capabilities. Failure modes like delamination and fractures often happen at the interfaces between the metallic substrate and ceramic top coats as the interfacial adhesion presents the limiting factor of the fracture toughness in the materials system.

We performed first-principles calculations to study the ideal work of separation and theoretical strength of Mo/SiC interfaces. In those calculations, bcc Molybdenum acts as a representative for Mo-Si-based alloys as a Mo solid solution phase is common in those alloys. Similarly, β-SiC was chosen as the second part of the interface since it is a typical high-temperature crystallization product of Si-based ceramic coatings.

MM 3.6 Mon 14:45 H2

Unravelling the lamellar size-dependent fracture behavior of fully lamellar intermetallic γ-TiAl — •Anupam Neogi and Rebecca Janisch — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Strengthening of metals by incorporating nano-scale coherent twin boundaries is one of the important breakthroughs in overcoming the strength-ductility trade-off in recent years. Also, nano-scale twin boundaries in the nano-lamellar in lightweight Ti-Al alloys promise great potential, but their contribution to the deformation and fracture behavior needs to be better understood for designing optimum microstructures. To this end, we carry out linear elastic fracture mechanics informed, large-scale atomistic simulations of fully lamellar γ-TiAl, and find, that nano-scale lamellae are not only effective in improving the fracture toughness and crack growth resistance, but the lamellar size possesses a significant controlling role on the crack tip mechanisms. The fracture initiation toughness exhibits an increasing trend with decreasing lamellar size until ~3 nm. In this regime, the crack tip events are mostly dislocation-based plasticity. Below the critical lamellar size of ~3 nm, the crack advances via a quasi-brittle manner, i.e., the cleavage of atomic bonds at the crack tip accompanied by some plasticity events, such as twin-boundary migration and dislocation nucleation. A layer-wise stacking fault energy-based analysis, including the quantitative analysis of dislocation barrier energy, elucidates the nano-scale lamellar size-dependent fracture behavior of γ-TiAl.

MM 4: Topical Session Interface-Dominated Phenomena - Diffusion

Time: Monday 15:15–16:15 Location: H2

Invited Talk MM 4.1 Mon 15:15 H2

Investigation of the early stage of reactive interdiffusion in the Cu-Al system by in-situ transmission electron microscopy — Florent Moisy[1], •Xavier Sauvage[2], and Eric Hug[1] — [1]CRISMAT Ensicaen, Caen, France — [2]GPM University Rouen Normandy, Rouen, France

The early stage of the reactive interdiffusion in the Al/Cu system was investigated by in-situ TEM at 350°C and 300°C. Original Al/Cu interfaces were created by a purely mechanical process using co-deformation at room temperature by drawing. During the reactive interdiffusion three IMCs were detected: Al2Cu and AlCu grew in the Al side and the Al4Cu9 in the Cu side. Systematic comparisons with ex-situ annealed samples and with regions out of the electron beam proved that there was no significant artefact (thin foil or beam effect). Although GBs may act as fast diffusion path, no preferential growth of IMC along these defects could be observed. The mean growth rates of all IMCs follow a classical parabolic law indicating that the kinetic of the transformation is controlled by diffusion mechanisms. A strong deviation was observed however in the early stage of the reaction. Nanoscaled Mg2Si particles located in the Al phase strongly interact with the transformation front. It leads to large fluctuations of the velocity of interphase boundaries at the nanoscale. The pinning effect in connection with change in local concentration gradients and driving forces will be discussed.

MM 4.2 Mon 15:45 H2

Silver-rich clusters reveal the initial ligament size during nanoporous gold dealloying via kinetic Monte Carlo simulation — •Yong Li[1,2], Jürgen Markmann[2,1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Hereon, Geesthacht, Germany

When nanoporous gold is made by dealloying Ag-Au, residual silver forms clusters that impact the material's functional properties. We point out that the clusters carry information on the geometry of the initial nanoscale network. Using atomistic kinetic Monte Carlo simulation, we studied the evolution of silver-rich clusters and ligament size for dealloying at various potentials. Our simulations demonstrate that dealloying involves two distinct stages. Primary dealloying generates the initial ligament network, while secondary dealloying brings coarsening of the ligaments and further dissolution. During primary dealloying, the sizes of clusters and ligaments are constant over time and they decrease with increasing dealloying potential with a Gibbs-Thompson type relation. At this stage, the ratio between ligament size and clusters size is 1.30±0.07 and independent of the potential. During secondary dealloying, the ligament size (L) for dealloying with various potentials converge to a common coarsening law, $L \propto t^{1/4}$. By contrast, the silver-clusters size still remains constant. That observation establishes that the surviving clusters provide a way to measure the initial ligament size.

MM 4.3 Mon 16:00 H2

Theoretical aspects of the reactive element effect — Andy Chen[1], Arthur Heuer[1], Matthew Foulkes[2], and •Michael Finnis[2] — [1]CWRU, Cleveland OH, U.S.A — [2]Imperial College London, UK

We are interested in the mechanism of growth of alumina scales on aluminium-containing alloys, and how the presence of certain elements such as Hf, Zr and Y operates to retard the growth of such scales, thereby improving their adherence and protective quality. These questions have been open for several decades, and are still not completely resolved [1]. We report here some recent results of experiments and theory, and in-sights that we have obtained. From tracer diffusion experiments, followed by Time of Flight - Secondary Ion Mass Spectroscopy (TOF-SIMS), diffusion coefficients of O and Al through alumina scales have been estimated and compared with measurements of weight-gain. Noting that grain boundaries are now believed to be the route for ion and electron diffusion, both of which are necessary for oxidation, we have applied Density Functional Theory to calculate the segregation energy of these reactive elements to a range of sites on grain boundaries in α-Al2O3,using our previous models of grain boundary structure [2]. Segregation of Hf and Zr and oxygen vacancies to the grain boundaries is favoured, with a spread of energies that we assess, and our calculations suggest how this may indirectly reduce the mobility of ions or electrons. Shortcomings of the classical theory of oxidation [3], originally due to Wagner, are discussed. The evidence is now overwhelming that the conventional hopping of cation and anion vacancies is not a relevant process.

[1] W. T. Chen, B. Gleeson, and A. Heuer. Oxidation of Metals, 92(3-4):137-150, 2019. [2] Hannes Guhl, Hak-Sung Lee, Paul Tangney, W. M. C. Foulkes, Arthur H. Heuer, Tsubasa Nakagawa, Yuichi Ikuhara, and Michael W. Finnis. Acta Materialia, 99:16-28, 2015. [3] A. Atkinson. Reviews of Modern Physics, 57:437-470, 1985.

MM 5: Topical Session Interface Dominated Phenomena - Poster

Time: Tuesday 10:00–12:45 Location: P

MM 5.1 Tue 10:00 P

Temperature and chemical bonding effects on the brittle-to-ductile transition in metal-metalloid glasses — •Daniel Şopu[1,2], Franco Moitzi[1], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science of the Austrian Academy of Sciences, Leoben, Austria — [2]Technische Universität Darmstadt, Darmstadt, Germany — [3]Montanuniversität Leoben, Leoben, Austria

The relationship between the deformation behavior of metal-metalloid glasses and their intrinsic properties is studied using large-scale molecular dynamics simulations. The influence of composition and temperature on the tensile deformation behavior of amorphous PdSi alloys is investigated. A transition from cracking perpendicular to the loading direction to shear banding can be achieved by increasing the temperature or decreasing the amount of silicon. A decrease in silicon content leads to fewer covalent bonds and, therefore, lower activation barriers for shear transformation zones and, consecutively, a high probability for shear band formation. On the other hand, at low temperatures these barrier cannot be overcome and cracking will dominate over shear banding. In this case, high activation barriers for local relaxation impedes stress redistribution into the glassy structure and, finally, cracking occurs. Additionally, the cracking path also depends on the degree of homogeneity. A corrugated fracture surface similar to experiment can be formed due to crack defection and cavitation ahead of the crack tip in chemically inhomogeneous samples. In contrast, a sharp cleavage-like fracture occurs for more homogeneous samples.

MM 5.2 Tue 10:00 P

Enabling materials design of ionic systems with automated corrections: AFLOW-CCE — •Rico Friedrich[1,2], Marco Esters[1], Corey Oses[1], Stuart Ki[1], Maxwell J. Brenner[1], David Hicks[1], Michael J. Mehl[1], Mahdi Ghorbani-Asl[2], Arkady Krasheninnikov[2], Cormac Toher[1], and Stefano Curtarolo[1,3] — [1]Center for Autonomous Materials Design, Duke University, USA — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Materials Science, Electrical Engineering, Physics and Chemistry, Duke University, USA

Materials databases such as AFLOW [1] leverage *ab initio* calculations for autonomous materials design. The predictive power critically relies on accurate formation enthalpies - quantifying the thermodynamic stability of a system. For ionic materials such as oxides and nitrides, standard DFT leads to errors of several hundred meV/atom [2,3].

We have recently developed the "coordination corrected enthalpies" (CCE) method yielding highly accurate room temperature formation enthalpies with mean absolute errors down to 27 meV/atom [3]. Here, we introduce AFLOW-CCE [4]: a tool where users can input a structure file and receive the CCE corrections, or even the CCE formation enthalpies if pre-calculated LDA, PBE or SCAN values are provided. The results can be used for the design of *e.g.* 2D materials.

[1] S. Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012).
[2] V. Stevanović *et al.*, Phys. Rev. B **85**, 115104 (2012).
[3] R. Friedrich *et al.*, npj Comput. Mater. **5**, 59 (2019).
[4] R. Friedrich *et al.*, Phys. Rev. Mater. **5**, 043803 (2021).

MM 5.3 Tue 10:00 P

Molecular Dynamics study of the influence of microstructure on reaction front propagation in Al-Ni multilayers — •Fabian Schwarz and Ralph Spolenak — Laboratory for Nanometallurgy, Department of Materials, ETH Zürich, CH-8093 Zürich, Switzerland

Reactive multilayers can be used for energy storage as well as releasing large amounts of heat in a short time. We use Molecular Dynamics (MD) simulations to study the influence of the crystal structure on the reaction front propagation in Al-Ni multilayers. Different microstructures, namely amorphous, single crystal, columnar grains and randomly oriented grains of varying size are investigated. The effect of the microstructure on the propagation speed is studied and compared to existing experimental results. Furthermore, MD simulations allow to study the inter-diffusion of the Al and Ni layers. We found that crystallinity has a significant impact on the front propagation speed, which is likely related to different diffusion mechanisms. The more disordered the individual layers become, e.g. by increasing the grain boundary density, the higher is the resulting propagation speed.

MM 5.4 Tue 10:00 P

Grain boundary segregation and precipitation in an Al-Zn-Mg-Cu alloy — •Huan Zhao[1], Baptiste Gault[1,2], Liam Huber[1], Wenjun Lu[1], Nicolas Peter[1], Dirk Ponge[1], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Department of Materials, Royal School of Mines, Imperial College London, London, United Kingdom

High-strength Al-Zn-Mg-Cu alloys are highly susceptible to intergranular embrittlement, which severely limits their lifetime. In this talk, I will present our recent work on the effect of solute segregation in the precipitation behavior at grain boundaries (GBs) compared to grain interiors. Solute segregation could accelerate the precipitation behavior at GBs, which causes the formation of coarse precipitates and precipitate free zones along GBs. Furthermore, the interplay of solute segregation and the local structure at GBs has been considered. We show that faceting occurs at GBs and that the distinct segregation and precipitation behavior occurs within the same GB. Investigations on the solute distribution inside the precipitates, matrix, and at GBs related to SCC resistance in Al-Zn-Mg-Cu alloys will also be discussed.

MM 5.5 Tue 10:00 P

On the role of rotational twin boundaries in lamellar TiAl on the deformation behavior — •Ashish Chauniyal and Rebecca Janisch — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Twin boundaries in lamellar TiAl alloys have a determining influence on their mechanical properties. During deformation, the twin boundaries prevent easy glide of dislocations, thereby contributing to strengthening. In nano-scale lamellae, twin boundaries can cause considerable dislocation pileups which contribute to strengthening, but compromise ductility. To maintain deformability, it is desirable to have movement of dislocations and sufficient dislocation sources to nucleate new dislocations. In this regard, the twin boundaries in lamellar TiAl are special as the tetragonality of the γ phase ($L1_0$) leads to several variants of rotational twin boundaries by rotating in steps of 60° around the [111] axis. While a $\gamma/\gamma_{180^\circ}$ boundary is fully coherent, γ/γ_{60° and $\gamma/\gamma_{120^\circ}$ boundaries exhibit a lattice misfit at the interface, which can result in coherency or semi-coherency. For a coherent interface a residual coherency stress is generated within the lamallae which can have a profound influence during deformation. For a semi-coherent interface, misfit dislocations at the interface can act as nucleation sources. In this work we model these interfaces atomistically and compare their deformation behavior by carrying out large scale atomistic simulations. Our simulations reveal the mechanisms of dislocation nucleation and propagation in lamellar layers with rotational twin boundaries.

MM 5.6 Tue 10:00 P

High hydrogen mobility in an amide-borohydride compound studied by quasielastic neutron scattering — •Neslihan Aslan[1], Sebastian Busch[1], Wiebke Lohstroh[2], Claudio Pistidda[3], and Martin Müller[1,4] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technical University Munich (TUM), Garching, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [4]Institute of Materials Physics, Helmholtz-Zentrum Hereon, Geesthacht, Germany

The hydrogen storage performance of reactive hydride composites Mg(NH2)2 + 2 LiH can be significantly improved by the addition of LiBH4 and the subsequent formation of the amide-borohydride compound Li4(BH4)(NH2)3 during hydrogen release. To understand the chemical behaviour and atomic motions of Li4(BH4)(NH2)3, we present an in situ phase analysis with X-ray synchrotron diffraction and quasielastic neutron scattering (QENS) during heating.

Li4(BH4)(NH2)3 melts at 494 K and the crystallization of a second phase is detected and identified as LiNH2. In molten phase, the neutron measurements confirm a long-range diffusive motion of hydrogen-containing species with the diffusion coefficient $D \sim 10^{-6}\,\frac{\mathrm{cm}^2}{\mathrm{s}}$. In solid phase, localized rotational motions are observed that have been attributed to (BH4)- tetrahedra units mainly undergoing rotations around C_3 axes.

MM 5.7 Tue 10:00 P

Substrate-Induced Anisotropic Superconductivity in Layered Materials: the role of Nonlocal Coulomb Interactions and Band Hybridisation — •Manuel Simonato[1], Anand Kamlapure[1], Emil Sierda[1], Manuel Steinbrecher[1], Umut Kamber[1], Elze. J. Knol[1], Peter Krogstrop[2,3], Mikhail I. Katsnelson[1], Alexander Khajetoorians[1], and Malte Rösner[1] — [1]Institute for Molecules and Materials, Radboud University, Nijmegen 6525AJ, Netherlands — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark — [3]Microsoft Quantum Materials Lab Copenhagen, 2800 Lyngby, Denmark

We investigate how anisotropic substrate materials, such as black-phosphorus (BP), can affect the properties of layered superconductors (SC), both via dielectric screening of the Coulomb interaction and via band hybridization. We employ generic lattice models to describe the SC in BCS theory and utilize Thomas-Fermi screening theory for the Coulomb interactions. The SC-substrate hybridization is studied by means of an effective two-band model, which yields an extension of conventional BCS theory in the Nambu-Gorkov formalism. We derive a new gap equation, from which the effective gap and other SC properties are evaluated. Our predictions for the spectral density function show great qualitative agreement with experimental data for thin Pb films on BP substrates.

MM 5.8 Tue 10:00 P

Sampling the parameter space of grain boundaries with a sequential sampling technique - Atomistics meets statistics — •Timo Schmalofski[1], Martin Kroll[2], Holger Dette[2], and Rebecca Janisch[1] — [1]ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany — [2]Department of Mathematics, Ruhr-University Bochum, 44780 Bochum, Germany

The grain boundary energy is a function of five degrees of freedom (DOF). Two DOF describe the inclination of the grain boundary plane and the remaining three DOF the misorientation between both grains (one for the misorientation angle and two for the rotation axis). The sampling of this grain boundary energy space or even subspaces of it has been shown to be very challenging due to the so-called "cusps", steep energy minima at special misorientations and/or inclinations. Several approaches have been tried to sample energy subspaces, but they mostly need a large amount of datapoints for sufficient accuracy, and in addition an a-priori knowledge of the positions of the energy cusps. Therefore, in this work, statistical methods are combined with atomistic simulations and a sequential sampling technique is designed. In this presentation this technique will be introduced and compared to a regular sampling technique, to prove its advantages when sampling a whole subspace with a minimal amount of datapoints and discovering unknown cusps automatically. The presentation will focus on the sampling of only one dimensional subspaces of symmetrical tilt grain boundaries to prove the concept, but the application can be generalized towards multidimensional subspaces.

MM 5.9 Tue 10:00 P

The methods of neutron diffraction intensity calculation — •Anastasiia Kuznetsova[1], Jie Luo[2], Hareesh Chavana[3], Veronika Reich[1], Sebastian Busch[1], and Martin Müller[4] — [1]GEMS at MLZ, Hereon, Lichtenbergstr. 1, 85748 Garching b. München, Germany — [2]ILL, 71 avenue des Martyrs, 38000 Grenoble, France — [3]ICG Place Eugene Bataillon, Bat. 15, 34095 Montpellier, France — [4]Hereon, Max-Planck-Str. 1, 21502 Geesthacht, Germany

Neutron diffraction intensity on a crystal is commonly calculated as crystal's structure factor squared. The SASSENA program, suitable for atomic movement modeling, and the Debye formula, applicable for any material, not obligatory a periodic one, were tested for calculation of diffraction on crystalline powders. Mono- and biatomic structures of cP, bcc, and fcc crystal lattices of two different sizes each were used as model crystals. Furthermore, for Po, which data on scattering length were not listed, it was set artificially and also varied. The first method sums up reflections from all crystalline planes for the same Q-vector; the second one takes into account both crystalline structure and atomic motions; the third one spherically averages all possible orientations of the system. The resulting curves were juxtaposed and for Debye formula, the intensities were also correlated with structure factors squared and plotted against Q to obtain some kind of dependence. Given their results' difference, one has to choose a proper calculation method and to justify their choice. Due to some Q-dependence of intensities ratios the presence of some explanation for the divergence among the results of both formulas was assumed.

MM 5.10 Tue 10:00 P

Broadband coupling of fast electrons with high-Q whispering gallery mode resonators — •Niklas Müller, Vincent Hock, Christopher Rathje, Nora Bach, Holger Koch, and Sascha Schäfer — Institute of Physics, University of Oldenburg, 26129 Oldenburg, Germany

The inelastic interaction of fast electrons with spatially confined intense light fields has recently enabled new techniques in ultrafast transmission electron microscopy (UTEM), enabling the coherent control of free-electron states. Advanced quantum control scenarios, including electron-light entanglement and non-trivial electron/photon counting statistics, become accessible if non-classical light states are applied. However, to mitigate the reduced coupling strength when considering few-photon-states, novel concepts for coupling electrons to high-Q optical resonators are required. Here, we demonstrate the excitation of high-Q whispering gallery modes in a silica microfiber taper in a transmission electron microscope by relativistic electrons (200 keV) passing close to the fiber surface. The evanescent electric field of the passing electron induces a femtosecond electric polarization in the silica, which can be decomposed into optical whispering gallery modes (WGM). The dtected coherent cathodoluminescence spectra consist of octave-spanning frequency combs with narrow-bandwidth peaks. By probing the WGM resonances for different distances from the taper apex, we demonstrate that the peaks within the comb exhibit a frequency spacing inversely scaling with the local fiber circumference. Q-factors up to 700 a measured, depending on the local taper angle.

MM 5.11 Tue 10:00 P

Large scale process for adjustable resonances as a versatile platform for SERS — •Marcel Below and Jörg Schilling — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06108 Halle, Germany

Samples on cm^2-scale with hexagonal lattices of gold nanoscatterers were created with different controlled periods by using three-beam interference lithography. The resulting nanoscatterers have an elliptical shape and the size of their semiaxes is linked to the period of the lattice.

Spectral transmission measurements show two broad drops of transmission at different wavelengths depending on the polarization of the light. These are identified as single particle plasmonic resonances and can be shifted from the visible to the mid-IR with increasing size of the nanoscatterers. FEM simulations reveal that both plasmonic resonances are caused by the shape of the individual nanoscatterers.

Additionally, considerably sharper and asymmetric drops of transmission, known as Fano resonances, were observed. These Fano resonances are caused by an overlap of the single particle plasmonic resonance of each nanoscatterer and the collective response of the lattice.

When a sample is immersed in a solution of 4-MBA molecules, the molecules bond to the surface of the gold nanoscatterers. Subsequent Raman measurements show a clear SERS signal and a strong dependency on the polarization of the excitation laser. These results present a possible route for large area SERS substrates with tunable plasmonic resonances.

MM 5.12 Tue 10:00 P

Influence of oxygen on the development of facets on the ligaments of nanoporous gold — •Ulrike Dette[1], Stefan A. Berger[1], Ling-Zhi Liu[2], Jürgen Markmann[1,3], and Jörg Weissmüller[3,1] — [1]Institut für Werkstoffmechanik, Helmholtz-Zentrum Hereon — [2]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences — [3]Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg

Even at comparably low temperatures, gold atoms diffuse on the surface of ligaments in nanoporous gold and create facets. Defects and residual silver act as pinning points for the diffusion and thus the facets. For a better understanding of the faceting mechanism and the role of oxygen in it, we annealed nanoporous gold in argon atmosphere at 500°C for 3 h with different oxygen partial pressures controlled by an electrolyzer. We used samples with and without residual silver on the surface. The results show that the higher the oxygen level the stronger the faceting and bigger the ligament size. Therefore, oxygen does support the faceting of nanoporous gold and the coarsening of the ligaments during annealing. We additionally found that the more residual silver on the surface the more silver clusters are formed during annealing and the smaller the facets become. It confirms that residual silver does act as a pinning point for the facets.

MM 5.13 Tue 10:00 P

Revealing highly stable copper based alloys using active learning — •Angel Diaz Carral[1], Azade Yazdan Yar[1], Siegfried Schmauder[2], and Maria Fyta[1] — [1]Institute for Computational Physics (ICP), Universität Stuttgart, Allmandring 3, 70569, Stuttgart, Germany — [2]Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF), Pfaffenwaldring 32 70569, Stuttgart, Germany

Copper based alloys, due to their high electrical conductivity and high strength, are of great importance for electric and electronic applications such as connectors or lead frames. To this end, we investigate the stability of Cu-Ni-Si-Cr alloys, that is copper alloys with nickel, silicon and chromium impurities. Through computational means, we scan a large number of impurities' concentration and configurations. A relaxation-on-the-fly active learning algorithm is applied in order to investigate the influence of this scanning and reveal the alloys of higher stability. The latter are used at a next step in larger scale simulations in order assist the design of alloys with pre-selected properties. Here, we mainly focus on the first part, the learning process and the stable alloy structures. We discuss the efficiency of this approach, the predictions that can be made and the impact in designing alloys.

MM 6: Topical Session Interface-Dominated Phenomena - Thermodynamics

Time: Wednesday 10:00–11:00 Location: H8

Invited Talk MM 6.1 Wed 10:00 H8

CALPHAD-informed density-based grain boundary thermodynamics — •Reza Darvishi Kamachali[1], Lei Wang[1], Linlin Li[2], Anna Manzoni[1], Birgit Skrotzki[1], and Gregory Thompson[3] — [1]Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin — [2]State Key Laboratory of Rolling and Automation, Northeastern University, Shenyang 110819, PR China — [3]University of Alabama, Department of Metallurgical Materials Engineering, 35487 Tuscaloosa, AL, USA

The Gibbs free energy of a grain boundary is a complex thermodynamic function of temperature, pressure, and composition. These complexities add to the intrinsic crystallographic and chemical constraints imposed by the adjacent bulk phase. Recently we have proposed a density-based model for assessing grain boundary thermodynamics that enables a CALPHAD-informed description of the grain boundary. As such, the Gibbs free energy of the grain boundary is directly linked to available CALPHAD thermodynamic data. In this talk, new aspects of interfacial segregation and phase transformation are revealed by benchmarking the current model for various experimental cases, including several steels, high-entropy alloys and aluminum alloys. The effects of elastic interactions on the grain boundary segregation and the application of the model to a nanocrystalline Pt-Au alloy, with numerous grain boundaries of various characters, will be discussed.

MM 6.2 Wed 10:30 H8

Methods for Gibbs triple junction excess determination: Ti segregation in CoSi2 thin film — •Hannes Zschiesche, Ahmed Charai, Claude Alfonso, and Dominique Mangelinck — CNRS, IM2NP, Faculté de Saint-Jérôme, Aix-Marseille Université, Marseille, France

Triple junctions (TJs) are present in poly crystalline material where three grain boundaries join together. They influence directly the thermodynamics and kinetics of the material and thereby its properties. Thus, their description by geometric and thermodynamic parameters is of great interest. One of these parameters is the Gibbs TJ segregation excess. Eich et al., Acta Mater, 2018 predicted TJ excess in a Fe-Cr alloy based on simulations. However, to compare such predictions on experimentally acquired TJs methods are needed for the determination of Gibbs TJ segregation excess.

We propose methods to determine Gibbs TJ segregation excess in an atomically resolved 3D volume where single atom counting is possible, as provided by atom probe tomography (APT). Firstly, we test the methods on a simulated model volume in which the excess value is known. Further, we investigate an APT volume of CoSi2 thin film that contains three grain boundaries and a TJ which show segregation of Ti. CoSi2 is well known as contact material in microelectronics and can grow in epitaxy on Si by the introduction of a Ti interlayer. The developed methods allow to quantify the Ti excess at the CoSi2 TJ.

This work offers new possibilities for fundamental characterization of materials and an example of its application.

MM 6.3 Wed 10:45 H8

A quantum-mechanical study of impact of vibrational entropy on the segregation of Cu to antiphase boundaries in Fe_3Al — •Martin Friák[1,2], Miroslav Černý[2,3], and Mojmír Šob[4,1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Central European Institute of Technology (CEITEC), Brno University of Technology, Brno, Czech Republic — [3]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

We have performed an *ab initio* study of segregation of Cu atoms towards antiphase boundaries (APBs) in Fe_3Al. The Cu atoms are predicted to segregate towards the studied APBs (the APB energy is then equal to 84 mJ/m^2) but the related energy gain is only 4 meV per Cu atom. Both Cu atoms (as point defects) and APBs (as extended defects) have their specific impact on local magnetic moments of Fe atoms (and they non-linearly combine when both types of defects are present). We have also performed phonon calculations and found all studied states mechanically stable. The band gap in phonon frequencies of Fe_3Al is barely affected by Cu substituents but reduced by APBs. The phonon contributions into segregation-related energy changes are significant, ranging from a decrease by 16 % at T = 0 K to an increase by 17 % at T = 400 K (changes with respect to the segregation-related energy difference between static lattices). Further, we have found non-linear trends in changes induced by the Cu segregation in the phonon entropy and phonon energy.

MM 7: Topical Session Interface-Dominated Phenomena - Segregation and Embrittlement

Time: Wednesday 11:15–12:45 Location: H8

Invited Talk MM 7.1 Wed 11:15 H8

Computational methods for grain boundary segregation in metallic alloys — •Lorenz Romaner[1], Daniel Scheiber[2], Vsevolod Razumovskiy[2], Oleg Peil[2], Christoph Dösinger[1], and Alexander Reichmann[1] — [1]Department Materials Science, Montanuniversität Leoben, A-8700 Leoben — [2]Materials Center Leoben Forschung GmbH, A 8700 Leoben

Modeling of grain boundary segregation phenomena is an important discipline of integrated computational materials design. Several computational methods, including in particular atomistic, thermokinetic or mechanical models are available to model grain boundary excess and to assess the associated material properties. Segregation energies plays a central role in this connection and large databases are being created to get a comprehensive overview over materials. With the availability of such databases, machine learning approaches can be used to learn the trends in the periodic table and get segregation energies even for alloys for which no data exist at present. We present an investigation on machine learning segregation energies obtained from density functional theory simulations. We will discuss the critical role of feature engineering and analyze different physical parameters including cohesive energies, solution energies, geometry of the segregation site and many more. Furthermore, we show results for a variety of metallic alloys focusing on the class of transition metals and on comparison with experiment. Finally, the challenges of machine learning of segregation energies and grain boundary engineering in general will be discussed.

MM 7.2 Wed 11:45 H8

Revealing in-plane grain boundary composition features through machine learning from atom probe tomography data — •Xuyang Zhou[1,2], Ye Wei[1], Markus Kühbach[1,3], Huan Zhao[1], Florian Vogel[4], Reza Darvishi Kamachali[5], Gregory B. Thompson[2], Dierk Raabe[1], and Baptiste Gault[1,6] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Department of Metallurgical & Materials Engineering, The University of Alabama, Tuscaloosa, USA — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [4]Institute of Advanced Wear & Corrosion Resistant and Functional Materials, Jinan University, Guangzhou, China — [5]Federal Institute for Materials Research and Testing (BAM), Berlin, Germany — [6]Department of Materials, Royal School of Mines, Imperial College London, London, UK

The structures of grain boundaries (GBs) have been investigated in great detail. However, much less is known about their chemical features, owing to the experimental difficulties to probe these features at the atomic length scale inside bulk material specimens. Atom probe tomography (APT) is a tool capable of accomplishing this task, with an ability to quantify chemical characteristics at near-atomic scale. Using APT data sets, we present here a machine-learning-based approach for the automated quantification of chemical features of GBs. This machine-learning-based approach provides quantitative, unbiased, and automated access to GB chemical analyses, serving as an enabling tool for new discoveries related to interface thermodynamics, kinetics, and the associated chemistry-structure-property relations.

MM 7.3 Wed 12:00 H8

How grain boundary doping affects the mechanical properties in ultra-fine grained tungsten and nanocrystalline tungsten composites — •Michael Wurmshuber[1], Simon Doppermann[1], Stefan Wurster[2], Severin Jakob[1], Markus Alfreider[1], Klemens Schmuck[1], Rishi Bodlos[3], Lorenz Romaner[1], Verena Maier-Kiener[1], Helmut Clemens[1], and Daniel Kiener[1] — [1]Department Materials Science, Montanuniversität Leoben, Jahnstraße 12, 8700 Leoben, Austria — [2]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, 8700 Leoben, Austria — [3]Materials Center Leoben GmbH, Roseggerstraße 12, 8700 Leoben, Austria

Brittle intercrystalline fracture due to weak grain boundaries is a major problem in both refractory metals as well as nanostructured metals. Naturally, it is therefore also the preferred failure mode in ultra-fine grained tungsten, which is a prime candidate for the divertor material in nuclear fusion. In this work, ultra-fine grained tungsten samples doped with various ab-initio informed elements are fabricated and characterized. A clear improvement of mechanical properties could be observed for samples doped with boron and hafnium. Furthermore, nanocrystalline W-Cu samples were fabricated and doped with the same elements. While boron and hafnium also have a positive effect on the mechanical properties in these samples, the addition of rhenium leads to an even more pronounced improvement, pushing the boundaries set by the strength-ductility paradigm.

MM 7.4 Wed 12:15 H8

Atomistic Insight into Hydrogen Trapping at MC/BCC-Fe Phase Boundaries: The Role of Local Atomic Environment — •Boning Zhang[1,2], Jie Su[2], Maoqiu Wang[2], Zhenbao Liu[2], Zhigang Yang[1], Matthias Militzer[3], and Hao Chen[1] — [1]Tsinghua University, Beijing, China — [2]Central Iron and Steel Research Institute, Beijing, China — [3]The University of British Columbia, Vancouver, Canada

A physical understanding of hydrogen trapping at microstructural defects such as grain boundaries (GBs) and phase boundaries (PBs) is vitally important for the design of hydrogen embrittlement (HE) resistant metals. As compared with GBs, the mechanism of hydrogen trapping at PBs is rather unclear due to the complex atomic environment. We perform systematic density functional theory (DFT) calculations to reveal the origin of hydrogen trapping at PBs between body centered cubic (BCC)-Fe and NaCl-type carbides (MCs). We found hydrogen trapping energetics at MC/BCC-Fe PBs depend not only on local volume dilation of the trapping sites, but also on the local atomic environment. An array of descriptors such as lattice strain, geometric volume, and charge density, which have been proven to effectively predict hydrogen trapping at GBs, fail to quantify hydrogen trapping at MC/BCC-Fe PBs. We analyzed the electronic interactions at PBs and found that they are closely related to hydrogen binding energies, and the Bader volume of hydrogen is a universal descriptor for assessing trapping energetics at PBs. This study provides a new insight into hydrogen trapping at microstructural defects.

MM 7.5 Wed 12:30 H8

Ab initio study of hydrogen segregation and embrittlement at grain boundaries in bcc Fe — •Abril Azócar Guzmán, Alexander Hartmaier, and Rebecca Janisch — ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

Hydrogen embrittlement is a fundamental problem in materials science that affects structural materials such as steel. Grain boundaries in ferritic microstructures play a dual role in the context of hydrogen embrittlement: they could act as H traps and thus reduce the amount of mobile H in the system. Alternatively, this trapping could promote hydrogen enhanced decohesion (HEDE) at the grain boundaries. Understanding the relationship between strain, hydrogen solubility, and cohesive strength can help elucidate the HEDE mechanism and influence the segregation process. We present the results of *ab initio* studies of the effect of H, as well as C, on Fe at $\Sigma5$ and $\Sigma3$ symmetrical tilt grain boundaries. The calculated results show that the presence of H significantly reduces both the work of separation and the intergranular cohesive strength; these quantities can aid to derive traction-separation laws for cohesive zone models in mesoscale simulations. Additionally, we analyse the solubility of H under mechanical load, which allows us to predict H distribution in microstructures with residual stresses, or under applied load.

MM 8: Annual General Meeting

Time: Wednesday 18:00–19:00 Location: MVMM

Annual General Meeting

Physics of Socio-economic Systems Division
Fachverband Physik sozio-ökonomischer Systeme (SOE)

Jens Christian Claussen
Mathematics EAS
Aston University
Aston Triangle,
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Marc Timme
Chair for Network Dynamics
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Overview of Invited Talks and Sessions

(Lecture hall H3; Poster P)

Young Scientist Award for Socio- and Econophysics (YSA) - Award Session and Prize Talks

SOE 1.1	Wed	15:00–15:45	YSA	**Quantifying science and art** — •Roberta Sinatra
SOE 1.2	Wed	15:45–16:30	YSA	**Multilayer modeling and analysis of complex socio-economic systems** — •Manlio De Domenico

Plenary talks related to SOE

PV III	Mon	16:30–17:15	Audimax 1	**Complex networks with complex nodes** — •Raissa D'Souza

Topical Talks

SOE 4.1	Thu	10:00–10:30	H3	**Felix Auerbach and Zipf's Law for Cities** — •Diego Rybski, Antonio Ciccone
SOE 4.2	Thu	10:30–11:00	H3	**Envy-induced class separation in societies of competing agents** — •Claudius Gros
SOE 7.1	Fri	10:00–10:30	H6	**Why Ergodicity Breaking from Climate Change matters in Ecosystems?** — •Jan Nagler

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium The Physics of CoViD Infections (SYCO)

See SYCO for the full program of the symposium.

SYCO 1.1	Mon	13:30–14:00	Audimax 1	**A Tethered Ligand Assay to Probe SARS-CoV-2:ACE2 Interactions** — Magnus Bauer, Sophia Gruber, Adina Hausch, Lukas Milles, Thomas Nicolaus, Leonard Schendel, Pilar Lopez Navajas, Erik Procko, Daniel Lietha, Rafael Bernadi, Hermann Gaub, •Jan Lipfert
SYCO 1.2	Mon	14:00–14:30	Audimax 1	**From molecular simulations towards antiviral therapeutics against COVID-19** — •Rebecca Wade
SYCO 1.3	Mon	14:45–15:15	Audimax 1	**The physical phenotype of blood cells is altered in COVID-19** — Markéta Kubánková, Martin Kräter, Bettina Hohberger, •Jochen Guck

SYCO 1.4	Mon	15:15–15:45	Audimax 1	**Extended lifetime of respiratory droplets in a turbulent vapor puff and its implications on airborne disease transmission** — •Detlef Lohse, Kai Leong Chong, Chong Shen Ng, Naoki Hori, Morgan Li, Rui Yang, Roberto Verzicco
SYCO 1.5	Mon	15:45–16:16	Audimax 1	**Beyond the demographic vaccine distribution: Where, when and to whom should vaccines be provided first?** — •Benno Liebchen, Jens Grauer, Fabian Schwarzendahl, Hartmut Löwen

Invited talks of the joint symposium Advanced neuromorphic computing hardware: Towards efficient machine learning (SYNC)

See SYNC for the full program of the symposium.

SYNC 1.1	Wed	10:00–10:30	Audimax 1	**Equilibrium Propagation: a Road for Physics-Based Learning** — •Damien Querlioz
SYNC 1.2	Wed	10:30–11:00	Audimax 1	**Machine Learning and Neuromorphic Computing: Why Physics and Complex Systems are Indispensable** — •Ingo Fischer
SYNC 1.3	Wed	11:00–11:30	Audimax 1	**Photonic Tensor Core Processor and Photonic Memristor for Machine Intelligence** — •Volker Sorger
SYNC 1.4	Wed	11:45–12:15	Audimax 1	**Material learning with disordered dopant networks** — •Wilfred van der Wiel
SYNC 1.5	Wed	12:15–12:45	Audimax 1	**In-memory computing with non-volatile analog devices for machine learning applications** — •John Paul Strachan

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Climate and energy: Challenges and options from a physics perspectiv (SYCE)

See SYCE for the full program of the symposium.

SYCE 1.1	Thu	13:30–14:00	Audimax 1	**The challenge of anthropogenic climate change - Earth system analysis can guide climate mitigation policy** — •Matthias Hofmann
SYCE 1.2	Thu	14:00–14:30	Audimax 1	**Towards a carbon-free energy system: Expectations from R&D in renewable energy technologies** — •Bernd Rech, Rutger Schlatmann
SYCE 1.3	Thu	14:30–15:00	Audimax 1	**Decarbonizing the Heating Sector - Challenges and Solutions** — •Florian Weiser

SYCE 1.4	Thu	15:15–15:45	Audimax 1	**A carbon-free Energy System in 2050: Modelling the Energy Transition** — •Christoph Kost, Philip Sterchele, Hans-Martin Henning
SYCE 1.5	Thu	15:45–16:15	Audimax 1	**The transition of the electricity system to 100% renewable energy: agent-based modeling of investment decisions under climate policies** — •Kristian Lindgren

Sessions

SOE 1.1–1.2	Wed	15:00–16:30	YSA	**Young Scientist Award for Socio-and Econophysics**
SOE 2.1–2.4	Wed	17:00–18:00	P	**Poster**
SOE 3	Wed	18:00–19:00	MVSOE	**Member's Assembly**
SOE 4.1–4.2	Thu	10:00–11:00	H3	**Dynamics and Scaling of Cities and Societies**
SOE 5.1–5.1	Thu	11:15–11:45	H3	**Financial Systems**
SOE 6.1–6.2	Thu	11:45–12:45	H3	**Dynamics of Social and Adaptive Networks I**
SOE 7.1–7.2	Fri	10:00–11:00	H6	**Socio-economic models of climate change impact**
SOE 8.1–8.3	Fri	11:15–12:45	H6	**Dynamics of Social and Adaptive Networks II**
SOE 9.1–9.4	Fri	13:30–16:00	ESS	**Symposium: Synchronization Patterns in Complex Dynamical Networks (organized by Jakub Sawicki, Sabine Klapp, Markus Bär and Jens Christian Claussen) (joint session DY/SOE)**

Annual General Meeting of the Physics of Socio-economic Systems Division

Wednesday 18:00–19:00 MVSOE

1. Report of the Chairpersons
2. Announcements and Discussion of future Activities
3. Elections
4. Miscellaneous

Sessions

– Invited Talks, Prize Talks, Topical Talks, Contributed Talks, and Posters –

SOE 1: Young Scientist Award for Socio-and Econophysics

Time: Wednesday 15:00–16:30 Location: YSA

Prize Talk SOE 1.1 Wed 15:00 YSA

Quantifying science and art — •Roberta Sinatra — NERDS, IT University of Copenhagen, Copenhagen, Denmark — SODAS, University of Copenhagen, Copenhagen, Denmark — Complexity Science Hub, Vienna, Austria

Performance, representing the objectively measurable achievements in a certain domain of activity, like the publication record of a scientist or the winning record of an athlete, captures the actions of an individual entity. In contrast, success, captured by impact or visibility, is a collective phenomenon, representing a community's reaction and acceptance of an individual entity's performance. We are often driven by the belief that the detection of extraordinary performance is sufficient to predict exceptional success. However, the link between these two measures, while often taken for granted, is actually far from being understood. Nevertheless, differently from performance, success is quantifiable and predictable: given its collective nature, its signatures can be uncovered from the many pieces of data around us using the tools of statistical physics, complex systems, network science, and data science. In this talk, I will focus on success in science and art as a way to test our ability to model and predict the collective phenomenon of success. I will discuss the role of luck in achieving success, and will address the relation between performance and success in a variety of settings, highlighting the challenges of gauging performance through success.

Prize Talk SOE 1.2 Wed 15:45 YSA

Multilayer modeling and analysis of complex socio-economic systems — •Manlio De Domenico — Complex Multilayer Networks Lab, Fondazione Bruno Kessler, Trento (Italy)

Complex systems are characterized by constituents – from neurons in the brain to individuals in a social network – which exhibit special structural organization and nonlinear dynamics. As a consequence, a complex system can not be understood by studying its units separately because their interactions lead to unexpected emerging phenomena, from collective behavior to phase transitions. Recently, we have discovered that a new level of complexity characterizes a variety of natural and artificial systems, where units interact, simultaneously, in distinct ways. For instance, this is the case of multimodal transportation systems (e.g., metro, bus and train networks) or of social networks, whose interactions might be of different type (e.g. trust, trade, virtual, etc.). The unprecedented newfound wealth of socio-economic data allows to categorize system's interdependency by defining distinct "layers", each one encoding a different network representation of the system. The result is a multilayer network model. In this talk we will discuss the most salient features of multilayer systems, with special attention to socio-ecological and socio-technical ones.

SOE 2: Poster

Time: Wednesday 17:00–18:00 Location: P

SOE 2.1 Wed 17:00 P

Scaling properties of bimodal on-demand public transportation — •Puneet Sharma[1,2], Stephan Herminghaus[1,2], Helge Heuer[1,2], Steffen Muehle[1], and Knut Heidemann[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Goettingen — [2]Georg-August-Universität Göttingen

While modern cities offer various modes of motorized transportation, considered separately, none of them is both efficient, i.e., sustainable, and convenient. A taxi service is convenient, in a sense, due to door-to-door service, but is inefficient since it usually serves one customer only. Demand responsive ride pooling (DRRP) with minibuses is more efficient, but leads to undue competition with line services (LS), which provide even better pooling (average number of passengers per vehicle) but are less convenient due to fixed routes and stops. A combination of both modes, DRRP and LS, may provide an ideal solution but is challenging to organize due to a trade-off between convenience and efficiency. Here we derive conditions for efficient and convenient transportation for a bimodal service based on a simple square-grid geometry. We relate the optimal mesh size, i.e., distance between stations, to external parameters like passenger density and traveling behavior.

SOE 2.2 Wed 17:00 P

Income inequality from multiple behavioural strategies — •Anjlee Gopiani and Jens Christian Claussen — Mathematics EPS, Aston University Birmingham

Income inequality, and thereby wealth inequality, is a societal problem on national and global scale. Here we investigate a monetary exchange model with interactions motivated from game theory. We assume a diversity of strategies and investigate through agent-based simulations the resulting income distributions in this artificial society. If the majority of agents is acting towards rationality and selflessness to fulfill personal and societal success, inequality is less prevalent.

SOE 2.3 Wed 17:00 P

The Principle of Largest Squares — •Martin Erik Horn — IU Internatinal University of Applied Sciences, Campus Berlin, and ISM International School of Management, Campus Berlin

Regression analysis is an important statistical tool to understand interdependencies between different variables in empirical sciences. And it is astonishing that this tool obviously is used only in Euclidean spaces - as if variables always have to act in an Euclidean way in the scientific world of socio economics and of other domains.

To critically question this Euclidean dominance, orthogonal regression will be transferred into spacetime. The didactical consequences are interesting: We are then discussing relativistic ideas with students who do not study physics, but economics, computer science or other subjects relying on empirical analysis. And the conceptual consequences are surprising: We will no longer apply the principle of least squares but have to switch to the principle of largest squares.

SOE 2.4 Wed 17:00 P

Complexity measures of small-world networks — •Yipei Zhao and Jens Christian Claussen — Mathematics EPS, Aston University Birmingham

While the notion of complexity is established for strings or texts, it is less clear how complexity of a network shall be defined, and various complexity measures have been defined and compared (Claussen 2007, Physica A 375, 365; Kim and Wilhelm 2008, Physica A 387, 2637). Here we compare several of the complexity measures listed in Kim and Wilhelm on small-world networks in comparison to random graphs. We compare Watts-Strogatz graphs in comparison to random graphs that fulfill the small-world property based on the small-world indes. The results are in line with the intuition that small-world structure can add to complexity, but reminescents of a lattice structure lower the complexity values.

SOE 3: Member's Assembly

Member's assembly - a Zoom link will be distributed to the SOE members of the DPG and displayed in the conference system.

Time: Wednesday 18:00–19:00 Location: MVSOE

Online only.

SOE 4: Dynamics and Scaling of Cities and Societies

Time: Thursday 10:00–11:00 Location: H3

Topical Talk SOE 4.1 Thu 10:00 H3

Felix Auerbach and Zipf's Law for Cities — •Diego Rybski[1,2,3] und Antonio Ciccone[4] — [1]Potsdam Institute for Climate Impact Research - PIK, Member of Leibniz Association, P.O. Box 60 12 03, Potsdam 14412, Germany — [2]University of California Berkeley, Department of Environmental Science, Policy and Management, 130 Mulford Hall #3114, Berkeley, CA 94720, USA — [3]Complexity Science Hub Vienna, Josefstädterstrasse 39, A-1090 Vienna, Austria — [4]Department of Economics, University of Mannheim, Mannheim, Germany

Power-law city size distributions are a statistical regularity researched in many countries and urban systems. In this history of science treatise we reconsider the paper by F. Auerbach published in 1913. Therefore, we review his empirical analysis and find (i) that a constant absolute concentration (AK), as introduced by him, is equivalent to a power-law distribution with exponent ≈ 1, (ii) the value of his AK relates to the size of the largest city, and (iii) the specific concentration (SpK), as also introduced by Auerbach, relates to the number of cities. We further investigate his legacy as reflected in citations and find that important follow-up work does give proper reference to his discovery – but other does not. A bibliographic analysis shows that almost all city-related works that cite Auerbach 1913 also cite Zipf 1949. However, only approximately 20 % of works citing Zipf 1949 also cite Auerbach 1913. To our best knowledge A.J. Lotka 1925 was the first to describe the power-law rank-size rule. Consequently, we suggest to use "Auerbach-Lotka-Zipf law" (or "ALZ-law") instead of "Zipf's law for cities".

Topical Talk SOE 4.2 Thu 10:30 H3

Envy-induced class separation in societies of competing agents — •Claudius Gros — Institute for Theoretical Physics, Goethe University Frankfurt

Everything is relative. This holds for Darwinian selection, which is based on relative fitness advantages, and today's social success and fairness criteria. The desire to compare own's own incomes and resources with that of others is the basis of envy. In game theoretical settings, envy is described by a psychological component, in addition to the monetary payoff function. We find that envy leads to a phase transition in societies of competing agents. Below the transition, most agents play pure strategies which follow from occupying the most yielding options. When approaching the transition, an increasing number of agents play mixed strategies, which eventually merge to a single encompassing mixed strategy played by a large number of agents, the lower class. All the while, upper-class agents continue to play high-rewarding pure strategies. Considering the Ultimatum game with envy, we estimate the strength of human envy from the respective laboratory results. One finds that envy is strongly relevant for humans societies.

C. Gros, "Collective strategy condensation: When envy splits societies", Entropy 23, 157 (2021).

C. Gros, "Self induced class stratification in competitive societies of agents: Nash stability in the presence of envy", Royal Society Open Science 7, 200411 (2020).

SOE 5: Financial Systems

Time: Thursday 11:15–11:45 Location: H3

SOE 5.1 Thu 11:15 H3

A New Attempt to Identify Long-term Precursors for Financial Crises in the Market Correlation Structures — •Anton J. Heckens and Thomas Guhr — Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

Prediction of events in financial markets is every investor's dream and, usually, wishful thinking. From a more general, economic and societal viewpoint, the identification of indicators for large events is highly desirable to assess systemic risks. Unfortunately, the non-stationarity nature of financial markets make this challenge a formidable one, leaving little hope for fully fledged answers. Nevertheless, it is called for to collect pieces of evidence in a variety of observables to be assembled like the pieces of a puzzle that eventually might help to catch a glimpse of precursors for large events - if at all in a statistical sense. Here, we present a new piece for this puzzle. We use the quasi-stationary market states which exist in the time evolution of the correlation structure in financial markets. Recently, we identified such market states relative to the collective motion of the market as a whole [1]. We study their precursor properties in the US stock markets over 16 years, including the pre-phase of the Lehman Brothers crash [2].

[1] A. J. Heckens, S. M. Krause, T. Guhr, Uncovering the Dynamics of Correlation Structures Relative to the Collective Market Motion J. Stat. Mech. 2020, 103402 (2020), preprint: arXiv:2004.12336

[2] A. J. Heckens, T. Guhr, A New Attempt to Identify Long-term Precursors for Financial Crises in the Market Correlation Structures (2021), preprint: arXiv:2107.09048

SOE 6: Dynamics of Social and Adaptive Networks I

Time: Thursday 11:45–12:45 Location: H3

SOE 6.1 Thu 11:45 H3

Understanding force directed layouts through latent space models — •Felix Gaisbauer, Armin Pournaki, Sven Banisch, and Eckehard Olbrich — Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany

This contribution brings together two strands of research: Latent space approaches to network analysis and force-directed layout algorithms. The former can be considered as extensions of spatial random graph models for social networks, which have the goal of embedding a graph/network in an underlying social space [1] and have been employed successfully in the estimation of ideological positions from follower networks on Twitter [2]. The latter are used ubiquitously for data exploration, illustration, and analysis. Nevertheless, an interpretation of the outcomes of graph drawings with force-directed algorithms is not straightforward. We show that interpretability can be provided by random graph models in which the nodes are positioned in a latent space. The closer the positions of the nodes, the more probable it is that they are connected. We show that force-directed layout algorithms can be considered as maximum likelihood estimators of such models. We also present ready-to-use implementation of the layout algorithm and show its application to Twitter retweet networks.

[1] P. D. Hoff, A. E. Raftery, and M. S. Handcock (2002). Latent space approaches to social network analysis. Journal of the American Statistical association, 97(460), 1090-1098. [2] P. Barberá (2015). Birds of the same feather tweet together: Bayesian ideal point estimation using Twitter data. Political analysis, 23(1), 76-91.

SOE 6.2 Thu 12:15 H3

Balanced Triad Formation explained by Dyadic Interactions — •Tuan Pham[1,2], Jan Korbel[1,2], Rudolf Hanel[1,2], and Stefan Thurner[1,2,3] — [1]Medical University of Vienna — [2]Complexity Science Hub Vienna — [3]Santa Fe Institute

The evolution of social (signed) triads towards so-called balanced states with either one or three positive links often results in the formation of clusters of positively-linked agents. We argue that –surprisingly– such cluster formation can emerge from *dyadic* interactions if homophily between agents is present. We show this in a Hamiltonian model, where every agent is linked to K others and holds binary opinions on G issues, in an opinion vector $\mathbf{s}_i$. If two agents i and j are connected by a link J_{ij} then $J_{ij} = \mathrm{sign}(\mathbf{s}_i \cdot \mathbf{s}_j)$. Without knowledge of the triads in their neighbourhoods, agents modify their opinions so as to minimize a social tension, $H^{(i)}$, defined via the weighted sum of opinion overlaps with friends and opinion discordance with enemies: $H^{(i)} = -\frac{\alpha}{G} \cdot \sum_{j:J_{ij}>0} \mathbf{s}_i \mathbf{s}_j + \frac{1-\alpha}{G} \cdot \sum_{j:J_{ij}<0} \mathbf{s}_i \mathbf{s}_j$, where α is the relative strength of positive interactions to that of negative ones. The model exhibits a transition from unbalanced- to balanced society at a critical temperature which depends on (G, K, α). As α exceeds 1/2, another transition between steady states with different fractions of balanced triads occurs. We show that the model explains actual data of triad statistics in social networks. The model produces z-scores for triads that is compatible with empirical values in real social networks, such as the *Pardus* computer game and the United Nations General Assembly.

SOE 7: Socio-economic models of climate change impact

Time: Friday 10:00–11:00 Location: H6

Topical Talk SOE 7.1 Fri 10:00 H6

Why Ergodicity Breaking from Climate Change matters in Ecosystems? — •Jan Nagler — Centre for Human and Machine Intelligence, Frankfurt

We show that and how ergodicity breaking due to temperature fluctuations adds up to the effects from rising temperatures and increasing fluctuations. Ergodicity breaking fluctuation-induced phenomena are well known in finance, where volatility can turn winning trading strategies into losing ones, or losing strategies into winning strategies. In physics, ergodicity breaking can result in an array of anomalous behaviours in stochastic systems. We show how ecosystems and evolutionary dynamics are affected. Ergodicity breaking in ecosystems may even dominate other effects from climate change. We report on a field study in nematodes on La Reunion Island that have adapted to temperature fluctuations. Ergodicity breaking leads to a shift of the adapted mean temperature, which we predict from first principles.

SOE 7.2 Fri 10:30 H6

Carbin dioxide emission quota attributions in a power system comprised of highly self-sufficient European actors — •Leon Joachim Schwenk-Nebbe[1,2], Marta Victoria[1,2], Gorm Bruun Andresen[1,2], and Martin Greiner[1,2] — [1]Department of Engineering, Aarhus University, Aarhus, Denmark — [2]iCLIMATE Interdisciplinary Centre for Climate Change, Aarhus University

The European countries all agree that carbon dioxide (CO2) emissions need to be decreased in the power sector. The ever dividing question is who must contribute by how much. We investigate possible near-future electricity system configurations where three aspects of collaboration between the individual countries are parametrized. First, the individual countries are attributed a CO2 emission quota in different ways. We show that a global carbon dioxide emission constraint with a global price leads to a particularly uneven emission distribution in a cost-optimal European electricity system. Different emission attributions are shown to strongly influence the required local emission prices. Second, they can collaborate by relaxing their need for autonomy and becoming less self-sufficient by placing generation capacity in countries with better prerequisites. Third, collaboration can also be strengthened by extending the cross-border transmission grid. We conclude that it is significantly easier for certain countries to decarbonize their electricity production than for others. We find that a deep collaboration between the European countries leads to not only a lowered total system cost but to CO2 emissions, and required CO2 prices that are much more equal between the European partners.

SOE 8: Dynamics of Social and Adaptive Networks II

Time: Friday 11:15–12:45 Location: H6

SOE 8.1 Fri 11:15 H6

Spinning faster and faster: acceleration of collective attention — •Philipp Hövel — University College Cork, Irlenad

Due to the advent of smart phones and other tools of modern communication, news are available in real time and social media reactions spread across the globe in seconds. As a consequence, the public discussion seems to be accelerated and its pace ever increasing. In longitudinal datasets across various domains (online and offline), covering multiple decades, we find significantly increasing gradients and shortened periods in the trajectories of how cultural items receive collective attention. Is this the inevitable conclusion of the way information is disseminated and consumed?

We present a simple mathematical model that is based on Lotka-Volterra dynamics with a memory kernel. The three main mechanisms are imitation/production, saturation/aging and competition. The common resource, for which different topics compete, is the collective attention of the userbase. The numerical time series are able to explain the empirical data remarkably well. Our modeling suggests that the accelerating ups and downs of popular content are driven by increasing production and consumption of content, resulting in a more rapid exhaustion of limited attention resources. In the interplay with competition for novelty, this causes growing turnover rates and individual topics receiving shorter intervals of collective attention.

SOE 8.2 Fri 11:45 H6

Evolutionary Reinforcement Learning Dynamics with Irreducible Environmental Uncertainty — •Wolfram Barfuss[1,2] and Richard P. Mann[2] — [1]University of Tübingen, Germany — [2]University of Leeds, United Kingdom

In this work we derive and present evolutionary reinforcement learning dynamics in which the agents are irreducibly uncertain about the current state of the environment. We evaluate the dynamics across different classes of partially observable agent-environment systems and find that irreducible environmental uncertainty can lead to better learning outcomes faster, stabilize the learning process and overcome social dilemmas. However, as expected, we do also find that partial observability may cause worse learning outcomes, for example, in the form of a catastrophic limit cycle. Compared to fully observant agents, learning with irreducible environmental uncertainty often requires more exploration and less weight on future rewards to obtain the best learning outcomes. Furthermore, we find a range of dynamical effects induced by partial observability, e.g., a critical slowing down of the learning processes between reward regimes and the separation of the learning dynamics into fast and slow directions. The presented dynamics are a practical tool for researchers in biology, social science and machine learning to systematically investigate the evolutionary effects of environmental uncertainty.

SOE 8.3 Fri 12:15 H6

Desynchronization Transitions in Adaptive Networks — •Rico Berner[1,2], Simon Vock[3], Serhiy Yanchuk[2], and Eckehard Schöll[1,4,5] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Institut für Mathematik, Technische Universität Berlin, Germany — [3]Charité-Universitätsmedizin Berlin, Germany — [4]Bernstein Center for Computational Neuroscience Berlin, Humboldt-Universität Berlin, Germany — [5]Potsdam Institute for Climate Impact Research, Potsdam, Germany

Adaptive networks change their connectivity with time, depending on their dynamical state [R. Berner, E. Schöll and S. Yanchuk, SIAM J. Appl. Dyn. Syst. 18, 2227 (2019)]. While synchronization in structurally static networks has been studied extensively, this problem is much more challenging for adaptive networks. In this work, we develop the master stability approach for a large class of adaptive networks [R. Berner, S. Vock, E. Schöll and S. Yanchuk, PRL 126, 028301 (2021)]. This approach allows for reducing the synchronization problem for adaptive networks to a low-dimensional system, by decoupling topological and dynamical properties. We show how the interplay between adaptivity and network structure gives rise to the formation of stability islands. Moreover, we report a desynchronization transition and the emergence of complex partial synchronization patterns induced by an increasing overall coupling strength. We illustrate our findings using adaptive networks of coupled phase oscillators and FitzHugh-Nagumo neurons with synaptic plasticity.

SOE 9: Symposium: Synchronization Patterns in Complex Dynamical Networks (organized by Jakub Sawicki, Sabine Klapp, Markus Bär and Jens Christian Claussen) (joint session DY/SOE)

The program of this session is embedded in a symposium supported by DPG section DY and SOE as well as TU Berlin, SFB 910 and the BCSCCS e.V in Honor of Professor Eckehard Schöll's 70th Birthday. Eckehard Schöll has been the local organizer of the DPG-SKM conferences in Berlin for many years and was awarded the DPG badge of honour (Ehrennadel) for his service to the community.

Time: Friday 13:30–16:00 Location: ESS

Invited Talk SOE 9.1 Fri 13:30 ESS

Network-Induced Multistability Through Lossy Coupling — •Jürgen Kurths — PIK, Potsdam, Germany — HU Berlin, Germany

The stability of synchronized networked systems is a multi-faceted challenge for many natural and technological fields, from cardiac and neuronal tissue pacemakers to power grids. For these, the ongoing transition to distributed renewable energy sources leads to a proliferation of dynamical actors. The desynchronization of a few or even one of those would likely result in a substantial blackout. Thus, the dynamical stability of the synchronous state has become a leading topic in power grid research. Here we uncover that, when taking into account physical losses in the network, the back-reaction of the network induces new exotic solitary states in the individual actors and the stability characteristics of the synchronous state are dramatically altered. These effects will have to be explicitly taken into account in the design of future power grids. We expect the results presented here to transfer to other systems of coupled heterogeneous Newtonian oscillators.

Invited Talk SOE 9.2 Fri 14:00 ESS

Control of synchronization in two-layer power grids — •Simona Olmi[1], Carl Totz[2], and Eckehard Schöll[2] — [1]Istituto dei Sistemi Complessi - CNR - Firenze, Italy — [2]Technische Universität Berlin - Germany

In this talk we suggest to model the dynamics of power grids in terms of a two-layer network, and use the Italian high voltage power grid as a proof-of-principle example. The first layer in our model represents the power grid consisting of generators and consumers, while the second layer represents a dynamic communication network that serves as a controller of the first layer. In particular, the dynamics of the power grid is modelled by the Kuramoto model with inertia, while the communication layer provides a control signal P_i^c for each generator to improve frequency synchronization within the power grid. We propose different realizations of the communication layer topology and different ways to calculate the control signal. Then we conduct a systematic survey of the two-layer system against a multitude of different realistic perturbation scenarios, such as disconnecting generators, increasing demand of consumers, or generators with stochastic power output. When using a control topology that allows all generators to exchange information, we find that a control scheme aimed to minimize the frequency difference between adjacent nodes operates very efficiently even against the worst scenarios with the strongest perturbations.

30 min. break.

Invited Talk SOE 9.3 Fri 15:00 ESS

Relay and complete synchronization of chimeras and solitary states in heterogeneous networks of chaotic maps — Elena Rybalova[1], Eckehard Schöll[2], and •Galina Strelkova[1] — [1]Institute of Physics, Saratov State University, Astrakhanskaya str. 83, Saratov 410012, Russia — [2]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

In this talk we discuss the phenomena of relay and complete synchronization in a heterogeneous three-layer network of chaotic maps. In the considered network two remote layers are not directly coupled but interact via a relay layer with which they are pairwise and symmetrically coupled. All the three layers represent rings of nonlocally coupled discrete-time oscillators but the relay layer is completely different in its spatiotemporal dynamics from that of the outer layers. We consider the cases when the individual elements of the relay layer and of the outer layers are described by Lozi maps and Henon maps, respectively, and vice versa. We establish and explore relay and complete synchronization of chimera structures and solitary state modes in a heterogeneous multiplex network and analyze the role of the relay layer structure in the resulted synchronous patterns. The results are illustrated by diagrams of desynchronized and synchronous regimes in the "inter-layer coupling - intra-layer coupling of the relay layer" parameter planes.

Invited Talk SOE 9.4 Fri 15:30 ESS

A bridge between the fractal geometry of the Mandelbrot set and partially synchronized dynamics of chimera states. — •Ralph G Andrzejak — Universitat Pompeu Fabra, Barcelona, Catalonia, Spain

A simple quadratic map with a complex-valued parameter c allows one to generate enormously rich dynamics and patterns. Fractal Julia sets and the Mandelbrot set divide the complex plane into stable and divergent regions of the map's initial conditions and parameters c. What happens if one couples several quadratic maps? We address this question using a minimal two-population network of two pairs of two quadratic maps. In dependence on c, the network enters into qualitatively different dynamical states. The network iterates can diverge to infinity or remain bounded. Bounded solutions can get fully synchronized, fully desynchronized, or enter into different partially synchronized states, including a symmetry-broken chimera state. We will at first inspect examples for these different dynamical states in the domain of the complex-valued iterates of the network. We then illustrate that the boundaries between different dynamical states form intriguing fractal patterns in the domain of the complex-valued c.

Low Temperature Physics Division
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Overview of Invited Talks and Sessions

(Lecture halls H6 and H7; Poster P)

Plenary Talks

PV II	Mon	9:00– 9:45	Audimax 2	**Quantum thermodynamics - superconducting circuit approach** — •Jukka Pekola
PV VI	Tue	9:00– 9:45	Audimax 1	**Correlated electrons with knots** — •Silke Bühler-Paschen
PV X	Wed	9:00– 9:45	Audimax 1	**Revealing the topological nature of transport at mesoscopic scales with quantum interferences** — •Helene Bouchiat
PV XI	Wed	9:00– 9:45	Audimax 2	**Quantum choreography to the beat of light** — •Rupert Huber
PV XII	Thu	9:00– 9:45	Audimax 1	**Quantum networks - from dreams to reality** — •Jian-Wei Pan
PV XVII	Fri	9:00– 9:45	Audimax 1	**Superconductivity near room temperature** — •Mikhail Eremets

Invited Talks

TT 2.4	Mon	11:45–12:15	H7	**Electronic instabilities of kagomé metals and density waves in the AV_3Sb_5 materials** — •Leon Balents
TT 4.4	Mon	14:45–15:15	H7	**2D Magnetism and Its Efficient Control** — •Cheng Gong
TT 6.1	Tue	10:00–10:30	H7	**Spin Triplet Superconductivity within Superconductors as Determined by FMR Spin pumping** — •Lesley Cohen
TT 21.1	Thu	13:30–14:00	H7	**A new class of charge density wave superconductors in the topological kagome metals AV_3Sb_5 (A=K, Rb, Cs)** — •Stephen Wilson

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium Potentials for NVs sensing magnetic phases, textures and excitations (SYNV)

See SYNV for the full program of the symposium.

SYNV 1.1	Mon	13:30–14:00	Audimax 2	**Harnessing Nitrogen Vacancy Centers in Diamond for Next-Generation Quantum Science and Technology** — •Chunhui Du
SYNV 1.2	Mon	14:00–14:30	Audimax 2	**Nanoscale imaging of spin textures with single spins in diamond** — •Patrick Maletinsky

SYNV 1.3	Mon	14:30–15:00	Audimax 2	**Spin-based microscopy of 2D magnetic systems** — •Jörg Wrachtrup
SYNV 1.4	Mon	15:15–15:45	Audimax 2	**Exploring antiferromagnetic order at the nanoscale with a single spin microscope** — •Vincent Jacques
SYNV 1.5	Mon	15:45–16:15	Audimax 2	**Nanoscale magnetic resonance spectroscopy with NV-diamond quantum sensors** — •Dominik Bucher

Invited talks of the joint symposium Novel phases and dynamical properties of magnetic skyrmions (SYMS)

See SYMS for the full program of the symposium.

SYMS 1.1	Tue	10:00–10:30	Audimax 2	**Imaging skyrmions in synthetic antiferromagnets by single spin relaxometry** — •Aurore Finco
SYMS 1.2	Tue	10:30–11:00	Audimax 2	**Microwave spectroscopy of the skyrmionic states in a chiral magnetic insulator** — •Aisha Aqeel
SYMS 1.3	Tue	11:15–11:45	Audimax 2	**Archimedean Screw in Driven Chiral Magnets** — •Nina del Ser
SYMS 1.4	Tue	11:45–12:15	Audimax 2	**Frustration-driven magnetic fluctuations as the origin of the low-temperature skyrmion phase in $Co_7Zn_7Mn_6$** — •Jonathan White
SYMS 1.5	Tue	12:15–12:45	Audimax 2	**Magnetic Skyrmions as Topological Multi-Media Influencers** — •Sebastián A. Díaz

Invited talks of the joint symposium Facets of many-body quantum chaos (SYQC)

See SYQC for the full program of the symposium.

SYQC 1.1	Tue	13:30–14:00	Audimax 2	**Holographic interpretation of SYK quantum chaos** — •Alexander Altland
SYQC 1.2	Tue	14:00–14:30	Audimax 2	**Non-Fermi liquids and the lattice** — •Sean Hartnoll
SYQC 1.3	Tue	14:30–15:00	Audimax 2	**Dual-unitary circuits: non-equilibrium dynamics and spectral statistics** — •Bruno Bertini
SYQC 1.4	Tue	15:15–15:45	Audimax 2	**Post-Ehrenfest many-body quantum interferences in ultracold atoms** — •Steven Tomsovic
SYQC 1.5	Tue	15:45–16:15	Audimax 2	**Dynamics in unitary and non-unitary quantum circuits** — •Vedika Khemani

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Attosecond and coherent spins: New frontiers (SYAS)

See SYAS for the full program of the symposium.

SYAS 1.1	Thu	10:00–10:30	Audimax 2	**Ultrafast Coherent Spin-Lattice Interactions in Iron Films** — •Steven Johnson
SYAS 1.2	Thu	10:30–11:00	Audimax 2	**Ultrafast spin, charge and nuclear dynamics: ab-initio description** — •Sangeeta Sharma
SYAS 1.3	Thu	11:15–11:45	Audimax 2	**Light-wave driven Spin Dynamics** — •Martin Schultze
SYAS 1.4	Thu	11:45–12:15	Audimax 2	**All-coherent subcycle switching of spins by THz near fields** — •Christoph Lange
SYAS 1.5	Thu	12:15–12:45	Audimax 2	**Ultrafast optically-induced spin transfer in ferromagnetic alloys** — •Stefan Mathias

Invited talks of the joint symposium Physics of van der Waals 2D heterostructures (SYWH)

See SYWH for the full program of the symposium.

SYWH 1.1	Thu	13:30–14:00	Audimax 2	**Spin interactions in van der Waals topological materials and magnets** — •Saroj Dash
SYWH 1.2	Thu	14:00–14:30	Audimax 2	**Exciton optics, dynamics and transport in atomically thin materials** — •Ermin Malic
SYWH 1.3	Thu	14:30–15:00	Audimax 2	**Correlated Electrons in van der Waals Superlattices: Control and Understanding** — •Tim Wehling
SYWH 1.4	Thu	15:15–15:45	Audimax 2	**Exciton manipulation and transport in 2D semiconductor heterostructures** — •Andras Kis
SYWH 1.5	Thu	15:45–16:15	Audimax 2	**Chern Insulators, van Hove singularities and Topological Flat-bands in Magic-angle Twisted Bilayer Graphene*** — •Eva Andrei

Invited talks of the joint symposium The Rise of Photonic Quantum Technologies – Practical and Fundamental Aspects (SYPQ)

See SYPQ for the full program of the symposium.

SYPQ 1.1	Fri	10:00–10:30	Audimax 2	**Quantum dots operating at telecom wavelengths for photonic quantum technology** — •Simone Luca Portalupi
SYPQ 1.2	Fri	10:30–11:00	Audimax 2	**Photonic graph states for quantum communication and quantum computing** — •Stefanie Barz
SYPQ 1.3	Fri	11:00–11:30	Audimax 2	**Rare-earth ion doped solids at sub-Kelvins: practical and fundamental aspects** — •Pavel Bushev
SYPQ 1.4	Fri	11:45–12:15	Audimax 2	**Quantum Light and Strongly Correlated Electronic States in a Moiré Heterostructure** — •Brian Gerardot
SYPQ 1.5	Fri	12:15–12:45	Audimax 2	**Quantum communication in fibers and free-space** — •Rupert Ursin

Sessions

TT 1.1–1.8	Mon	10:00–12:45	H6	**Focus Session: Disordered and Granular Superconductors: Fundamentals and Applications in Quantum Technology I**
TT 2.1–2.5	Mon	10:00–12:45	H7	**Focus Session: Exotic Charge Density Wave States of Matter: Correlations and Topology (joint session TT/HL)**
TT 3.1–3.7	Mon	13:30–16:15	H6	**Focus Session: Entanglement as a Probe for Correlated Quantum Matter**
TT 4.1–4.8	Mon	13:30–16:15	H7	**Focus Session: Correlated van-der-Waals Magnets**
TT 5.1–5.32	Mon	13:30–16:00	P	**Poster Session: Superconductivity**
TT 6.1–6.6	Tue	10:00–12:45	H7	**Focus Session: Emerging Phenomena in Superconducting Low Dimensional Hybrid Systems I**
TT 7.1–7.8	Tue	13:30–16:15	H6	**Focus Session: Disordered and Granular Superconductors: Fundamentals and Applications in Quantum Technology II**
TT 8.1–8.10	Tue	13:30–16:15	H7	**Focus Session: Emerging Phenomena in Superconducting Low Dimensional Hybrid Systems II**
TT 9.1–9.43	Tue	13:30–16:00	P	**Poster Session: Correlated Electrons**
TT 10.1–10.9	Wed	10:00–12:45	H4	**Materials and devices for quantum technology (joint session HL/TT)**
TT 11.1–11.11	Wed	10:00–13:00	H6	**Focus Session: Facets of Many-Body Quantum Chaos (organised by Markus Heyl and Klaus Richter) (joint session DY/TT)**
TT 12.1–12.4	Wed	10:00–11:00	H7	**New Experimental Techniques**

TT 13.1–13.7	Wed	11:15–13:00	H7	**Quantum Computing (joint session TT/DY)**
TT 14.1–14.4	Wed	13:30–14:45	H6	**Many-Body Quantum Dynamics I (joint session DY/TT)**
TT 15.1–15.6	Thu	10:00–11:30	H2	**Many-Body Quantum Dynamics II (joint session DY/TT)**
TT 16.1–16.7	Thu	10:00–12:45	H5	**PhD Focus Session: Symposium on Strange Bedfellows - Magnetism Meets Superconductivity" (joint session MA/AKjDPG) (joint session MA/TT)**
TT 17.1–17.4	Thu	10:00–11:00	H6	**Charge Density Wave Materials**
TT 18.1–18.10	Thu	10:00–12:45	H7	**Frustrated Magnets**
TT 19.1–19.6	Thu	11:15–12:45	H6	**Unconventional Superconductors**
TT 20.1–20.10	Thu	13:30–16:30	H4	**Quantum Dots and Wires (joint session HL/TT)**
TT 21.1–21.7	Thu	13:30–16:00	H7	**Focus Session: Topological Kagome Metals**
TT 22.1–22.9	Thu	13:30–15:30	P	**Poster Session: Disordered and Granular Superconductors: Fundamentals and Applications in Quantum Technology**
TT 23.1–23.3	Thu	13:30–15:30	P	**Poster Session: Emerging Phenomena in Superconducting Low Dimensional Hybrid Systems**
TT 24.1–24.11	Thu	13:30–16:00	P	**Poster Session: Transport**
TT 25.1–25.18	Thu	13:30–16:00	P	**Poster Session: Topology**
TT 26	Thu	18:00–19:30	MVTT	**Annual General Meeting of the Low Temperature Physics Division**
TT 27.1–27.10	Fri	10:00–12:45	H7	**Topological Insulators and Semimetals (joint session TT/KFM)**
TT 28.1–28.6	Fri	13:30–15:00	H6	**Transport (joint session TT/DY)**
TT 29.1–29.6	Fri	13:30–15:00	H7	**Topological Superconductors**

Annual General Meeting of the Low Temperature Physics Division

Thursday 18:00–19:30 MVTT

- Bericht
- Wahl
- Verschiedenes

Sessions

– Invited Talks, Contributed Talks, and Posters –

TT 1: Focus Session: Disordered and Granular Superconductors: Fundamentals and Applications in Quantum Technology I

Superconducting qubits and quantum circuits are traditionally fabricated from simple superconductors such as aluminum or niobium. Recently, strongly disordered and granular superconductors have become a promising alternative for quantum devices that seek a combination of large impedance and low losses: here, the high kinetic inductance of disordered and granular superconductors is a key asset. While these particular materials are in the focus of fundamental superconductivity materials research already for a long time, their application in quantum technologies now motivates a tight interaction of these two research fields.

Organizers: Marc Scheffler (University of Stuttgart), Joachim Ankerhold (Ulm University)

Time: Monday 10:00–12:45 Location: H6

TT 1.1 Mon 10:00 H6

Fate of the superfluid density near the SIT in amorphous superconductors — •Benjamin Sacepe — Néel Institute, CNRS Grenoble, France

Superconducting films of amorphous Indium Oxide (a:InO) thin films undergo a transition to insulation upon increasing disorder, driven by the localization of preformed Cooper pairs. The continuous decrease of the critical temperature as the critical disorder approaches indicates a similarly continuous suppression of the superfluid density. In this talk I discuss the fate of the superfluid density in the vicinity of this transition to insulation. We have accurately measured the superfluid density by a systematic study of the plasmon dispersion spectrum of microwave resonators made of a:InO, combined with DC resistivity measurements, as a function of disorder. We observed that the superfluid stiffness defines the superconducting critical temperature over a wide range of disorder, highlighting the dominant role of phase fluctuations. Furthermore, we found that the superfluid density remains surprisingly finite at the critical disorder, indicating an unexpected first-order nature of the disorder-driven quantum phase transition to insulator.

TT 1.2 Mon 10:30 H6

Superconducting silicon: material and devices — •Francesca Chiodi[1], Pierre Bonnet[1], Daniel Flanigan[2], Raphaelle Delagrange[1], Dominique Débarre[1], and Hélène le Sueur[2] — [1]C2N, Université Paris-Saclay, CNRS, Palaiseau, France — [2]SPEC, Université Paris-Saclay, CEA, CNRS, Gif-sur-Yvette, France

Silicon is one of the most well-known materials, and the main actor in today electronics. Despite this, silicon superconductivity was only discovered in 2006 in laser doped Si:B samples. Laser annealing is instrumental to cross the superconductivity threshold, as the required doping is above the solubility limit, and cannot be reached using conventional micro-electronic techniques. Laser doping allows the realisation of epitaxial, homogeneous, thin silicon layers (5-300 nm) with extreme active doping as high as 11 at. %, and without the formation of B aggregates.

Silicon is a disordered superconductor, with a lower carrier density (1e20 to 5e21 cm-3) than metallic superconductors, a critical temperature modulable with doping from 0 to 0.8 K, and a relatively high resistivity that allows to easily match the devices to the void impedance.

We have realised microwave silicon resonators, working in the 1-12 GHz range and with quality factors about 4000. We have shown a strong non-linear response with power, observing a Kerr coefficient of the order of 300 Hz/photon where less than 1 Hz/photon was expected. To better understand the losses and recombination mechanisms, we have measured the relaxation dynamics of the resonators following a light or a microwave pulse.

TT 1.3 Mon 10:45 H6

Nanocrystalline boron-doped diamond as a model granular superconductor — •Georgina Klemencic[1], David Perkins[2], Jon Fellows[3], Soumen Mandal[1], Chris Muirhead[2], Robert Smith[2], Sean Giblin[1], and Oliver Williams[1] — [1]Cardiff University, UK — [2]University of Birmingham, UK — [3]University of Bristol, UK

We present results of an experimental investigation into Boron-doped Nanocrystalline Diamond (BNCD), which we argue to be an exemplary model for granularity in a low-temperature superconducting system.

Through measurement of the fluctuation conductivity [1], we have indirectly measured the inter- and intragrain diffusion lengths, in an experimental application of the theoretically proposed 'fluctuation spectroscopy' technique. The fluctuation conductivity is well predicted by theories of granular superconductors and the magnetoresistance exhibits the same glassy behaviour as high-T_c samples [2]. In this respect, we find that BNCD is a good system for distinguishing high-T_c behaviours from granular superconductor behaviours.

A special feature of BNCD is its morphology, in which grains extend vertically through the film, making the bulk material structurally akin to a naturally occurring Josephson junction array. In recent work, we have found evidence of metastable phase slip-like excitations in the current-voltage characteristics of macroscopic bridges fabricated from BNCD, which we attribute to this morphology [3].

[1] G. M. Klemencic et al., Phys. Rev. Mater. 1.4 (2017): 044801
[2] G. M. Klemencic et al., Sci. Rep. 9.1 (2019): 1-6
[3] G. M. Klemencic et al., Carbon 175 (2021): 43-49

TT 1.4 Mon 11:00 H6

Distribution of the order parameter in strongly disordered superconductors: analytic theory — •Anton V. Khvalyuk[1,2] and Mikhail V. Feigel'man[2,3] — [1]Skolkovo Institute of Science and Technology, 143026 Skolkovo, Russia — [2]L. D. Landau Institute for Theoretical Physics, 119334 Moscow, Russia — [3]Moscow Institute of Physics and Technology, 117303 Dolgoprudny, Russia

We present an analytic theory of inhomogeneous superconducting pairing in strongly disordered materials, which are moderately close to Superconducting-Insulator Transition. Within our model, single-electron eigenstates are assumed to be Anderson-localized, with a large localization volume. Superconductivity then develops due to coherent delocalization of originally localized preformed Cooper pairs. The key assumption of the theory is that each such pair is coupled to a large number $Z \gg 1$ of similar neighboring pairs. We derived integral equations for the probability distribution $P(\Delta)$ of local superconducting order parameter $\Delta(\boldsymbol{r})$ and analyzed their solutions in the limit of small dimensionless Cooper coupling constant $\lambda \ll 1$. The shape of the order-parameter distribution is found to depend crucially upon the effective number of "nearest neighbors" $Z_{\text{eff}} = 2\nu_0 \Delta Z$. The solution we provide is valid both at large and small Z_{eff}; the latter case is nontrivial as the function $P(\Delta)$ is heavily non-Gaussian. One of our key findings is the discovery of a broad range of parameters where the distribution function $P(\Delta)$ is non-Gaussian but also free of "fat tails" and other features of criticality. The analytic results are supplemented by numerical data, and good agreement between them is observed.

15. min. break

TT 1.5 Mon 11:30 H6

Spectroscopy of a single Josephson impurity in a high kinetic inductance array — •Serge Florens[1], Sébastien Léger[1], Théo Sépulcre[1], Denis Basko[2], Izak Snyman[3], and Nicolas Roch[1] — [1]Néel Institute, CNRS, Grenoble, France — [2]LPMMC, UGA, Grenoble, France — [3]Wits University, Johannesburg, South Africa

Superconducting arrays constitute a promising platform to explore a large class of physical phenomena, from quantum phase transitions to non-linear quantum optics in the microwave domain. We design a fully-tunable model system where a long chain of several thousands linear Josephson elements, acting as a high inductance transmission line, is terminated by a small Josephson junction endowed with a strong non-linearity, acting as a single impurity. From microwave spectroscopic measurements, we extract the phase shift and the inelastic losses induced by the impurity onto the linear modes of the array. In agreement with a microscopic modeling of the circuit, we put into evidence a huge renormalization of the Josephson tunnel energy at the impurity site, and show that the associated enhancement of phase fluctuations provides the dominant dissipation mechanism in the array.

TT 1.6 Mon 12:00 H6

Low energy electrodynamics of strongly disordered superconductors — •Götz Seibold[1], Lara Benfatto[2], and Claudio Castellani[2] — [1]BTU Cottbus-Senftenberg, Cottbus, Germany — [2]University of Rome 'La Sapienza', Rome, Italy

In this contribution we will discuss the static and dynamical response of strongly disordered superconductors based on investigations of the attractive Hubbard model with strong on-site disorder and by including fluctuations beyond the Bogoljubov-de Gennes approach. It turns out that paramagnetic processes mediate the response of all collective modes, with a substantial contribution of charge/phase fluctuations [1,2,3]. In particular, we show that for strongly disordered superconductors phase modes acquire a dipole moment and appear as a subgap spectral feature in the optical conductivity which even survives long-range Coulomb interactions. The same processes turn out to dominate also the third-order current at strong disorder [5]. In this regard we show that disorder strongly influences the polarization dependence of the non-linear response, with a marked difference between the homogenous and the disordered case. Our results are particularly relevant for recent experiments in cuprates, whose band structure is in a first approximation reproduced by our lattice model.

[1] G. Seibold et al., Phys. Rev. B 92, 064512 (2015)
[2] T. Cea et al., Phys. Rev. B 89, 174506 (2014)
[3] G. Seibold et al., Phys. Rev. Lett. 108, 207004 (2012)
[4] G. Seibold et al., Phys. Rev. B 103, 014512 (2021)

TT 1.7 Mon 12:15 H6

Decoupling of the Quasiparticle Number and Lifetime in a Disordered Superconductor Probed by Quasiparticle Fluctuation Measurements — •Steven A. H. de Rooij[1,2], Kevin Kouwenhoven[1,2], Jochem J. A. Baselmans[1,2], Vignesh Murugesan[2], David J. Thoen[1,3], and Pieter J. de Visser[2] — [1]SRON - Netherlands Institute for Space Research, Leiden, The Netherlands — [2]Department of Microelectronics, Delft University of Technology, The Netherlands — [3]Kavli Institute of NanoScience, Delft University of Technology, Delft, The Netherlands

In a superconductor, the number of quasiparticles (N_{qp}) decreases exponentially when lowering the temperature, while the quasiparticle lifetime increases, i.e. $\tau_{qp} \sim 1/N_{qp}$. Measuring quasiparticle fluctuations, induced by thermal fluctuations, give access to both τ_{qp} and N_{qp}. In disordered superconductors, these fundamental quasiparticle properties have hardly been studied, although these materials are widely applied in high kinetic inductance quantum circuits and kinetic inductance detectors. We measured quasiparticle fluctuations in the disordered superconductor β-Ta, embedded in a NbTiN microwave resonator, probing both the dissipation (i.e. quasiparticles) and kinetic inductance (i.e. Cooper-pairs). We observe a non-conventional temperature dependence of τ_{qp}, i.e. $\tau_{qp} \nsim 1/N_{qp}$, which results in a strong reduction of the quasiparticle fluctuations with decreasing temperature. This behavior is similar to that of the conventional superconductor Al, where we relate it to quasiparticle trapping [arXiv:2103.04777], which may also play a role in disordered superconductors.

TT 1.8 Mon 12:30 H6

Current-enhanced superfluid stiffness near the Berezinskii-Kosterlitz-Thouless transition in strongly disordered NbN-films — •Alexander Weitzel[1], Lea Pfaffinger[1], Klaus Kronfeldner[1], Thomas Huber[1], Lorenz Fuchs[1], Sven Linzen[2], Evgenii Il'ichev[2], Nicola Paradiso[1], and Christoph Strunk[1] — [1]Experimental and Applied Physics, Uni Regensburg, Germany — [2]Leibniz Institute of Photonic Technology, Jena, Germany

We investigate resistivity and kinetic inductance in long and ultra-thin NbN strips near the superconductor-insulator transition. Resistive transition is dominated by superconducting fluctuations of both amplitude and phase of the order parameter. Near the foot of the transition, the resistivity displays a square-root cusp divergence of the conductance expected for the Berezinski-Kosterlitz-Thouless (BKT) transition. The superfluid stiffness of the very same strip (measured using an RLC-resonator technique) displays a sharp drop close to the universal value of $2T_{\mathrm{BKT}}/\pi$. Current voltage (IV) characteristics become non-linear below T_c, with a complex back-bending shape that signals a heating instability. At lower temperatures, IV-characteristics feature a peculiar negative curvature in a log-log representation. This indicates a reduction of dissipation with respect to the standard power-law behavior of the IV-characteristics and is corroborated by the observation of an unexpected increase of kinetic inductance near the critical current.

TT 2: Focus Session: Exotic Charge Density Wave States of Matter: Correlations and Topology (joint session TT/HL)

The recent observation of charge density waves (CDW) in a variety of topological materials ranging from two-dimensional dichalcogenides, Weyl semimetals and metallic kagome systems has prompted intensive research on the origin and effects of such states. In these systems charge order forms the basis for correlated and topological states of quantum matter: Mott Hubbard correlations, tentative spin-liquid physics and chiral superconductivity in two-dimensional dichalcogenides, the emergence of axionic CDWs in Weyl semimetals and an interplay of Z2 topology, charge order and superconductivity in kagome metals. At the same time topology and electron correlations feed back on the CDW formation and dynamics. In this Focus Session we bring together theorists and experimentalists working in the field to discuss the interplay of charge order, correlations and topology in representative model systems, to identify major open challenges in our understanding of these systems and ultimately reach out for controlling CDW physics in correlated topological states of matter.

Organizers: Roser Valenti (Frankfurt University), Tim Wehling (Bremen University)

Time: Monday 10:00–12:45 Location: H7

TT 2.1 Mon 10:00 H7

Chiral superconductivity in the alternate stacking compound 4Hb-TaS$_2$ — •Amit Kanigel — Technion. Haifa, Israel

We study 4Hb-TaS$_2$, which naturally realizes an alternating stacking of 1T-TaS$_2$ and 1H-TaS$_2$ structures. The former is a well-known Mott insulator, which has recently been proposed to host a gapless spin-liquid ground state. The latter is a superconductor known to also host a competing charge density wave state. We find a superconductor with a T$_c$ of 2.7 Kelvin and anomalous properties, of which the most notable one is a signature of time-reversal symmetry breaking, abruptly appearing at the superconducting transition. This observation is consistent with a chiral superconducting state.

TT 2.2 Mon 10:30 H7

Non-local electronic correlations in 1T-TaS$_2$ out of equilibrium — •Uwe Bovensiepen — University of Duisburg-Essen, Faculty of Physics and Center for Nanointegration (CENIDE), 47048 Duisburg, Germany

Transition metal dichalcogenides with a d^1 transition metal electron configuration exhibit broken symmetry ground states and distorted structures. The formation of charge density wave (CDW) states in conjunction with Mott physics in 1T-TaS$_2$ is a well know example. Current efforts aim at microscopic understanding of the intertwined electronic and lattice effects. In this regard experiments in the time domain provide direct insights because the characteristically different timescales of electronic hopping with a time constant $\hbar/J$ ≈2 fs and the CDW amplitude period of 400 fs can be well distinguished. In this talk time-resolved photoelectron spectroscopy results will be presented in connection with theoretical results to discuss electronic excitations and their dynamics. Excitation and relaxation of doubly occupied sites is mediated by intersite hopping and coupling to delocalized electrons [1,2]. Comparison with literature indicates that such electron dynamics can be excited selectively, separate from lattice excitations. First experiments towards bulk sensitive, time-resolved photoelectron spectroscopy [3] will be discussed as well.

Funding by the DFG through SFB 1242 is gratefully acknowledged. [1] Ligges et al., PRL **120**, 166401 (2018)
[2] Avigo et al., PR Research **2**, 022046(R) (2020)
[3] Beyazit et al., PRL **125**, 076803 (2020)

15 min. break

TT 2.3 Mon 11:15 H7

Axionic charge density wave in the Weyl semimetal $(TaSe_4)_2I$ — •Johannes Gooth — Max Planck Institut für Chemische Physik fester Stoffe, Dresden, Germany

An axion insulator is a correlated topological phase, which is predicted to arise from the formation of a charge-density wave in a Weyl semimetal that is, a material in which electrons behave as massless chiral fermions. The accompanying sliding mode in the charge-density-wave phase - the phason - is an axion and is expected to cause anomalous magnetoelectric transport effects. However, this axionic charge-density wave has not yet been experimentally detected. Here, we report the observation of a large positive contribution to the magnetoconductance in the sliding mode of the charge-density-wave Weyl semimetal $(TaSe_4)_2I$ for collinear electric and magnetic fields. The positive contribution to the magnetoconductance originates from the anomalous axionic contribution of the chiral anomaly to the phason current, and is locked to the parallel alignment of the electric and magnetic fields. By rotating the magnetic field, we show that the angular dependence of the magnetoconductance is consistent with the anomalous transport of an axionic charge-density wave. Our results show that it is possible to find experimental evidence for axions in strongly correlated topological condensed matter systems, which have so far been elusive in any other context.

Invited Talk TT 2.4 Mon 11:45 H7

Electronic instabilities of kagomé metals and density waves in the AV_3Sb_5 materials — •Leon Balents — University of California, Santa Barbara

Recently, a new class of kagomé metals, with chemical formula AV_3Sb_5, where A = K, Rb, or Cs, have emerged as an exciting realization of quasi-2D correlated metals with hexagonal symmetry. These materials have been shown to display several electronic orders setting in through thermodynamic phase transitions: multi-component (*3Q*) hexagonal charge density wave (CDW) order below a T_c of 90K, and superconductivity with critical temperature of 2.5K or smaller, and some indications of nematicity and one-dimensional charge order in the normal and superconducting states. Other experiments show a strong anomalous Hall effect, suggesting possible topological physics. I will discuss a theory of these phenomena based in part on strong interactions between electrons at saddle points, as well as ideas related to different competing density wave orders.

TT 2.5 Mon 12:15 H7

Charge density waves and superconductivity in kagome metals — •Titus Neupert — Univertity of Zurich, Zurich, Switzerland

Strongly correlated itinerant electron systems exhibit an intertwining of interactions and electronic band fermiology, including flat bands and van Hove points with diverging density of states, nesting patterns, or band degeneracies –for instance of Dirac type or quadratic band touching. The kagome lattice stands out in that it combines all these characteristics, and has thus been subject to many theoretical investigations. However, material realizations of kagome metals with interaction-induced Fermi instabilities have largely been elusive. The recently discovered family of kagome materials AV3Sb5 has filled this gap, displaying charge ordered and superconducting phases with unconventional properties. In my talk, I will discuss the status quo understanding of these instabilities emanating from a critical synopsis of experiments and theoretical studies.

TT 3: Focus Session: Entanglement as a Probe for Correlated Quantum Matter

The interplay of quantum fluctuations and correlations in many-body systems can result in novel phases with exciting physical phenomena. Celebrated examples are the fractional quantum Hall effect and quantum spin liquids. A generic property of such phases is their non- local entanglement that manifests itself in topological order and fractionalized particle-like excitations. Excitingly, it has been proposed that such topologically ordered phases might be an ideal building block for a fault-tolerant quantum computer. While recent experiments pinpointed the presence of fractionalized excitations in spin-liquid materials, the characteristic underlying property of non-local entanglement remains elusive and evades a direct experimental probe.

Organizers: Alexander Tsirlin (Augsburg University), Frank Pollmann (Technical University Munich)

Time: Monday 13:30–16:15 Location: H6

TT 3.1 Mon 13:30 H6

Measuring quantum entanglement with neutrons — •Alan Tennant — Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

The quantification of entanglement without the need for underlying models and theoretical solutions is an open challenge for measurement in condensed matter. This is particularly important in the case of quantum magnets such as spin liquids where we often lack theories that can connect with measurement. Three quantum entanglement witnesses relevant to neutron scattering have been proposed in the form of one-tangle, two-tangle (concurrence), and quantum Fisher information. We have recently applied these to real quantum magnets and found the one-tangle and quantum Fisher information to be particularly promising. I will show how the entanglement witnesses can be determined using experiment and what can be learned from them about the underlying quantum states.

TT 3.2 Mon 14:00 H6

Observation of E_8 particles in Ising chain quantum magnets — •Zhe Wang — Department of Physics, TU Dortmund University, Dortmund, Germany

Near the transverse-field-induced quantum critical point of the Ising chain, an exotic dynamic spectrum consisting of exactly eight particles was predicted [1], which is uniquely described by an emergent quantum integrable field theory with the E_8 Lie algebra, but rarely explored experimentally. By performing high-resolution terahertz spectroscopy of quantum spin dynamics and comparing to analytical calculation of the dynamical spin correlations, we revealed evidence for the E_8 particles in the Ising chain antiferromagnet $BaCo_2V_2O_8$ [2] as well as in the Ising chain ferromagnet $CoNb_2O_6$ [3] under an applied transverse field. In particular, higher-energy E_8 particles were observed above the low-lying two-particle continua, featuring the quantum many-body effects in the exotic dynamic spectrum [2,3].

[1] A. B. Zamolodchikov, Int. J. Mod. Phys. A 4, 4235 (1989).
[2] Z. Zhang et al., Phys. Rev. B 101, 220411 (2020).
[3] K. Amelin et al., Phys. Rev. B 102, 104431 (2020).

15 min. break

TT 3.3 Mon 14:45 H6

Topologically ordered systems on the digital quantum processor — Kevin Satzinger[3], •Yujie Liu[1,2], Adam Smith[4], Christina Knapp[5,6], Michael Knap[1,2], Kirill Schtengel[7], Pedram Roushan[3], and Frank Pollmann[1,2] — [1]Department of Physics, Technical University of Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology, M{\"u}nchen, Germany — [3]Google Quantum AI, Mountain View, CA, USA — [4]Centre for the Mathematics and Theoretical Physics of Quantum Non-Equilibrium Systems, University of Nottingham, Nottingham, UK — [5]Department of Physics and Institute for Quantum Informationand Matter, California Institute of Technology, Pasadena, CA, USA — [6]Walter Burke Institute for Theoretical Physics, California Institute of Technology, Pasadena, CA, USA — [7]Department of Physics and Astronomy, University of California, Riverside, California, USA

In the first part of the talk, we will discuss the experiment on Sycamore quantum processor where we prepare the ground state of the toric code Hamiltonian using an efficient quantum circuit. We measure a topological entanglement entropy near the expected value of ln 2 and simulate anyon interferometry to extract the braiding statistics of the emergent excitations. We further investigate key aspects of the surface code, including logical state injection and the decay of the nonlocal order parameter. In the second part of the talk. We generalize our protocol to the more general class of string-net states which host doubled topological order, rendering the braiding of non-abelian anyons possible, as a tool to probe and simulate topological quantum field theory.

TT 3.4 Mon 15:15 H6

Robustness of the thermal Hall effect close to half-quantization in a field-induced spin liquid state — •Jan Bruin[1], Ralf Claus[1], Yosuke Matsumoto[1], Nobuyuki Kurita[2], Hidekazu Tanaka[2], and Hidenori Takagi[1,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Department of Physics, Tokyo Institute of Technology, Tokyo, Japan — [3]Department of Physics, The University of Tokyo, Bunkyo, Tokyo, Japan

Thermal signatures of fractionalized excitations are a fingerprint of quantum spin liquids (QSLs). In the J_{eff}=1/2 honeycomb magnet α-$RuCl_3$, a QSL state emerges upon applying an in-plane magnetic field $H_{||}$ greater than the critical field $H_{C2} \approx 7$ T along the a-axis, where the thermal Hall conductivity (k_{XY}/T)

was reported to take on the half-quantized value k_{HQ}/T. This finding was discussed as a signature of an emergent Majorana edge mode predicted for the Kitaev QSL. The $H_{||}$- and T-range of the half-quantized signal and its relevance to a Majorana edge mode are, however, still under debate.

Here we present a comprehensive study of k_{XY}/T in α-$RuCl_3$ with $H_{||}$ up to 13 T and T down to 250 mK, which reveals the presence of an extended region of the phase diagram with $k_{XY}/T \approx k_{HQ}/T$ above H_{C2}. The results are in support of a topological state with a half-quantized k_{XY}/T and suggest an interplay with crossovers or weak phase transitions beyond H_{C2} in α-$RuCl_3$.

TT 3.5 Mon 15:30 H6

Angle-dependent thermodynamic measurements on α-$RuCl_3$ — •Sebastian Bachus[1], David Kaib[2], Anton Jesche[1], Yoshifumi Tokiwa[1], Vladimir Tsurkan[1], Alois Loidl[1], Stephen Winter[2], Alexander Tsirlin[1], Roser Valentí[2], and Philipp Gegenwart[1] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg — [2]Institute of Theoretical Physics, Goethe University Frankfurt

For several years, the field-dependence of the Kitaev material α-$RuCl_3$ has been subject to controversial discussions. Recently, a field-induced Kitaev spin liquid state has been proposed above the critical field for long-range magnetic order. This scenario, however, requires another phase transition towards the partially polarized state upon leaving the spin liquid phase. We utilize a high-resolution alternating field method to precisely determine the magnetic Grüneisen parameter down to 0.5 K in magnetic fields up to 14 T. In combination with specific heat measurements, this allows us to determine the entropy evolution into and out of the presumed topological Kitaev quantum spin liquid regime. We compare our thermodynamic measurements to exact diagonalization results and carefully establish the temperature-field phase diagram. Finally, we discuss implications on the suggested spin liquid phase.

[1] S. Bachus et al., Phys. Rev. B 103, 054440 (2021)
[2] S. Bachus et al., Phys. Rev. Lett. 125, 097203 (2020)

TT 3.6 Mon 15:45 H6

Comparative study of the triangular spin-liquid candidates $NaYbO_2$, $KYbO_2$ and $KYbS_2$ — •Franziska Grussler, Sebastian Bachus, Noah Winterhalter-Stocker, Philipp Gegenwart, and Alexander Tsirlin — Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

Spin liquid is an entangled state of matter. $NaYbO_2$, $KYbO_2$ and $KYbS_2$ feature the same space group $R\bar{3}m$ as the spin-liquid candidate $YbMgGaO_4$ but evade structural disorder pertinent to that compound. We report a comparative study of the polycrystalline $NaYbO_2$ and $KYbO_2$ and single crystalline $KYbS_2$ including their structural characterization and thermodynamic properties in the milli-K temperature range. The compounds reveal the reduction in magnetic couplings upon replacing Na by K and the enhanced easy-plane anisotropy upon replacing O by S. They show no signs of magnetic order in zero field, but undergo field-induced magnetic order. For $KYbS_2$ a detailed B-T phase diagram is deduced from heat capacity, dilatometry and magnetization measurements for B‖c. By studying specific heat of $NaYbO_2$ and $KYbS_2$ at milli-K temperatures, we conclude that between 0.5 T and 2 T, within the putative spin-liquid phase, magnetic specific heat follows quadratic behavior expected for the gapless Dirac spin liquid. Our observations establish gapless nature of the spin-liquid phase of triangular antiferromagnets but show strong similarities to 120-degree ordered triangular antiferromagnets when B‖c is applied.

TT 3.7 Mon 16:00 H6

Structural and thermodynamic properties of the spin-liquid candidate $Na_2BaCo(PO_4)_2$ — •Vera P. Bader[1], Alexander A. Tsirlin[1], Ivo Heinmaa[2], Raivo Stern[2], Noah Winterhalter-Stocker[1], and Philipp Gegenwart[1] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg — [2]National Institute of Chemical Physics and Biophysics, Tallinn

The first report of $Na_2BaCo(PO_4)_2$ as a spin liquid candidate [1] brought the compound to the fore. One structural prerequisite is fulfilled as the Co^{2+} ions with an effective spin 1/2 form a frustrated triangular lattice. The low temperature properties found in the literature are rather controversial. On the one hand a clear transition is observed in the heat capacity data in zero magnetic field at 140 mK [2]. One the other hand AC magnetic susceptibility data and ZF-μSR measurements indicate a dynamically fluctuating ground state down to 80 mK [3]. The spin-liquid state is highly sensitive to details of the crystal structure and may be suppressed upon structural disorder. Here, we revise both crystal structure and low-T temperature-field phase diagram of $Na_2BaCo(PO_4)_2$. Using high-resolution synchrotron XRD and NMR, we show symmetry lowering and signatures of structural disorder. Moreover, our milli-K heat capacity, thermal expansion and magnetostriction measurements confirm magnetic order in zero field and reveal field-induced phases expected from a nearest-neighbor triangular antiferromagnet.

[1] Zhong *et al.*, PNAS 116 29 (2019)
[2] Li *et al.*, Nat. Commun 11 4216 (2020)
[3] Lee *et al.*, Phys. Rev B 103 024413 (2021)

TT 4: Focus Session: Correlated van-der-Waals Magnets

Reducing the dimensionality of electronic materials often yields novel phenomena and exceptional physical properties. In layered van-der-Waals (vdW) materials which are formed by structurally stable but out-of-plane only weakly coupled crystalline layers this is, e.g., demonstrated by the presence of long-range magnetic order down to the bilayer in $Cr_2Ge_2Te_6$ and down to the monolayer in CrI_3. For VSe_2, the presence of ferromagnetism even at room temperature has been reported for monolayers while the bulk material is paramagnetic. Due to their quasi-2D, layered vdW-magnets do not only allow to investigate fundamental aspects of electronic correlation in structurally reduced dimensionality, but also hold a promise for technological applications, as demonstrated, e.g., by $Cr_2Ge_2O_6$/NiO heterostructures or $NiPS_3$-based field-effect transistors. Furthermore, the recent discovery of magnetic topological insulators (MTIs) in the $(MnBi_2Te_4)(Bi_2Te_3)$n (n = 0, 1, 2) family of vdW compounds has provided a rich experimental basis for the realization of new emerging physical phenomena such as the quantum anomalous Hall effect, the topological magnetoelectric effect, and majorana fermions emerging in MTIs due to a coexistence of the long-range magnetic order and the topologically nontrivial electronic band structure.

Organizers: Bernd Büchner (IFW Dresden), Rüdiger Klingeler (Heidelberg University)

Time: Monday 13:30–16:15 Location: H7

TT 4.1 Mon 13:30 H7

Topological states in $MnBi_2Te_4$-based magnetic van der Waals materials — •Hendrik Bentmann[1], Raphael. C. Vidal[1], Philipp Kagerer[1], Sebastian Buchberger[1], Celso Fornari[1], Anna Isaeva[2], and Friedrich Reinert[1] — [1]Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [2]Van der Waals – Zeeman Institute, IoP, University of Amsterdam, 1098 XH Amsterdam, The Netherlands

Magnetic van der Waals materials down to a single monolayer have attracted considerable attention in recent years. In this talk, we will discuss electronic and magnetic properties of $MnBi_2Te_4$-based systems, in which Mn local moments and strong spin-orbit interaction of Bi and Te yield an interplay of magnetism and non-trivial band topology. Using angle-resolved photoemission and X-ray magnetic dichroism, we provide evidence that 3D $MnBi_2Te_4$ realizes an antiferromagnetic topological insulator [1]. Incorporation of non-magnetic Bi_2Te_3 spacer layers in $MnBi_4Te_7$ and $MnBi_6Te_{10}$ yields modified magnetic properties and surface-termination-dependent topological surface states [2]. In the 2D regime, $MnBi_2Te_4$ is a candidate for realizing the quantum anomalous Hall state. We will present ongoing efforts to grow $MnBi_2Te_4$ thin films using molecular beam epitaxy (MBE) [3].

[1] Nature 576, 416 (2019)
[2] Phys. Rev. X 9, 041065 (2019), Phys. Rev. Lett. 126, 176403 (2021)
[3] J. Appl. Phys. 128, 135303 (2020)

TT 4.2 Mon 14:00 H7

Static and dynamic magnetic properties of $(MnBi_2Te_4)(Bi_2Te_3)_n$ ($n = 0, 1$) probed by electron spin resonance technique. — •Alexey Alfonsov[1], Kavita Mehlawat[1,2], Jorge I. Facio[1], Ali G. Moghaddam[1,3], Rajyavardhan Ray[1], Alexander Zeugner[4,5], Manuel Richter[1,5], Anna Isaeva[1,6], Jeroen van den Brink[1,2,5], Bernd Büchner[1,2,5], and Vladislav Kataev[1] —

[1]Leibniz IFW Dresden, 01069 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]IASBS, Zanjan 45137-66731, Iran — [4]H.C. Starck Tungsten GmbH, 38642 Goslar, Germany — [5]TU Dresden, 01062 Dresden, Germany — [6]University of Amsterdam, 1098 XH Amsterdam, The Netherlands

$(MnBi_2Te_4)(Bi_2Te_3)_n$ ($n = 0, 1$) represent a family of van der Waals materials which exhibit a coexistence of topologically nontrivial surface states with intrinsic magnetism. Such unusual combination of properties renders this natural heterostructures very attractive for investigations since it enables a number of exotic phenomena. In this work we address static and dynamic magnetic properties of the title materials in the ordered and disordered states using multifrequency and high field electron spin resonance technique. We show that the spin dynamics of the magnetic building blocks of these compounds, the Mn-based septuple layers (SLs), is inherently ferromagnetic (FM) featuring persisting short-range FM correlations far above the magnetic ordering temperature as soon as the SLs get decoupled either by introducing a nonmagnetic quintuple interlayer, as in $MnBi_4Te_7$, or by applying a moderate magnetic field, as in $MnBi_2Te_4$.

TT 4.3 Mon 14:15 H7

Tuning Magnetic and Transport Properties in Quasi-2D $(Mn_{1-x}Ni_x)_2P_2S_6$ Single Crystals — •S. Aswartham[1], Y. Shemerliuk[1], Y. H. Zhou[2], Z. R. Yang[2], G. Cao[3], A.U.B. Wolter[1], and B. Büchner[1,4] — [1]Institut für Festkörperforschung, Leibniz IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Anhui Province Key Laboratory of Condensed Matter Physics at Extreme Conditions, High Magnetic Field Laboratory, Chinese Academy of Sciences, Hefei 230031, China — [3]Department of Physics, University of Colorado at Boulder, Boulder, CO 80309, USA — [4]Institut für Festkörper-und Materialphysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

We report an optimized chemical vapor transport method to grow single crystals of $(Mn_{1-x}Ni_x)_2P_2S_6$ where x = 0, 0.3, 0.5, 0.7, and 1. The structural characterization shows that all crystals crystallize in monoclinic symmetry with the space group $C2/m$ (No. 12). The magnetic measurements of the all as-grown single crystals show long range antiferromagnetic order along all principal crystallographic axes. Overall, the Néel temperature T_N is non-monotonous; with increasing Ni^{2+} doping, the temperature of the antiferromagnetic phase transition first decreases from 80 K for pristine ($Mn_2P_2S_6$ (x = 0) up to x= 0.5 and then increases again to 155 K for pure $Ni_2P_2S_6$ (x = 1). We show that, the magnetic anisotropy switches from out-of-plane to in-plane as a function of composition.

15. min. break

Invited Talk TT 4.4 Mon 14:45 H7

2D Magnetism and Its Efficient Control — •Cheng Gong — University of Maryland, College Park, USA

Magnetism, one of the most fundamental physical properties, has revolutionized significant technologies such as data storage and biomedical imaging, and continues to bring forth new phenomena in emerging materials of reduced dimensionalities. The recently discovered magnetic 2D van der Waals materials provide ideal platforms to enable the atomic-thin, flexible, lightweight magneto-optical and magnetoelectric devices. Though many have hoped that the ultra-thinness of 2D magnets should allow an efficient control of magnetism, the state-of-the-art has not achieved notable breakthroughs to this end. In this talk, I will speak on our experimental discovery of the first 2D ferromagnet, and discuss the strategies of the efficient control of 2D magnetism.

TT 4.5 Mon 15:15 H7

Coulomb-Engineered Magnetism in CrI_3 Monolayer — David Soriano, Alexander Rudenko, Mikhail Katsnelson, and •Malte Rösner — Radboud University, Nijmegen, Netherlands

We present a detailed study on the microscopic origin of magnetism in suspended and dielectrically embedded CrI_3 monolayer. To this end, we downfold minimal generalized Hubbard models from *ab initio* calculations using the constrained random phase approximation. Within mean-field approximation, we show that these models are capable of describing the formation of localized magnetic moments in CrI_3 and of reproducing electronic properties of full *ab initio* calculations. We find a multi-orbital super-exchange mechanism as the origin of magnetism in CrI_3 resulting from a detailed interplay between effective ferro- and anti-ferromagnetic Cr-Cr d coupling channels, which is decisively affected by the ligand (I) p orbitals. We show how environmental screening such as resulting from encapsulation with hexagonal boron nitride (hBN) of the CrI_3 monolayer affects the Coulomb interaction in the film and how this successively controls its magnetic properties. Driven by a non-monotonic interplay between nearest and next-nearest neighbour exchange interactions we find the magnon dispersion and the Curie temperature to be non-trivially affected by the environmental dielectric screening.

TT 4.6 Mon 15:30 H7

Magnetoelastic coupling in the ferromagnetic van-der-Waals material CrI_3 — •Jan Arneth[1], Martin Jonak[1], Sven Spachmann[1], Mahmoud Abdel-Hafiez[2], Yaroslav Kvashnin[3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University, Germany — [2]Department of Physics and Astronomy, X-ray Photon Science, Uppsala University, Sweden — [3]Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden

We present high-resolution thermal expansion and magnetostriction studies on the layered van-der-Waals (vdW) ferromagnet CrI_3 in magnetic fields up to 15 T. Distinct anomalies in the thermal expansion coefficient at the ferromagnetic ordering temperature signal magnetoelastic coupling and allow us to quantify the uniaxial pressure dependencies $\partial T_C/\partial p_i$. While T_C reduces at a rate of −0.4 K/GPa upon the application of in-plane pressure, ferromagnetism is stabilized and the effect is about 4 times larger for out-of-plane pressure. The results are compared with numerical studies. We also observe macroscopic length changes associated with field-induced flipping of antiferromagnetically coupled surface layers in the magnetostriction data. We construct the magnetic phase diagram of bulk CrI_3 and show that magnetostriction is also sensitive to the saturation fields of the FM bulk and AFM surface phases.

TT 4.7 Mon 15:45 H7

Probing magnetic states in 2D layered van-der- Waals materials under pressure — Anirudha Gosh[1], Deobrat Singh[1], Qingge Mu[2], Sergey Medvedev[2], Rajeev Ahuja[1], Olle Eriksson[1], and •Mahmoud Abdel-Hafiez[1] — [1]Uppsala University, Department of Physics and Astronomy, Box 516, SE-751 20 Uppsala, Sweden — [2]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany

Two-dimensional van der Waals materials offer a plethora of functional properties that are not only of fundamental interest but are essential for the development of new technological applications. Through combined complementary experimental techniques supplemented with theoretical calculations on high quality CrI3 single crystals, we derive a previously not discussed pressure-temperature phase diagram. TC increases to ~ 66 K with pressure up to ~ 3 GPa and then decreases to ~ 10 K at 21.2 GPa. The origin of this behavior is associated with a decrease in the calculated bond angle from 95^o at ambient pressure to ~ 85^o at 25 GPa. At a pressure above ~ 22 GPa, the magnetically ordered state is highly quenched, possibly driving the system to a Kitaev spin-liquid state at low temperature. Pressure-dependent Raman and resistivity measurements also reveal suppression of the phonon modes and semiconductor to metal transition, respectively above ~ 22 GPa. Furthermore, we will describe our recent experiments on CrCl3 single crystals.

TT 4.8 Mon 16:00 H7

Magnetic- and structural properties of α-$RuCl_3$ under hydrostatic He-gas pressure — •Bernd Wolf[1], Anja Wolter-Giraud[3], Gael Bastien[3], Anna Isaeva[4], David Kaib[2], Aleksandar Razpop[2], Kira Riedl[2], Sananda Biswas[2], Roser Valentí[2], Bernd Büchner[3], and Michael Lang[1] — [1]Physikalisches Institut, GU, SFB/TR 288, D-60438 Frankfurt (M) — [2]Institut für theoretische Physik, GU, SFB/TR 288, D-60438 Frankfurt (M) — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, 01171 Dresden, Germany — [4]Fakultät für Chemie und Lebensmittelchemie, TUD, 01062 Dresden, Germany

α-$RuCl_3$ is a material to probe fundamental aspects of Kitaev physics despite the occurrence of magnetic order at low temperatures. We followed the idea that the suppression of magnetic order in α-$RuCl_3$ by using external parameters like magnetic field or pressure gives rise to a range where Kitaev physics prevails. We present magnetic susceptibility measurements on α-$RuCl_3$ single crystals under almost ideal hydrostatic pressure conditions. We find that the susceptibility strongly increases with increasing pressure. Furthermore, the magnetic ordering temperature T_N becomes rapidly reduced with pressure but cannot be fully suppressed to $T_N = 0$ due to the occurrence of a pressure-induced dimerization transition. We explain both results microscopically by employing a combination of first principles and finite-temperature Lanczos methods. Importantly, thorough investigations of the experimentally observed magnetic transition at varying pressure and magnetic fields reveal clear indications for a first order transition.

TT 5: Poster Session: Superconductivity

Time: Monday 13:30–16:00 Location: P

TT 5.1 Mon 13:30 P

Proximity effects of superconducting Nb thin films on chiral magnetic substrates — •Julius Grefe[1], Rodrigo de Vasconcellos Lourenço[2], Philip Schröder[1], Jannis Willwater[1], Mauricio de Melo[3], Jochen Litterst[1], Stefan Süllow[1], and Dirk Menzel[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Institut für Angewandte Physik, TU Braunschweig, Germany — [3]Departamento de Física, Universidade Estadual de Maringá, Brazil

Superconducting spin valves consisting only of a single magnetic layer and a thin superconducting film promise simple and compact devices in comparison to established GMR systems. Theory has suggested that the critical temperature T_C of a superconductor can be controlled via the proximity effect with a magnetic system exhibiting a non-collinear spin structure [1]. MnSi being a member of the non-centrosymmetric B20 structure shows helimagnetic spin order below $T_N = 29.5$ K and $B_{C1} = 100$ mT. In the related system $Fe_{1-x}Co_xSi$ the Néel-temperature can be tuned in a range of 0 K - 55 K by variation of the Co concentration. Superconducting Nb thin films have been deposited by molecular beam epitaxy on oriented monocrystalline substrates grown by the Triarc-Czochralski method. The surface quality of the substrates and the Nb films has been investigated by atomic force microscopy resulting in a surface roughness of approximately 2 nm.

[1] N. G. Pugach et al., Appl. Phys. Lett. **111**, 162601 (2017)

TT 5.2 Mon 13:30 P

Substrate enhanced superconductivity in layered materials — •Yann in 't Veld[1], Roelof Groenewald[2], Jan Berges[3], Stephan Haas[2], Mikhail Katsnelson[1], Tim Wehling[3], Ryotaro Arita[4], and Malte Rösner[1] — [1]Radboud University, Nijmegen, The Netherlands — [2]University of Southern Calidornia, Los Angeles, USA — [3]Universität Bremen, Bremen, Germany — [4]University of Tokyo, Tokyo, Japan

External dielectric screening can be used to efficiently tune the Coulomb interaction and plasmonic excitations in layered materials. At the same time, two-dimensional plasmons couple strongly to electrons due to their gapless square-root-like dispersion, which renders them particularly interesting for tunable superconductivity in layered materials. Here, we extend density functional theory for superconductors (SC-DFT) to account for both the full dynamic Coulomb interaction and phonon contributions in two dimensions. We apply this scheme to monolayer MoS_2 and find that external screening indeed strongly enhances the superconducting critical temperature in the low-doping regime.

TT 5.3 Mon 13:30 P

Relativistic first principles theory of Yu–Shiba–Rusinov states: Mn dimers on Nb(110) — •Bendegúz Nyári[1], András Lászlóffy[2], László Szunyogh[1], and Balázs Újfalussy[2] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Wigner RCP, ELKH, Budapest, Hungary

The local magnetic moments of magnetic impurities at superconducting surfaces break the Cooper pairs leading to the formation of localized bound states within the superconducting gap, called as Yu–Shina–Rusinov (YSR) states. In the present work we introduce an *ab initio* theory based on the Green's function embedding technique within the Korringa–Kohn-Rostoker method to solve the Bogoliubov–de Gennes equations for the impurities. We present a detailed study of a Mn adatom and various Mn dimers at the surface of Nb(110), as the building blocks of atomic chains expected to host Majorana zero modes. From the calculated local density of states (LDOS) the spatial distribution of the YSR states is determined and compared with scanning tunneling spectroscopy (STS) measurements. The dimers are calculated in several geometric and magnetic configurations, while also the effect of the spin-orbit coupling (SOC) is investigated. We also study the effect of a relative angle between the atomic spins on the YSR states, where we find that for certain values a zero bias peak can exist in some dimer geometries.

TT 5.4 Mon 13:30 P

Development of an ab initio Bogoliubov-de Gennes method with applications to Nb(110) — •Philipp Rüssmann and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany

Ab initio calculations based on density functional theory (DFT) play a major role in understanding and improving quantum materials. Recently, material platforms for topological superconductivity have attracted a lot of attention. Typically materials require a combination of topological insulator, superconductor and magnetic materials and are promising candidates for the realization of Majorana-based qubits.

In this work we present the Bogoliubov-de Gennes extension of the JuKKR code that is based on the all-electron full-potential relativistic Korringa-Kohn-Rostoker Green-function method (https://jukkr.fz-juelich.de). We demonstrate the features of our code using bulk Nb and Nb(110) surfaces as examples, discussing the importance of spin-orbit coupling and showing calculations of the superconducting gap through the layers of thin films of Nb(110). These calculations establish the computational technology that opens the doors to studying the interfaces of superconductors and topological materials and gain insights into the proximity effect and the interplay of the electronic structure in quantum materials from first-principles calculations.

We acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – Cluster of Excellence Matter and Light for Quantum Computing (ML4Q) EXC 2004/1 – 390534769.

TT 5.5 Mon 13:30 P

Impurities in inhomogeneous superconductors from Density Functional Theory — •David Antognini Silva, Philipp Rüssmann, and Stefan Blügel — Peter Grünberg Institute and Institute for Advanced Simulation, FZ Jülich and JARA, 52425 Jülich, Germany

As impurities in a given material can change the electronic properties of the pristine material and give rise to new unique behaviors, their study is crucial in material science. Very timely examples are impurities, atomic chains or nanostructures in superconductor heterostructures [1] where these defects can be instrumental to in-gap states or *e.g.* identifying Majorana modes in Yu-Shiba-Rusinov chains [2]. The relativistic full-potential Korringa-Kohn-Rostoker Green function (KKR-GF) method, used in the Density Functional Theory (DFT) framework, is particularly suited to perfectly embed impurities in materials. We extend the JuKKR code (https://jukkr.fz-juelich.de) by the Bogoliubov-de Gennes (BdG) formalism to treat inhomogeneous superconductors. In this poster we present an extension of the implementation to the impurity problem and present first results of magnetic impurities on superconductors.

This work was funded by the Deutsche Forschungsgemeinschaft (DFG) under Germany's Excellence Strategy - Cluster of Excellence Matter and Light for Quantum Computing (ML4Q) EXC 2004/1 - 390534769.

[1] Z. Yan, Phys. Rev. B **100**, 205406 (2019)
[2] L. Schneider *et al.*, Nat. Phys. (2021)

TT 5.6 Mon 13:30 P

Relativistic and non-relativistic Ginzburg-Landau models in two-dimensional curved films — •Igor Bogush[1,2] and Vladimir M. Fomin[2,3] — [1]Theoretical Physics, Faculty of Physics, Lomonosov Moscow State University, Leninskie Gory, Moscow, 119991, Russia — [2]Moldova State University, Chisinau MD-2009, Republic of Moldova — [3]Institute for Integrative Nanosciences, Leibniz IFW Dresden, D-01069 Dresden, Germany

Superconductor nanoarchitectures, including self-rolled films, are highly promising for advancements in nano- and meso-scale devices. Superconductivity strongly depends on the external magnetic field applied to thin films. Managing the profile of the magnetic field is a challenging technical problem. To get around this problem, one can give a complex shape to the film such that the normal component of the magnetic field has the desired profile. We solve relativistic and non-relativistic time-dependent Ginzburg-Landau models for two-dimensional curved manifolds by applying the tool of General Relativity, differential geometry. The arbitrary geometry opens the way to manipulate the effective normal component of the magnetic field to control the regions with normal or superconducting state and, as a consequence, to manage the superconducting properties of films, transitions between vortex-chain and phase-slip regimes. We describe numerically nontrivial vortex and phase-slip dynamics and topological transitions in cylindric films and membranes with a deep well.

The present work has been supported by the DFG project #FO 956/6-1 and by the COST Action CA16218 (NANOCOHYBRI).

TT 5.7 Mon 13:30 P

^{125}Te NMR studies of 1T-$MoTe_2$ under pressure -Towards superconductivity mediated by Weyl Fermions — •Takuto Fujii[1], Hiroshi Yasuoka[1], M.O. Ajeesh[1], Marcus Schmidt[1], Takeshi Mito[2], Michael Nicklas[1], Claudia Felser[1], Andrew Mackenzie[1], and Michael Baenitz[1] — [1]MPI for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]School of Science, University of Hyogo Hyogo, Japan

1T-$MoTe_2$ is claimed to be one of the type-II Weyl semimetals, and has attracted much attention due to its exotic physical properties stemming from the topological (line nodal) band structure where the electron and hole pockets are touching at the E_F. One of the most preeminent features is the occurrence of superconductivity which is stabilized under pressure up to around T_c=7K. In order to understand the superconductivity, we have employed the ^{125}Te NMR technique under pressure (up to 2.17 GPa) and measured the NMR line profile and T_1, determining the Knight shift and low lying magnetic excitations. Using the same NMR tuning circuit, we have also measured the pressure and temperature (T)

dependences of the resonant frequency, and extracted the T-dependence of the H_{c2}. The results are not in accord with simple WHH model, but are well fit to an empilical formula, $H_{c2}(T) = H_{c2}(0)[1 - \frac{T}{T_c}]^{\alpha}$. By doing this, we obtained $H_{c2}(0)$=1.50T, T_c= 3.81K, and α=1.1 at 2.17 GPa. A superconducting signature has been observed in $K(T)$ and $1/T_1T(T)$ at around 2.5 K (2.17GPa). We present detailed NMR results and try to explore the superconductivity from the microscopic point of view.

TT 5.8 Mon 13:30 P

Critical current suppression via electrostatic field effect in epitaxial grown nanodevice — •Sohaila Z Noby, Roman Hartmann, Elke Scheer, and Angelo Di Bernardo — Physics department, Universität Konstanz, Germany

Quantum devices based on superconducting materials provide various technological applications, such as e.g. current limiters, electronic filters, routers, digital receivers, and photon detectors. Superconductors demonstrate unconventional pronounced performance under their critical temperatures in industrial electronic circuits in a comparison with semiconductors. However, controlling the electrical conductivity in nanoscale semiconductor devices considers as one of the cornerstones of such technology. This is attributed to the week screening effect, which allows the penetration of the electric field into a lower charge density semiconductor material. Although that phenomenon was believed that can not be realized in superconductor materials due to their higher charge density, which eliminate the field effect on the surface. Recent studies show that the strong electrostatic field can manipulate superconductor characteristics, which their origin still controversial between scientists. This effect has been seen in suppression of the critical current via the application of higher electrostatic field in different material. One such example is niobium (Nb), a well-established suitable elemental superconductor in circuit operation due to its highest critical temperature (~9.2K). In our study the mechanism of field effect, which introduced as a gate voltage, is being studied in a four-terminal nanowire device based on epitaxial grown Nb material.

TT 5.9 Mon 13:30 P

Unconventional Dynamical Scaling close to a Nematic Quantum Critical Point in $FeSe_{0.89}S_{0.11}$ — •Pascal Reiss[1,2], David Graf[3], Amir-Abbas Haghighirad[4], Thomas Vojta[5], and Amalia Coldea[1] — [1]Clarendon Laboratory, University of Oxford, UK — [2]MPI-FKF, Stuttgart, Germany — [3]NHMFL, Tallahassee, USA — [4]IQMT, Karlsruhe Institute of Technology, Germany — [5]Department of Physics, Missouri University of Science and Technology, USA

In the vicinity of quantum critical points, the interplay between electronic and structural order can lead to new and unconventional phases. Of particular interest is the electronic nematic order, with its predicted long-range interactions mediated through the lattices shear modes. Here, we first review the nature of the nematic QCP in $FeSe_{0.89}S_{0.11}$ under hydrostatic pressure. Then, we will demonstrate that the magnetoresistivity close to the QCP obeys a scaling relation over two decades in temperature with diverging critical exponents at low temperatures, in stark contrast to the usual ansatz using fixed exponents. We discuss our findings in the context of disconnected static and dynamic quantum fluctuations, a coupling between electronic and phononic modes, and topological changes of the Fermi surface. These lead to the emergence of an atypical non-zero energy scale at the QCP which strongly affects superconductivity. arXiv:2103.07991

We acknowledge funding from the EPSRC (EP/I004475/1, EP/I017836/1, EP/M020517/1, EP/N01085X/1), the NSF (DMR-1157490, DMR-1828489), the State of Florida, and the John Fell Fund.

TT 5.10 Mon 13:30 P

Growth and characterisation of substitution variants of LaOFeAs single crystals — •Felix Anger[1], Christian Blum[1], Anja Wolter-Giraud[1], Sebastian Gass[1], Hans-Joachim Grafe[1], Saicharan Aswartham[1], Sabine Wurmehl[1,2], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, Dresden, Germany

Facetted LaOFeAs single crystals with considerably growth in the crystallographic c direction were first reported by R. Kappenberger et al. [1]. The growth process takes place via diffusion in solid state, the so-called Solid State Crystal Growth (SSCG) method. The single crystals are grown from a polycrystalline matrix by the introduction of NaAs as a liquid phase to aid the crystallization process.1 Here, we present some additional experimental findings regarding growth temperature, initial microstructure and the role of NaAs for the growth. Furthermore, we are aiming to grow novel series of crystals of substitution variants as, e.g., Co-doped SmOFeAs and LaO1-xFxFeAs. The crystals were characterized regarding their composition, structure and magnetic properties.

[1] R. Kappenberger et al., Journal of Crystal Growth 483, 9-15 (2018)

TT 5.11 Mon 13:30 P

Anomalous softening of phonon-dispersion in the under-doped cuprate superconductors — •Saheli Sarkar[1,2], Maxence Grandadam[1], and Catherine Pépin[1] — [1]Institut de Physique Théorique, Gif-sur Yvette, France — [2]Current affiliation: Institut für QuantenMaterialien und Technologien, Karlsruhe Institute of Technology, Karlsruhe, Germany

Cuprate superconductors possess a complex phase diagram with various other phases like charge density wave (CDW) in the underdoped region. Interestingly, the CDW order has become fundamentally important due to growing evidences of its close relation to the pseudo-gap phase. One leading approach to unravel the relation, is to study the phonon-spectrum which couples to electronic degrees of freedom, thus leaving fingerprints associated with the electronic-structure. Several experiments have observed a softening of the phonon-dispersion in the underdoped cuprates at the CDW ordering wave vector, but only below the superconducting transition temperature. The phonon-softening in cuprates is considered 'anomalous' since it is in sharp contrast to the situation in metallic systems where such softening occurs for temperatures below the onset of CDW order. By employing a perturbative approach, we find that a complex interplay among the CDW order, superconductivity and a finite quasi-particle lifetime arising from an unusually connected thermal fluctuations of these orders, can explain the 'anomalous' nature of the phonon-softening, also giving good accounts for other features observed in recent inelastic-Xray scattering experiments.

TT 5.12 Mon 13:30 P

Enhanced Higgs oscillations in unconventional superconductors — •Matteo Puviani[1], Dirk Manske[1], and Rudi Hackl[2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Walther Meissner Institut, Bayerische Akademie der Wissenschaften, Garching, Germany

In superconductors the Anderson-Higgs mechanism allows for the existence of a collective amplitude (Higgs) mode which can couple to eV-light mainly in a non-linear Raman-like process. While the observed properties of the Higgs mode in clean, conventional, isotropic superconductors can be explained within a BCS picture, strong interaction effects with other modes in anisotropic d-wave superconductors are likely. In our work we have calculated the Raman contribution of the Higgs mode from a new perspective, including many-body Higgs oscillations effects and their consequences in steady-state Raman spectroscopy [1]. This solves the long-standing problem of the A1g symmetry Raman spectrum in d-wave superconductors [2]. In order to test our theory, we predicted the presence of measurable characteristic oscillations in THz quench-optical probe time-dependent reflectivity experiments[1,3].

[1] M. Puviani et al., arxiv: 2012.01922
[2] T.P. Devereaux et al., Phys. Rev. Lett. 72, 396 (1994)
[3] S. Nakamura et al., Phys. Rev. Lett. 122, 257001 (2019)

TT 5.13 Mon 13:30 P

Higgs mode mediated enhancement of interlayer transport in high-T_c cuprate superconductors — •Guido Homann[1], Jayson G. Cosme[1,2,3], Junichi Okamoto[4,5], and Ludwig Mathey[1,2] — [1]Zentrum für Optische Quantentechnologien and Institut für Laserphysik, Universität Hamburg, Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [3]National Institute of Physics, University of the Philippines, Diliman, Philippines — [4]Institute of Physics, University of Freiburg, Freiburg, Germany — [5]EUCOR Centre for Quantum Science and Quantum Computing, University of Freiburg, Freiburg, Germany

We put forth a mechanism for enhancing the interlayer transport in cuprate superconductors, by optically driving plasmonic excitations along the c axis with a frequency that is blue-detuned from the Higgs frequency [1]. The plasmonic excitations induce a collective oscillation of the Higgs field which induces a parametric enhancement of the superconducting response, as we demonstrate with a minimal analytical model. Furthermore, we perform simulations of a particle-hole symmetric $U(1)$ lattice gauge theory and find good agreement with our analytical prediction. Our numerical results show that the Higgs mode mediated enhancement can be larger than 50%. We investigate how the renormalization of the interlayer coupling depends on the parameters of the optical field and discuss possible challenges brought by damping.

[1] G. Homann, J. G. Cosme, J. Okamoto, L. Mathey, Phys. Rev. B 103, 224503 (2021)

TT 5.14 Mon 13:30 P

Optimization of Sr_2RuO_4 thin films grown by pulsed laser deposition — •Priyana Puliyappara Babu, Roman Hartmann, Alfredo Spuri, Sohaila Zaghloul Nabi Mohammed, Elke Scheer, and Angelo Di Bernardo — University of Konstanz, 78457 Konstanz, Germany

Since its discovery in 1994, $Sr_2RuO_4$4 has been the subject of intensive studies aiming at shedding light on the nature of its superconducting order parameter (OP). Despite earlier reports suggesting an unconventional nature of the Sr_2RuO_4 superconductivity, conflicting results have been recently reported and a definitive conclusion about the superconducting OP symmetry has not been yet achieved. To address some of the open questions, it is crucial to fabricate superconducting devices based on high-quality superconducting thin films of Sr_2RuO_4. However, this task has proven challenging due the sensitivity of Sr_2RuO_4 to disorder and impurities. We have carried out a systematic study to optimize the transport properties of Sr_2RuO_4 thin films grown by pulsed laser deposition using Sr_3RuO_7 single crystals as the material source. Thin films with very low density of defects, high residual resistivity ratio (> 20) and fully metallic down to low temperatures have been grown. The growth parameters that can be further optimized to get fully superconducting thin films have also been identified.

TT 5.15 Mon 13:30 P

Spin torque in a Josephson junction between two superconducting magnetic impurity states — •Fabian Ziesel[1], Ciprian Padurariu[1], Björn Kubala[1,2], and Joachim Ankerhold[1] — [1]ICQ and IQST, Ulm University, Germany — [2]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany

Superconducting tunneling between spin-polarized Yu-Shiba-Rusinov (YSR) impurity states can be realized using a functionalized mK-STM [1], which can be further developed as a local probe of electronic spins for spintronics applications. Here, we consider a Josephson junction containing two magnetic impurities and show that the Josephson current is spin-dependent and accompanied by a spin torque. The torque acts to align the two impurities either parallel or anti-parallel, depending on the parity of YSR states occupation.

Using standard Green's functions techniques, we derive the spin-torque and spin-current as function of the superconducting phase difference ϕ and the relative angle θ between the impurity spins, modeled as classical magnets. Our results are also relevant for recent realizations of double quantum dot superconducting junctions with YSR states [2]. Finally, we provide a discussion on spin dynamics with a possible relevance to spin chains that show topological superconductivity.

[1] H. Huang *et al.*, Nat. Phys. **16**, 1227 (2020)
[2] J.C.E. Saldaña *et al.*, Phys. Rev. Lett. **121**, 257701 (2018)

TT 5.16 Mon 13:30 P

Fluxoid dynamics in high impedance long Josephson junctions — •Micha Wildermuth[1], Lukas Powalla[1], Jan Nicolas Voss[1], Yannick Schön[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2,3] — [1]Institute of Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

The dynamics of Josephson vortices in long Josephson junctions is a well-known example of soliton physics and allows to study highly nonlinear effects on a mesoscopic scale. We experimentally study the characteristics of a Josephson junction with electrodes having a large kinetic inductance fraction which provides an additional degree of freedom. The London penetration depth exceeds the stack thickness which results in an incomplete screening of magnetic fields and in fluxoids with an altered shape. We present transport measurements of long Josephson junctions with electrodes made from disordered oxidized aluminum showing current steps with and without external magnetic fields and the IV-characteristics resemble the Fiske and zero-field steps. Magnetic field dependent measurements also show a very similar behavior to conventional long Josephson junctions.

TT 5.17 Mon 13:30 P

Exponential speedup of incoherent tunneling via dissipation — •Dominik Maile[1,2,4], Sabine Andergassen[2], Wolfgang Belzig[1], and Gianluca Rastelli[3] — [1]Fachbereich Physik, Universität Konstanz — [2]Institut für Theoretische Physik and Center for Quantum Science, Universität Tübingen — [3]INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento — [4]Institut für komplexe Quantensysteme, Universität Ulm

We study the escape rate of a particle in a metastable potential in the presence of a dissipative bath coupled to the momentum of the particle. Using the semiclassical bounce technique, we find that this rate is exponentially enhanced. In particular, the influence of momentum dissipation depends on the slope of the barrier that the particle is tunneling through. We investigate also the influence of dissipative baths coupled to the position, and to the momentum of the particle, respectively. In this case the rate exhibits a nonmonotonic behavior as a function of the dissipative coupling strengths. Remarkably, even in the presence of position dissipation, momentum dissipation can enhance exponentially the escape rate in a large range of the parameter space. Our theoretical findings can be directly tested in superconducting quantum circuits in which dissipative position and momentum interactions translate to dissipative phase or charge couplings. In particular, momentum/charge dissipation can be readily implemented simply using capacitances and resistances.

TT 5.18 Mon 13:30 P

Electron cooling by phonons in mesoscopic superconducting systems — •Danilo Nikolic[1], Denis M. Basko[2], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78467 Konstanz, Germany — [2]Université Grenoble Alpes and CNRS, LPMMC, 25 Rue des Martyrs, 38042 Grenoble, France

We investigate the electron-phonon cooling power in disordered electronic systems with a special focus on mesoscopic superconducting proximity structures. Employing the quasiclassical Keldysh Green's function method, we obtain a general expression for the cooling power perturbative in the electron-phonon coupling but valid for arbitrary electronic systems out of equilibrium. We apply our theory to several disordered electronic systems valid for an arbitrary relation between the thermal phonon wavelength and the electronic mean-free path due to impurity scattering. In addition to recovering the known results for bulk normal metals and BCS superconductors, we consider two experimentally relevant geometries of superconductor-normal-metal proximity contacts. Both structures feature a significantly suppressed cooling power at low temperatures related to the existence of a minigap in the quasiparticle spectrum. This improved isolation low cooling feature in combination with the high tunability makes such structures highly promising candidates for quantum calorimetry.

This project has received funding from the EU Horizon 2020 program (Marie Sklodowska-Curie action QuESTech 766025).

[1] D. Nikolić, D. M. Basko, W. Belzig, Phys. Rev. B **102**, 214514 (2020)

TT 5.19 Mon 13:30 P

Charge dynamics in quantum-circuit refrigeration: thermalization and microwave gain — •Hao Hsu and Gianluigi Catelani — JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, Jülich, Germany

Recently, a quantum circuit refrigerator (QCR) consisting of a voltage biased superconductor-insulator-normal metal-insulator-superconductor (SINIS) tunnel junction has been experimentally demonstrated to cool superconducting resonators [1] and theoretically predicted to reset superconducting qubits [2] fast and accurately. Here we derive a master equation for a QCR-two level system dynamics. We find that starting with a steady state charge distribution on the normal-metal island, thanks to slower charge relaxation rate than the bare qubit decoherence rate at the off mode and the QCR-induced qubit decay rate, it always remains in its steady state, thus validating the former-presented theory [2, 3]. Replacing the normal-metal island with a quantum dot, we find a voltage regime where the photon-assisted tunnelings serve as a pumping mechanism. Also using the master equation approach, we investigate the possible microwave gain application by coupling the quantum dot QCR to a resonator.

[1] K. Y. Tan et.al., Nat. Commun. 8 15189 (2017)
[2] H. Hsu et.al., Phys. Rev. B 101, 235422 (2020)
[3] M. Silveri et.al., Phys. Rev. B 96, 094524 (2017)

TT 5.20 Mon 13:30 P

Heat transport in quantum overdamped systems — •sadeq s. kadijani, thomas l. schmidt, massimiliano esposito, and nahuel freitas — Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

In classical and statistical physics, the overdamped limit of systems interacting with their environments is a very useful approximation allowing for the simplification of the Fokker-Plank equation in phase space to the Smoluchowski equation for the position variable alone. For quantum systems, the same limit leads to the quantum version of the Smoluchowski equation for systems in thermal equilibrium with only one thermal bath. However, to study the stochastic and quantum thermodynamics, one needs to deal with systems in a nonequilibrium situation where the quantum Smoluchowski equation is not valid anymore.

We are interested in studying the properties of the heat current in the overdamped limit where dissipation dominates. We obtain an analytical expression for the heat current between two overdamped quantum oscillators interacting with local thermal baths at different temperatures. The total heat current is split into classical and quantum contributions. We show how to evaluate both contributions by taking advantage of the timescale separation associated with the overdamped regime and without assuming the usual weak-coupling and Markovian approximations. We find that nontrivial quantum corrections survive even when the temperatures are high compared to the frequency scale relevant for the overdamped dynamics of the system.

TT 5.21 Mon 13:30 P

Emission of photon multiplets by a dc-biased superconducting circuit — •Björn Kubala[1,2], Gerbold Menard[3], Ambroise Peugeot[3], Ciprian Padurariu[2], Chloe Rolland[3], Zubair Iftikhar[3], Yuri Mukharsky[3], Carles Altimiras[3], Helene le Sueur[3], Philippe Joyez[3], Denis Vion[3], Patrice Roche[3], Daniel Esteve[3], Joachim Ankerhold[2], and Fabien Portier[3] — [1]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany — [2]ICQ and IQST, Ulm University, Germany — [3]SPEC, CEA Paris-Saclay, France

We show experimentally that a dc-biased Josephson junction in series with a high-impedance microwave resonator can emit up to $k = 6$ photons simultaneously for each Cooper pair tunneling through the junction. Our resonator is made of a simple micro-fabricated spiral coil that resonates at 4.4 GHz and reaches a 1.97 kΩ characteristic impedance, corresponding to an effective fine-structure constant, $\alpha \sim 1$. Measuring the second order correlation function of the emission from the resonator allows computing the Fano factor F of the emitted photons, found to coincide with the naive prediction $F = k$ in the weak driving regime. At higher emission, the feedback of the population of the resonator on the emission dynamics yields a non-monotonous behavior, hallmark of parametric transitions. Results are found in quantitative agreement with our theoretical predictions. This simple scheme highlights the ability of superconducting devices operating in the microwave domain to reach strong-coupling regimes of matter-light coupling inaccessible to conventional quantum optics experiments in the visible domain.

TT 5.22 Mon 13:30 P

Microwave photonics in High Kinetic Inductance Microstrip Networks — •Niklas Gaiser[1], Samuel Goldstein[2], Guy Pardo[2], Naftali Kirsh[2], Ciprian Padurariu[1], Björn Kubala[1,3], Nadav Katz[2], and Joachim Ankerhold[1] — [1]ICQ and IQST, University of Ulm, Ulm, Germany — [2]The Racah Institute of Physics, The Hebrew University of Jerusalem, Israel — [3]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany

Microwave photonics based on superconducting circuits is a promising candidate for many quantum-technological applications. Progress towards compact integrated photonics devices in the microwave regime, however, is constrained by their long wavelengths.

Here, we discuss a solution to these difficulties via compact networks of high-kinetic inductance microstrip waveguides and coupling wires with strongly reduced phase velocities experimentally realized in [1]. We describe, how the Kirchhoff equations of a periodic network map to a tight-binding model, which allows a description in term of Bloch waves and band structures, to explain experimental features. Furthermore, we present first steps towards exploiting versatility and unique properties of this new platform - compactness and reduced speed of light, strong nonlinear features, and band-structure design - to develop fundamental building blocks for integrated microwave photonics for technology applications and for exploring fundamental physics in such diverse areas as non-linear waves and topological lattice phases.

[1] S. Goldstein, G. Pardo, N. Kirsh, N. Gaiser, C. Padurariu, B. Kubala, J. Ankerhold, and N. Katz, arXiv:2106.15951

TT 5.23 Mon 13:30 P

Quantum Locking and Synchronization in Josephson Photonics Devices — •Florian Höhe[1], Lukas Danner[1,2], Ciprian Padurariu[1], Björn Kubala[1,2], and Joachim Ankerhold[1] — [1]ICQ and IQST, Ulm University, Ulm, Germany — [2]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany

Phase stability is an important characteristic of radiation sources. For quantum sources exploitation and characterization of many quantum properties, such as entanglement and squeezing, may be hampered by phase instability. Josephson photonics devices, where microwave radiation is created by inelastic Cooper pair tunneling across a *dc-biased* Josephson junction connected in-series with a microwave resonator are particularly vulnerable lacking the reference phase provided by an ac-drive. To counter this issue, sophisticated measurement schemes have been used in [1] to prove entanglement, while in [2] a weak ac-signal was put in to lock phase and frequency of the emission.

Here, we extend a recent classical theory [3] to describe locking and the synchronization of several Josephson-photonics devices to the quantum regime. Our description relies on linking the current shot-noise at a residual in-series resistor, which is crucial for phase diffusion, to the Full Counting Statistics of emitted radiation. From this full numerical description, phenomenological Adler-type equations for locking are derived to analyze quantum locking and synchronization.

[1] A. Peugeot et al., Phys. Rev. X 11, 031008 (2021).
[2] M. C. Cassidy et al., Science 355, 939 (2017).
[3] L. Danner et al., arXiv:2105.02564 (see also contribution here).

TT 5.24 Mon 13:30 P

Injection locking and synchronization in Josephson photonics devices — •Lukas Danner[1,2], Ciprian Padurariu[2], Joachim Ankerhold[2], and Björn Kubala[1,2] — [1]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany — [2]ICQ and IQST, Ulm University, Ulm, Germany

Injection locking can stabilize a source of radiation, leading to an efficient suppression of noise-induced spectral broadening and therefore, to a narrow spectrum. The technique is well established in laser physics, where a phenomenological description due to Adler is usually sufficient. Recently, locking experiments were performed in Josephson photonics devices, where microwave radiation is created by inelastic Cooper pair tunneling across a dc-biased Josephson junction connected in-series with a microwave resonator. An in-depth theory of locking for such devices however is lacking.

Here, we study injection locking in a typical Josephson photonics device where the environment consists of a single mode cavity, operated in the classical regime [1]. We show that an in-series resistance, however small, is an important ingredient in describing self-sustained Josephson oscillations and enables the locking region. We derive a dynamical equation describing locking, similar to an Adler equation, from the specific circuit equations. Phase slips due to noise are also studied. The synchronization of two Josephson photonics devices can be described by the Kuramoto model. For an extension of this classical analysis to the quantum regime, see the contribution by F. Höhe.

[1] L. Danner et al., arXiv:2105.02564 (submitted to PRB).

TT 5.25 Mon 13:30 P

Characterization of harmonic modes and parasitic resonances in multi-mode superconducting coplanar resonators — •Cenk Beydeda, Konstantin Nikolaou, Marius Tochtermann, Nikolaj G. Ebensperger, Gabriele Untereiner, Ahmed Farag, Philipp Karl, Monika Ubl, Harald Giessen, Martin Dressel, and Marc Scheffler — Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany

Planar superconducting microwave transmission line resonators can be operated at multiple harmonic resonance frequencies, which allows covering wide spectral regimes with high sensitivity, as is desired e.g. for cryogenic microwave spectroscopy. A common complication of such experiments is the presence of undesired "spurious" additional resonances. Identifying the nature of individual resonances ("designed" vs. "spurious") can become challenging for higher frequencies or if elements with unknown material properties are included, as is common for microwave spectroscopy. Here various experimental strategies are discussed to distinguish designed and spurious modes in a broad frequency range up to 20 GHz. These strategies include tracking resonance evolution as a function of temperature, magnetic field, and microwave power. It is also demonstrated that applying minute amounts of dielectric or ESR(electron spin resonance)-active materials on the resonator lead to characteristic signatures in the various resonance modes, which depend on the local strength of the electric or magnetic microwave fields.

TT 5.26 Mon 13:30 P

Josephson Optomechanics — •Surangana Sen Gupta[1], Björn Kubala[1,2], Ciprian Padurariu[1], and Joachim Ankerhold[1] — [1]ICQ and IQST, Ulm University, Germany — [2]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany

Optomechanics at optical frequencies typically uses sources of light in a classical state, e.g. coherent states from lasers, to control mechanical vibrations. Cavity optomechanics can also be realised in the microwave regime using superconducting cavities and Josephson junctions. Inelastic tunneling in a Josephson junction biased by a dc-voltage can provide a bright source of quantum states of light, that can then be used for optomechanics. Experiments [1] have shown that the nonlinearity of Josephson junctions allows for various photon creation processes including single photon and multi-photon resonances.

Here, we theoretically investigate an optomechanical system consisting of a single-mode superconducting cavity, which is parametrically driven by a dc-biased Josephson junction at the two-photon resonance, and a mechanical resonator. The optomechanical coupling is treated in the spirit of mean field where the cavity is deep in the quantum regime, while the mechanics is considered semi-classical. We show that squeezed microwaves lead to regimes of heating and cooling for the mechanics and identify their signatures in the spectrum. We contrast these signatures with those of conventional optomechanics.

[1] M. Hofheinz, F. Portier, Q. Baudouin, P. Joyez, D. Vion, P. Bertet, P. Roche, D. Esteve, Phys. Rev. Lett. **106**, 217005 (2011)

TT 5.27 Mon 13:30 P

Transmission spectra of the driven, dissipative Rabi model in the USC regime — •Luca Magazzu[1], Pol Forn-Diaz[2,3,4], and Milena Grifoni[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institut de Física d'Altes Energies (IFAE) — [3]The Barcelona Institute of Science and Technology (BIST), Bellaterra (Barcelona) 08193, Spain — [4]Qilimanjaro Quantum Tech SL, Barcelona, Spain

We present theoretical transmission spectra of a strongly driven, damped, flux qubit coupled to a dissipative resonator in the ultrastrong coupling regime. Such a qubit-oscillator system, described within a dissipative Rabi model, constitutes the building block of super-conducting circuit QED platforms. The addition of a strong drive allows one to characterize the system properties and study novel phenomena, leading to a better understanding and control of the qubit-oscillator system. The calculated transmission of a weak probe field quantifies the response of the qubit, in frequency domain, under the influence of the quantized resonator and of the strong microwave drive. We find distinctive features of the entangled driven qubit-resonator spectrum, namely resonant features and avoided crossings, modified by the presence of the dissipative environment. The magnitude, positions, and broadening of these features are determined by the interplay among qubit-oscillator detuning, the strength of their coupling, the driving amplitude, and the interaction with the heat bath. This work establishes the theoretical basis for future experiments in the driven ultrastrong coupling regime.

[1] arXiv:2104.14490 (2021)

TT 5.28 Mon 13:30 P

Probing the Density of States of Defects in Superconducting Flux Qubits — •Benedikt Berlitz[1], Alexander Neumann[1], Alexey V. Ustinov[1,2,3], and Jürgen Lisenfeld[1] — [1]Physikalisches Institut Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany) — [2]National University of Science and Technology MISIS, Moscow, Russia — [3]Russian Quantum Center, Skolkovo, Moscow, Russia

Material defects forming two-level-systems (TLS) present a source of decoherence and unwanted degrees of freedom in superconduncting quantum systems. Current theoretical models make different assumptions about the frequency dependence of the TLS' density-of-states (DOS). We intend to measure the TLS' DOS in a wide frequency range, spanning ~0.1 to 20 GHz, using widely tunable flux-qubits specifically designed as TLS-scanners. Measuring the DOS will enhance our understanding of the underlying physics of TLS in amorphous materials.

TT 5.29 Mon 13:30 P

Two-qubit gates between two transmons via parametrically driven coupling circuits — •Miriam Resch[1,2], Aneirin J. Baker[3], and Michael J. Hartmann[1,4] — [1]Physics Department, Friedrich-Alexander-University Erlangen Nürnberg, Germany — [2]ICQ and IQST, Ulm University, Germany — [3]Institute of Photonics and Quantum Sciences, Heriot-Watt University Edinburgh EH14 4AS, United Kingdom — [4]Max Planck Institute for the Science of Light, 91058 Erlangen, Germany

One important ingredient of quantum computation is the ability to implement gates that are efficient as well as precise to perform various operations on qubits. In the case of superconducting qubits, two-qubit gates can be implemented using a tunable coupler, where interaction terms in the Hamiltonian can be turned on and off. In this work we study the effective coupling of two transmon qubits through a coupler whose parameters are externally driven with a frequency ω_D. Depending on the drive frequency, the excitation number conserving interaction of an iSWAP gate, $\sigma_1^+\sigma_2^- + \sigma_1^-\sigma_2^+$, or the interaction of a bSWAP gate, $\sigma_1^+\sigma_2^+ + \sigma_1^-\sigma_2^-$, which does not conserve excitation numbers, can be created. Using an approach that considers the time dependent magnetic modulation of the coupler in a non-perturbative way, we find that the interaction of the bSWAP gate can be realized by driving the system with the average of the two qubit transition-frequencies. This result eliminates the demand for external drives at frequencies above 6 or 7 GHz for realizing interactions that break excitation number conservation and can thus realize bSWAP gates.

TT 5.30 Mon 13:30 P

Nuclear Spin Readout in a Cavity-Coupled Hybrid Quantum Dot-Donor System — •Jonas Mielke[1], Jason R. Petta[2], and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, Konstanz D-78457, Germany — [2]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

Nuclear spins show long coherence times and are well isolated from the environment, which are properties making them promising for quantum information applications. Here, we present a method for nuclear spin readout by probing the transmission of a microwave resonator. We consider a single electron in a silicon quantum dot-donor device interacting with a microwave resonator via the electric dipole coupling and subjected to a homogeneous magnetic field and a transverse magnetic field gradient. In our scenario, the electron spin interacts with a ^{31}P defect nuclear spin via the hyperfine interaction. We theoretically investigate the influence of the P nuclear spin state on the microwave transmission through the cavity and show that nuclear spin readout is feasible with current state-of-the-art devices. Moreover, we identify optimal readout points with strong signal contrast to facilitate the experimental implementation of nuclear spin readout.

TT 5.31 Mon 13:30 P

Bose condensation of squeezed light — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

Light with an effective chemical potential and no mass is shown to possess a general phase-transition curve to Bose-Einstein condensation. This limiting density and temperature range is found by the diverging in-medium potential range of effective interaction. While usually the absorption and emission with Dye molecules is considered, here it is proposed that squeezing can create also such an effective chemical potential. The equivalence of squeezed light with a complex Bogoliubov transformation of interacting Bose system with finite lifetime is established with the help of which an effective gap is deduced. This gap phase creates a finite condensate in agreement with the general limiting density and temperature range. The phase diagram for condensation is presented due to squeezing and the appearance of two gaps is discussed.

[1] Phys. Rev. B 99 (2019) 205124

TT 5.32 Mon 13:30 P

Collisionless drag for a one-dimensional two-component Bose-Hubbard model — •Daniele Contessi[1,4], Donato Romito[2,3], Matteo Rizzi[4,5], and Alessio Recati[1,2] — [1]Dipartimento di Fisica, Università di Trento, 38123 Povo, Italy — [2]INO-CNR BEC Center, 38123 Povo, Italy — [3]Mathematical Sciences, University of Southampton, Highfield, Southampton, SO17 1BJ, United Kingdom — [4]Forschungszentrum Jülich, Institute of Quantum Control (PGI-8), 52425 Jülich, Germany — [5]Institute for Theoretical Physics, University of Cologne, D-50937 Köln, Germany

We theoretically investigate the elusive Andreev-Bashkin collisionless drag for a two-component one-dimensional Bose-Hubbard model on a ring. By means of Tensor Network algorithms, we calculate superfluid stiffness matrix as a function of the interactions and of the lattice filling. We focus on the region close to the so-called pair-superfluid phase, where we observe that the drag can become comparable with the total superfluid density. We elucidate the importance of the drag in determining the long-range behavior of the correlation functions and the spin speed of sound. In this way we are able to provide an expression for the spin Luttinger parameter K_S in terms of drag and the spin susceptibility. Our results are promising in view of implementing the system by using ultra-cold Bose mixtures trapped in deep optical lattices. Importantly the mesoscopicity of the system appears to favour a large drag, avoiding the Berezinskii-Kosterlitz-Thouless jump at the transition to the pair superfluid phase which would reduce the region where a large drag can be observed.

TT 6: Focus Session: Emerging Phenomena in Superconducting Low Dimensional Hybrid Systems I

Low-dimensional superconducting hybrid systems belong to the most intensively studied nanoelectronic devices and building blocks to date. On one hand they reveal and allow to study in detail a plethora of novel transport phenomena discovered only recently. These include, among others, studies of stacked two-dimensional hybrid systems, phenomena arising from the interplay between superconducting and magnetic order, single-particle or spin excitations excitations in zero- or one-dimensional systems, the competition of superconductivity and charging phenomena, Majorana bound states, or Ising superconductivity. On the other hand, some of these novel phenomenal are already under discussion for quantum information applications. This focus session aims at addressing selected aspects of the field thereby mainly focussing on the fundamental physical mechanisms rather than on the application aspects.

Organizers: Elke Scheer and Wolfgang Belzig (Konstanz University)

Time: Tuesday 10:00–12:45 Location: H7

Invited Talk TT 6.1 Tue 10:00 H7

Spin Triplet Superconductivity within Superconductors as Determined by FMR Spin pumping — •Lesley Cohen — Blackett Laboratory Imperial College London

Superconductor (SC)/ ferromagnet (FM) interfaces are of great interest as potential candidates to exploit the spin degree of freedom in superconducting phenomena, leading to potential applications for cryogenic memory and novel computing technologies. Over the last decade, experimental and theoretical studies have established that long-range spin polarized triplet supercurrents can be generated in superconducting/ferromagnetic heterostructures in the presence of magnetic inhomogeneities (e.g. spatially varying magnetization) via the proximity effect in combination with spin mixing and spin rotation processes. Separately it has been predicted that spin-orbit coupling in combination with the ferromagnetic exchange interaction can also generate conditions for the formation of spin triplet superconductivity. In this talk I will introduce the use of ferromagnetic resonance to inject a pure spin current in an interfacial material in close proximity, when that material is a superconductor. At a clean interface spin currents should be blocked from entering the superconductor by the Andreev process. I will discuss the conditions where the opposite appears to be the case and aspects we have learnt so far about using this technique to determine the strength of the spin triplet current within the superconductor under these conditions.

TT 6.2 Tue 10:30 H7

Tunneling Spectroscopy of Layered Superconductors — •Hadar Steinberg — Hebrew University of Jerusalem, Jerusalem, Israel

Tunnel junctions consisting of van der Waals (vdW) materials are realized by placement of thin barriers on top layered superconductors such as $NbSe_2$, TaS_2, and others. The atomic mating of the tunnel barrier and superconductor gives rise to a stable junction, which allows probing of the spectrum at high resolution, revealing clear signatures of the quasiparticle structure and of the sub-gap features. I will show how the use of such devices allows us to differentiate between dynamic properties of carriers in multi-gap superconductors. At ultrathin superconductors, we are able to track the evolution of the gap function up to very high in-plane magnetic field, where the gap feature hints at the onset of a triplet order. I will also show how defects in the barriers can give rise to quantum dot states, which can couple to the superconductor, forming Andreev bound states, and can be utilized as energy probes. Finally, I will show new data demonstrating the use of $NbSe_2$ as a source-drain electrode in a graphene-based Josephson device, which can sustain high in-plane fields.

15. min. break

TT 6.3 Tue 11:15 H7

Interplay of magnetism and Ising superconductivity: mirage gap and Josephson junction — •Gaomin Tang[1], Raffael L. Klees[2], Christoph Bruder[1], and Wolfgang Belzig[2] — [1]Department of Physics, University of Basel, Switzerland — [2]Fachbereich Physik, Universität Konstanz, Germany

Superconductivity is commonly destroyed by a magnetic field due to orbital or Zeeman-induced pair breaking. Surprisingly, the spin-valley locking in an Ising superconductor makes the superconducting state resilient to large magnetic fields. In the presence of an in-plane magnetic field, the emerging finite-energy pairing correlations manifest themselves in the occurrence of "mirage" gaps: at (high) energies of the order of the spin-orbit coupling strength, a gaplike structure in the spectrum emerges that mirrors the main superconducting gap. These mirage gaps are signatures of the equal-spin triplet finite-energy pairing correlations.

In a Josephson junction formed by two Ising superconductors that are in proximity to ferromagnetic layers, the supercurrent due to the triplet pairing correlations is controlled by the magnetic exchange fields. We show that both the charge and spin supercurrents can be modulated by the exchange fields.

[1] G. Tang, C. Bruder, W. Belzig, Phys. Rev. Lett. 126, 237001 (2021)

TT 6.4 Tue 11:30 H7

A Josephson junction supercurrent diode — •Christian Baumgartner[1], Lorenz Fuchs[1], Andreas Costa[1], Simon Reinhardt[1], Sergei Gronin[2], Geoffrey Gardner[2], Tyler Lindemann[2], Michael Manfra[2], Paulo Faria Junior[1], Denis Kochan[1], Jaroslav Fabian[1], Nicola Paradiso[1], and Christoph Strunk[1] — [1]University of Regensburg — [2]Purdue University

The combination of Rashba spin-orbit interaction and superconductivity leads to the appearance of an anomalous phase shift (φ_0) in the current phase relation (CPR) of Josephson junctions, as experimentally demonstrated by several groups in recent years. However, if the CPR is sinusoidal, the φ_0 shift does not affect the symmetry between positive and negative branch of the CPR. Here, we demonstrate that in short ballistic Josephson junctions application of an in-plane field perpendicular to the current induces an asymmetry between positive and negative branch of the CPR. Such magnetochiral anisotropy (MCA) is at the basis of the so-called supercurrent diode effect, here shown for the first time in Josephson junctions. We quantify MCA by measuring the kinetic inductance, whose in-plane field dependence allows us to determine the MCA coefficient for the superfluid. The experimental value compares well with the results of tight-binding simulations based on realistic material parameters for epitaxial Al/InAs 2DEGs.

TT 6.5 Tue 11:45 H7

Majorana bound states in magnetic impurity chains on conventional superconductors — •Annica Black-Schaffer — Uppsala University, Uppsala, Sweden

Magnetic impurities on the surface of spin-orbit coupled but otherwise conventional superconductors offer the possibility to create topological phases with Majorana bound states (MBSs) without having to apply an external magnetic field. In this talk I will present some of our resent results in modeling both magnetic impurity wires and islands on the surface of spin-orbit coupled superconductors, including a self-consistent treatment of the superconductivity, which results in a local π-shift of superconducting order parameter near magnetic impurities. In particular, I will show how MBSs at wire end points very strongly hybridize with in-gap Yu-Shiba-Rusinov (YSR) states, causing large oscillations in the MBSs energies that are significantly enhanced within the self-consistent treatment. Still, by treating the MBSs as topological boundary modes dependent only on the effective mass gap, we can arrive at a fully parameter-free fitting of the Majorana localization length, which stays very short. I will also show how the wire end point MBSs are very robust against disorder within a self-consistent treatment, despite individual YSR states being extremely sensitive to disorder. Finally, despite the importance of a self-consistent treatment of superconductivity for the properties of the MBSs, I will show how the π-shift cannot easily be measured using the Josephson effect.

TT 6.6 Tue 12:15 H7

Evidence for *p*-wave pairing and precursors of Majorana modes in artificial Shiba chains — •Jens Wiebe — Department of Physics, Universität Hamburg, Hamburg, Germany

Magnetic chains on *s*-wave superconductors hosting spin spirals or spin-orbit coupling may realize one-dimensional topological superconductors with Majorana modes on their edges. We study artificial spin chains built atom-by-atom [1] with respect to such phenomena. By variation of substrate and adatom species and interatomic distances in the chain [2-5], we adjust the energies of multi-orbital Yu-Shiba Rusinov states induced by the adatoms [2,3], their hybridizations [4], as well as the chains' spin structures [5]. This enables to tailor the emerging multi-orbital Shiba bands such that *p*-wave gaps open [6]. We measure the length dependent energy oscillations of precursors of Majorana modes in short chains [7].

We acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) via the Cluster of Excellence 'Advanced Imaging of Matter' (EXC 2056-project ID 390715994), via the SFB-925-project 170620586, and by the ERC via the Advanced Grant ADMIRE (No. 786020).

[1] D.-J. Choi *et al.*, Rev. Mod. Phys. **91**, 041001 (2019)
[2] L. Schneider *et al.*, npj Quantum Materials **4**, 42 (2019)
[3] L. Schneider *et al.*, Nature Commun. **11**, 4707 (2020)
[4] P. Beck *et al.*, Nat. Commun. **12**, 2040 (2021)
[5] L. Schneider *et al.*, Science Advances **7**, eabd7302 (2021)
[6] L. Schneider *et al.*, Nat. Phys. (2021) https://doi.org/10.1038/s41567-021-01234-y
[7] L. Schneider *et al.*, arXiv:2104.11503 (2021)

TT 7: Focus Session: Disordered and Granular Superconductors: Fundamentals and Applications in Quantum Technology II

Time: Tuesday 13:30–16:15 Location: H6

TT 7.1 Tue 13:30 H6

Granular Aluminum: a superconducting material with amenable nonlinearity for quantum circuits — •Ioan Pop — KIT, Karlsruhe, germany

The electrodynamics of granular Aluminum (grAl) can be modeled based on an effective Josephson junction array with high kinetic inductance and amenable nonlinearity[1,2]. This recommends grAl for various applications in quantum technology, including kinetic inductance detectors, parametric amplifiers and quantum bits. One illustration of grAl's utility in quantum circuit design is the remarkable resilience of grAl fluxonium qubits[3] to photons populating its dispersively coupled readout resonator. This resilience allows single shot QND measurements[4] and quantum state preparation via active feedback with fidelities exceeding 90

[1] Maleeva et al. Nature Comm. 9, 3889 (2018)
[2] Winkel et al. Phys. Rev. X 10, 031032 (2020)
[3] Grunhaupt, Spiecker et al. Nature Materials 18, 816-819 (2019)
[4] Takmakov, Winkel, et al. Phys. Rev. App. 15, 064029 (2021)
[5] Gusenkova, Spiecker, et al. Phys. Rev. App. 15, 064030 (2021)
[6] Cardani, Valenti et al. Nat. Commun. 12, 2733 (2021)

TT 7.2 Tue 14:00 H6

Novel Quantum state at the interface between graphene and disordered superconductor — •Gopi Nath Daptary, Eyal Walach, Efrat Shimshoni, and Aviad Frydman — Department of Physics, Bar-Ilan University, Ramat-Gan 5290002, Israel

Over the past decades, there have been considerable interest in electronic properties of low dimensional systems, in particular the quantum effects that manifest themselves as the dimensions of a device approaches a microscopic length scale. Two-dimensional (2D) materials, composed of single atomic layers, have attracted vast research interest since the breakthrough discovery of graphene. One major benefit of such systems is the simple ability to tune the Fermi level through the charge neutrality point between electron and hole doping. For 2D

Superconductors, this means that one may potentially achieve the regime described by Bose Einstein Condensation (BEC) physics of small bosonic tightly bound electron pairs. In my talk I will describe an experiment showing that single layer graphene, in which superconducting pairing is induced by proximity to a low density superconductor, can be tuned from hole to electron superconductivity through an ultra-law carrier density regime. We have studied, both experimentally and theoretically, the vicinity of this "Superconducting Dirac point" and found an unusual situation where reflections at interfaces between normal and superconducting regions within the graphene, suppress the conductance. In addition, the Fermi level can be adjusted so that the momentum in the normal and superconducting regimes perfectly match giving rise to ideal Andreev reflection processes.

TT 7.3 Tue 14:15 H6

Impact of Kinetic Inductance on the Critical Curren Oscillations of Nanobridge SQUIDs — •Heleen Dausy, Lukas Nulens, Bart Raes, Margriet Van Bael, and Joris Van de Vondel — Quantum Solid-State Physics, Department of Physics and Astronomy, KU Leuven, Celestijnenlaan 200D, B-3001 Leuven, Belgium

We study lithographically fabricated MoGe nanobridges and their current phase relation (CΦR), which is linked to the nanobridge kinetic inductance. We do this by imbedding the nanobridges in a SQUID. We observe that for temperatures far below the critical temperature, the CΦR is linear as long as the condensate is not weakened by the presence of supercurrent. Another result is that the nanobridge kinetic inductance scales with its aspect ratio. We demonstrate that the SQUID $I_c(B)$ characteristic is tuneable through lithographic control over the nanobridge dimensions. These observations can be of use for the design and operation of future superconducting devices such as magnetic memories or flux qubits.

TT 7.4 Tue 14:30 H6

Disorder-enhanced inelastic relaxation in thin NbN films — Andrey Lomakin[1,2], Elmira Baeva[1,2], Philipp Zolotov[1,2], Alexandra Triznova[2], •Anna Kardakova[1,2], and Gregory Goltsman[1,2] — [1]National Research University Higher School of Economocs, Moscow, Russia — [2]Moscow Pedagogical State University, Moscow, Russia

Disordered superconducting films is a building block for superconducting nanowire single-photon detectors. A complex physics of such detectors implies a non-equilibrium response, determined by energy relaxation of electrons, namely electron-phonon (e-ph) scattering and phonon escaping times. In practice, one prefers to reduce these values along with optimization of other detector parameters.

Here, we report on experimental study of inelastic relaxation in thin disordered NbN films by measuring of magnetoconductance in the temperature range $T_c < T < 3T_c$. The studied 2.5-nm thick NbN films are characterized by a moderate level of disorder, expressed as $3 < k_F l < 6$. From magnetoconductance data, we find out the phase-breaking rate is a sum of two terms, electron-electron (e-e) and e-ph scattering, $\tau_\phi^{-1} \sim A_{e-e}T + A_{e-ph}T^n$, where $n = 3.5 - 4$ is similar as in work of Sidorova et.al, 2020. We also observe that both e-e and e-ph rates gradually increase with film disorder. The trend for increase of e-e rate with disorder is consistent with scenario of fermionic suppression of superconductivity in NbN films.

15. min. break

TT 7.5 Tue 15:00 H6

Magnetic-field-compatible hybrid superconducting circuits — •Marta Pita-Vidal — Qutech, Delft university of Technology, The Netherlands

Hybrid superconducting circuits, which integrate semiconducting elements into a circuit quantum electrodynamics (cQED) architecture, provide new insights into mesoscopic superconductivity. Extending the capabilities of hybrid circuits to work in large magnetic fields would enable the investigation and control of spin-polarized and topological phenomena. Here, I will discuss our work on magnetic-field-compatible hybrid cQED devices based on NbTiN. In particular, we exploit the high kinetic inductance of thin NbTiN to build a fluxonium which includes an electrostatically-tuned semiconducting nanowire as its nonlinear element. We in-situ tune its Josephson energy with an electrostatic gate and demonstrate operation of the fluxonium in magnetic fields up to 1T. This combination of gate-tunability and field-compatibility demonstrates the utility of hybrid superconducting circuits for exploring mesoscopic physics and enables the use of the fluxonium as a readout device for topological qubits.

TT 7.6 Tue 15:30 H6

Disordered superconducting NbN thin films and their quantum device application — •Evgeni Il'ichev[1], Sven Linzen[1], Oleg Astafiev[2,3], Rais Shaikhaidarov[3], Kyungho Kim[3], Jacob Dunstan[3], Ilya Antonov[3], Vladimir Antonov[2,3], Mario Ziegler[1], Gregor Oelsner[1], and Ronny Stolz[1] — [1]Leibniz Institute of Photonic Technology, Jena, Germany — [2]Skolkovo Institute of Science and Technology, Bolshoy Boulevard 30, bld. 1, Moscow, Russia 121205 — [3]Physics Department, Royal Holloway, University of London, United Kingdom

Within the past years we optimized and studied the properties of superconducting niobium nitride films fabricated with plasma-enhanced atomic layer deposition (PEALD). The films are polycrystalline and consist mainly of cubic δ-niobium-nitride grains of only a few nanometers in size. A superconductor to insulator transition (SIT) can be observed within ultrathin PEALD-NbN films by reducing the film thickness from 3.1 to 2.8 nm. Well-adjusting the film thickness slightly above the SIT point the films show high values of the kinetic inductance and the normal state resistance. Such films were used to fabricate nanowires in which the coherent quantum phase slips (CQPS) can be observed. Observation of the Aharonov-Casher effect as well as the dynamics of the CQPS are discussed.

This work was supported by European Union Horizon 2020 Research and Innovation Programme under Grant No. 862660/QUANTUM E-LEAPS.

TT 7.7 Tue 15:45 H6

High-kinetic-inductance superconducting nanowires for ultra-compact microwave devices — •Marco Colangelo[1], Daniel F. Santavicca[2], Carleigh R. Eagle[2], Brenden A. Butters[1], Owen Medeiros[1], Maitri P. Warusawithana[2], and Karl K. Berggren[1] — [1]Massachusetts Institute of Technology, Department of Electrical Engineering and Computer Science, 77 Massachusetts Avenue, Cambridge, Massachusetts 02139, USA — [2]University of North Florida, Department of Physics, 1 UNF Dr, Jacksonville, FL 32224

Superconducting nanowires made of disordered thin films can achieve a kinetic inductance which is several orders of magnitude higher than their magnetic inductance. Nanowires, integrated into transmission-line architectures, feature a characteristic impedance ~kΩ, an effective phase velocity a few percent of the speed of light in vacuum, and a strong compression of the microwave wavelength. We exploit these properties to demonstrate a balanced forward coupler at 4.73GHz based on coupled nanowire stripline with < 500 μm2 footprint, more than one order of magnitude lower than traditional modules. Interfacing high-impedance nanowire devices to 50 Ω electronics requires a large matching structure, which can, in principle, spoil the miniaturization achieved with nanowires. We address this challenge by combining high-inductance nanowires with high dielectric constant substrates. We demonstrate nanoscale resonators operating natively at 50Ω featuring a wavelength compression of almost 200 times. This demonstration paves the way to 50Ω ultra-compact cryogenic microwave devices.

TT 7.8 Tue 16:00 H6

Eliminating Quantum Phase Slips in Superconducting Nanowires — •Jan Nicolas Voss[1], Yannick Schön[1], Micha Wildermuth[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2,3,4] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Quantenmaterialien und Technologien (IQMT), Karlrsruher Institut für Technologie, Karlsruhe, Germany — [3]Russian Quantum Center, Skolkovo, Moscow, Russia — [4]National University of Science and Technology MISIS, Moscow, Russia

Superconducting nanowires made from granular aluminium have unique electrical properties at low temperatures. They originate from the intrinsic network of Josephson junctions in the material and the spatial restrictions to dimensions that are of the order of the superconducting coherence length. We present a novel method, which allows changing the nanowire resistance by modifying the intrinsic junction network by electrical pulses.

At low temperatures, we have observed a transition from an insulating over a metallic to a superconducting response in about a two hundred individual resistance steps. The measurement results are compared with the quantum phase slip model for superconducting nanowires [1].

[1] J. N. Voss, Y. Schön, M. Wildermuth, D. Dorer, J. H. Cole, H. Rotzinger and A. V. Ustinov, ACS Nano 15, 4108 (2021)

TT 8: Focus Session: Emerging Phenomena in Superconducting Low Dimensional Hybrid Systems II

Time: Tuesday 13:30–16:15 Location: H7

TT 8.1 Tue 13:30 H7

Theory of Shiba-Shiba tunneling at the edge of a Majorana chain — •Ciprian Padurariu[1], Haonan Huang[2], Björn Kubala[1,3], Christian R. Ast[2], and Joachim Ankerhold[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany

The realization of the Majorana chain [1], a 1D-chain of Yu-Shiba-Rusinov (YSR) impurity states on the surface of a superconductor, suggests that Majorana states emerging at the edges can be probed by an STM. Recently, we have developed an ideal tool to probe and manipulate the edge states of a Majorana chain. It consists of a superconducting STM tip functionalized with its own in-gap YSR state created by a magnetic impurity on the tip. With this device we have studied the sharp resonant transport between the YSR state on the tip and another YSR on the sample, and have developed its theory [2].

This presentation will expand on the theory of Shiba-Shiba tunneling and present the possibilities to manipulate edge states of the Majorana chain. In certain parameter regimes theory predicts that the edge state will transfer from the chain to the tip. This may provide a first step towards realizing braiding of edge states using the STM.

[1] S. Nadj-Perge, *et al.*, Science **346**, 602 (2014)
[2] H. Huang, *et al.*, Nat. Phys. **16**, 1227 (2020)

TT 8.2 Tue 13:45 H7

Spin-polarized zero bias peak from a single magnetic impurity at a s-wave superconductor — •Kyungwha Park[1], Bendeguz Nyari[2], Andras Laszloffy[3], Laszlo Szunyogh[2], and Balazs Ujfalussy[3] — [1]Virginia Tech, Blacksburg, United States — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]Wigner RCP, ELKH, Budapest, Hungary

Topological superconductivity has emerged a promising platform for quantum computing using Majorana modes. Since intrinsic topological superconductors are rare, various heterostructures including ferromagnetic atomic chains on s-wave superconductors have been proposed to realize topological superconductivity. So far, most theoretical studies in heterostructures were done using effective models. Here we investigate the Yu-Shiba-Rusinov (YSR) states of a single magnetic impurity at the surface of superconducting Pb using the fully relativistic first-principles simulations including DFT band structure of Pb and 3d orbitals of the impurity in the superconducting state. For the single Fe and Co impurities, we observe strong effects of spin-orbit coupling on the YSR states as the impurity moment rotates. As the rotation angle varies, we show that two symmetric same-spin YSR states of electron character merge and form a zero-bias peak (ZBP) with large spin polarization. According to effective models, whether a ZBP has net spin polarization or not is often used to determine its topological nature. Our results reveal importance of including realistic band structure and multiple 3d orbitals of the impurity in the calculations.

TT 8.3 Tue 14:00 H7

Conductance anomalies in magnetization-controlled superconductor-ferromagnet-superconductor proximity junctions — •Lukas Kammermeier, Elke Scheer, Angelo di Bernardo, and Maik Kerstingskötter — Universität Konstanz, Konstanz, Germany

A key building block in superconducting spintronics is a controllable superconducting spin triplet device. We study superconducting aluminium contacts, the superconducting properties of which are locally modulated by the inverse proximity effect of an adjacent ferromagnet (cobalt in this case). We show that the zero-field current-voltage characteristics of these devices can be in situ controlled by polarizing the magnet in a parallel magnetic field.

The measurements reveal that we can drive the system into different conductance states controlled by the magnetization state of the ferromagnet. One of these states shows a significant differential conductance increase, which even increases more while the magnetic field is applied, possibly indicating a spin-triplet-dominated transport regime.

TT 8.4 Tue 14:15 H7

Heat-charge separation and nonlocal response in superconductor-InAs nanowire hybrid devices — Artem Denisov[1], Gregor Koblmueller[2], and •Vadim Khrapai[3] — [1]Department of Physics, Princeton University, Princeton — [2]Walter Schottky Institut, Physik Department, and Center for Nanotechnology and Nanomaterials, TU Muenchen — [3]Osipyan Institute of Solid State Physics of the Russian Academy of Sciences

Nonlocal quasiparticle transport in normal-superconductor-normal (NSN) hybrid structures probes sub-gap states in the proximity region. Here we show that a non-local shot noise is a complementary to conductance measurement in superconducting proximity devices. Using NSN InAs nanowire based devices we demonstrate that quasiparticle response is practically charge-neutral. This is qualitatively explained by numerous Andreev reflections of a diffusing quasiparticle, that makes its charge completely uncertain. As a result, the sub-gap response is dominated by the heat transport component with a thermal conductance being on the order of the conductance quantum. By contrast, strong fluctuations and sign reversal are observed in the nonlocal conductance, including occasional Andreev rectification signals. Our results evidence effective heat-charge separaion at the central S-terminal.

We are grateful to our colleagues A. Bubis, S. Piatrusha, N. Titova, A. Nasibulin, J. Becker, J. Treu, D. Ruhstorfer and E. Tikhonov for their contribution to the preprint arXiv:2101.02128 on which this presentation is based.

15 min. break

TT 8.5 Tue 14:45 H7

Supercurrent-enabled Andreev reflection in a chiral quantum Hall edge state — •Andreas Bock Michelsen[1,2], Patrik Recher[3], Bernd Braunecker[1], and Thomas Schmidt[2] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews KY16 9SS, UK — [2]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg — [3]Institut für Mathematische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany

A chiral, spinless quantum Hall edge state placed in proximity to an s-wave superconductor experiences induced superconducting correlations. This effect provides a promising pathway to the realization of Majorana zero-modes and their parafermionic generalizations as non-Abelian anyons. Recent experiments have observed the phenomenon through conductance signatures of the mediating process of Andreev reflection, where electrons tunnel in pairs. We develop a tunneling model of the system and demonstrate that this process is enabled by the superconductor surface hosting spin-orbit coupling and a supercurrent induced by the strong magnetic field. By integrating out the superconductor we develop an effective model of the proximitized edge state, and derive an expression for the probability of an electron being transported as a hole through the edge state. This lets us analytically predict the outcome of conductance measurements given external experimental parameters.

TT 8.6 Tue 15:00 H7

Majorana zero modes in one- and two-dimensional magnet-superconductor hybrid systems — •Stephan Rachel — School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

Majorana zero modes, exotic quasiparticles in topological superconductors, are considered as the fundamental building blocks of future fault-tolerant quantum computers. The list of candidate materials is, however, short. Magnet-superconductor hybrid (MSH) systems represent one of the most promising platforms for topological superconductivity: magnetic atoms are placed on the surface of a conventional superconductor with spin-orbit coupling, leading to a topologically non-trivial system. Here we report recent theoretical progress on one- and two-dimensional MSH systems, and discuss them in the light of the latest experiments. By combining ab initio modeling and toy-model calculations on the theoretical side with atom-manipulation techniques via STM on the experimental side, we are getting closer to a complete understanding of Majorana zero modes in MSH systems.

TT 8.7 Tue 15:15 H7

Josephson and Andreev transport in a superconducting single electron transistor with a normal lead (SSN-SET) — •Laura Sobral Rey[1,2] and Elke Scheer[1,2] — [1]Physics department, University of Konstanz, 78464, Konstanz, Germany — [2]QuESTech consortium

An island coupled via a tunnel barrier to two leads and a gate forms a single electron transistor (SET) that shows Coulomb blockade. All-superconducting SETs (SSS-SETs) have shown to enable a multitude of possible charge transport processes which are not well understood, in particular in the strong-coupling regime [1]. To disentangle these processes, we study here the conceptually simpler SSN-SET, which has never been investigated experimentally before.

The SSN-SETs studied here consist of an S island coupled to an N lead via an oxide tunnel barrier, and to an S lead with a mechanically controlled break junction (MCBJ). Via the MCBJ, different coupling regimes can be studied: from a tunnel contact when the MCBJ is broken to a point contact when it is closed. In that limit the MCBJ has a small number of highly transmissive transport channels.

For weak coupling, our experimental findings can be understood in terms of the orthodox theory [2]. For stronger coupling, we observe Andreev and Josephson transport, as well as a renormalization of the charging energy and dynamical Coulomb blockade, which are also observed in the N state.

[1] T. Lorenz, J. Low Temp. Phys. 191, 301 (2017)
[2] T.A. Fulton, Phys. Rev. Lett. 59, 109 (1987)

TT 8.8 Tue 15:30 H7

Unconventional Meissner screening induced by chiral molecules in a conventional superconductor — Hen Alpern[1], Morten Amundsen[2], •Roman Hartmann[3], Nir Sukenik[1], Alfredo Spuri[3], Shira Yochelis[1], Thomas Prokscha[4], Vitaly Gutkin[1], Yonathan Anahory[1], Elke Scheer[3], Jacob Linder[2], Zaher Salman[4], Oded Milo[1], Yossi Paltiel[1], and Angelo Di Bernardo[3] — [1]The Hebrew University of Jerusalem — [2]Norwegian University of Science and Technology — [3]Universität Konstanz — [4]Paul Scherrer Institut

Superconducting spintronics is emerging as an alternative technology that can overcome the main limitation of conventional spintronic devices, their high current dissipation. It has developed after the discovery that Cooper pairs with parallel-aligned spins (spin-triplets) can be generated at the interface between a conventional superconductor (S) and a magnetically inhomogeneous ferromagnet (F). More recently, by performing low-temperature scanning tunneling spectroscopy measurements of chiral molecules (ChMs) adsorbed on the surface of a Nb (S) thin film, we have observed subgap features due to spin-triplet states. Motivated by these results, we have performed low-energy muon spectroscopy on ChMs/Nb which shows evidence for an unconventional Meissner screening effect. Our experimental data and theoretical analysis show that the unconventional Meissner screening is due to the generation of spin-triplet pairs, as a result of the ChMs acting as a spin active interface. These results pave the way for the realisation of novel devices based on ChMs/S hybrids for superconducting spintronics.

TT 8.9 Tue 15:45 H7

Magic angles and current-induced topology in twisted nodal superconductors — •Pavel Volkov, Justin Wilson, and Jed Pixley — Rutgers University

We propose twisted bilayers of two-dimensional nodal superconductors as a new platform to realize topological and correlated superconducting phases. We show that the Fermi velocity of the Dirac excitations in the Bogoliubov-De Gennes quasiparticle dispersion is strongly renormalized by the interlayer hopping, vanishing at a "magic angle", where time-reversal breaking superconductivity is induced. We demonstrate that magnetic field, electric gating, and current bias can be used for versatile control of the system. In particular, an interlayer current bias opens a topological gap, with the system being characterized by a non-zero Chern number.

TT 8.10 Tue 16:00 H7

Vortex inductance as a probe of symmetry breaking in Rashba superconductors — •Lorenz Fuchs[1], Denis Kochan[1], Simon Reinhardt[1], Christian Baumgartner[1], Sergei Gronin[2], Geoffrey Gardner[2], Tyler Lindemann[2], Michael Manfra[2], Christoph Strunk[1], and Nicola Paradiso[1] — [1]University of Regensburg (Germany) — [2]Purdue University (USA)

In this work, we demonstrate the use of vortices as directional probes of the superconducting condensate symmetry via vortex inductance measurements. We investigate Al/InAs heterostructures containing a high-mobility InAs quantum well that is proximitized by the epitaxially grown Al top layer. In out-of-plane magnetic field, ac-current-driven oscillations of vortices around pinning centers give rise to an additional inductance, which is orders of magnitude larger than the bare kinetic inductance of the superfluid. We find that the application of an additional in-plane magnetic field induces a surprising increase of the pinning potential and demonstrate that such increase obeys a characteristic two-fold anisotropy when changing the angle between the in-plane field and the ac-current. The observed counter-intuitive behavior can be theoretically explained by introducing Lifshitz-invariant terms (resulting from the Rashba interaction and the in-plane field) in the Ginzburg-Landau free energy.

TT 9: Poster Session: Correlated Electrons

Time: Tuesday 13:30–16:00 Location: P

TT 9.1 Tue 13:30 P

Electronic Nematicity in 4f electron systems — •Mario Malcolms de Oliveira[1], Pascoal Pagliuso[2], and Eduardo Miranda[2] — [1]Max Planck Institute for Solid State Research — [2]Unicamp

In this work, we show that the interplay between the Neel order and the spin-orbit coupling present in 4f electron systems are key ingredients to give rise to the emergence of an electronic nematic state in this kind of system. Our result can shed light on the understanding of the experimental results observed for the heavy-fermion compound $CeRhIn_5$.

TT 9.2 Tue 13:30 P

Spin excitations in the fully gapped hybridized two band superconductor — •Alireza Akbari and Peter Thalmeier — Max Planck Institute for the Chemical Physics of Solids, D-01187 Dresden, Germany

In f-electron heavy fermion superconductors, the presence of a spin resonance in the inelastic magnetic response is commonly associated with an unconventional nodal gap function that is not fully symmetric. However, it appears possible that the resonance is still observed even when the low-temperature thermodynamic behavior suggests a fully gapped state. We investigate such possibility within a two-dimensional toy model of a hybridized superconductor with a fully symmetric unconventional symmetry with a different sign of the gap function on disjoint Fermi surface sheets. We compute the collective magnetic response function in the hybridized superconducting state of the two-band model and show that the appearance of the resonance is also possible for the fully gapped state.[1]

[1] A. Akbari, P. Thalmeier, Annals of Physics 428, 168433 (2021)

TT 9.3 Tue 13:30 P

Probing the electron-lattice coupling near the valence transition of $EuPd_2Si_2$ — •Jan Zimmermann, Steffi Hartmann, Bernd Wolf, Marius Peters, Cornelius Krellner, and Michael Lang — PI, SFB/TR288, Goethe Univ., Frankfurt/M., Deutschland

The thermodynamic properties of materials close to a second-order critical endpoint in strongly correlated electron systems are a field of high interest. Within the strong-coupling regime, it is expect to find cross-correlations between electronic and lattice properties like the recently proposed phenomena of critical elasticity, which implies a strong lattice softening and strongly nonlinear strain-stress relations. [1] Intermetallic compounds from the EuT_2X_2 family show various types of phase transitions such as valence- or structural instabilities that make it possible to study collective phenomena resulting from such a particularly strong coupling of electrons to phonons [2]. In this work electron lattice coupling near the second-order critical endpoint of the valence transition in $EuPd_2Si_2$ is investigated via thermodynamic methods. Recently published measurements [2] indicate the unique possibility of experimental access to the critical endpoint of the valence transition using helium gas pressure. We present measurements of thermal expansion and compressibility in a pressure range from 0 MPa up to 40 MPa and temperatures from 90 K to 210 K. Results are compared to specific heat measurements and analyzed for sample-to-sample variations.

[1] E. Gati *et al.*, Sci. Adv. **2**, e1601646 (2016)

[2] Y. Onuki *et al.*, Philosophical Magazine **97**, 3399 (2017)

TT 9.4 Tue 13:30 P

Magnetic and electronic phases of $U_2Rh_3Si_5$ — •Jannis Willwater[1], Nico Steinki[1], Dirk Menzel[1], Ricarda Reuter[1], Hiroshi Amitsuka[2], Vladimír Sechovsky[3], Michal Valiska[3], Marcelo Jaime[4], Franziska Weickert[5], and Stefan Süllow[1] — [1]TU Braunschweig, Braunschweig, Germany — [2]Hokkaido University, Sapporo, Japan — [3]Charles University, Prague, Czech Republic — [4]Los Alamos National Laboratory, Los Alamos, USA — [5]Florida State University, Tallahassee, USA

It has been demonstrated that the intermetallic uranium compound $U_2Rh_3Si_5$ exhibits a unique first-order antiferromagnetic transition accompanied by a structural transition. This was explained with the so-called bootstrapping effect. Here, we present a detailed study of the magnetic and electronic properties of this compound.

Based on the results of magnetization and magnetostriction measurements in high magnetic fields, we establish the complex magnetic phase diagram of $U_2Rh_3Si_5$ up to 60 T. For the first time, various steps in the high-field magnetization of the a axis have been observed. These effects are probably due to several metamagnetic transitions. In addition, the electrical resistivity exhibits a unique anomaly in a narrow temperature range above the Néel temperature. Since there is no associated signature in the magnetic susceptibility or the structural parameters for all three crystallographic axes, this anomaly in the resistivity cannot be caused by a magnetic, but rather by an electronic phase transition.

[1] J. Willwater et al., Phys. Rev. B **103**, 054408 (2021)

TT 9.5 Tue 13:30 P

Anisotropic magnetic and thermodynamic properties of single crystals of antiferromagnetic $CePdAl_3$ — •Vivek Kumar[1], Andreas Bauer[1], Christian Franz[2,3], Rudolf Schönmann[1], Michal Stekiel[1], Astrid Schneidewind[1], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [2]JCNS at MLZ, FZ Jülich GmbH, Lichtenbergstr. 1, D-85747 Garching — [3]TUM at MLZ, Technische Universität München, D-85748 Garching, Germany

Recently, the class of $CeTAl_3$ (T is a transition metal) attracted considerable scientific attention when strong coupling between phonons and crystal electric field excitations was demonstrated in $CeCuAl_3$ and $CeAuAl_3$ [1,2]. Here, we report on the magnetic and thermodynamic properties of single-crystalline $CePdAl_3$ studied by means of ac susceptibility, magnetization, and specific heat measurements. The compound crystallizes in an orthorhombic crystal structure and displays antiferromagnetic order below $T_N = 5.6$ K. A strong anisotropy was observed in magnetic properties. We obtained a large electronic specific heat coefficient, $\gamma = 121$ mJ K^{-2} mol^{-1}, characteristic of heavy-fermion behavior. Field-driven magnetic transitions were detected for fields applied along the easy basal plane, which leads to a complex magnetic phase diagram.

[1] Franz *et al.*, J. Alloys Compd. **688**, 978 (2016).
[2] Čermák *et al.*, Proc. Natl. Acad. Sci. U.S.A. **116**, 6695 (2019).

TT 9.6 Tue 13:30 P

Low-Temperature Properties of the Non-Centrosymmetric Heavy-fermion Compound $CeAl_2$ — •Christian Oberleitner, Alexander Regnat, Christian Franz, Jan Spallek, Georg Benka, Michael Petrov, Marc Andreas Wilde, Andreas Bauer, and Christian Pfleiderer — Physik-Department, Technische Universitaet Muenchen, 85748 Garching, Germany

We report a comprehensive study of the non-centrosymmetric heavy-fermion compound $CeAl_2$ with $T_N = 3.8$ K. The metallurgical characterization by Laue x-ray scattering and powder x-ray diffraction shows the excellent crystalline quality, which is confirmed by very high residual-resistivity ratios (RRR). Magnetization, specific heat, torque magnetometry, resistivity, and Hall-effect measurements down to 50 mK and up to 18 T were carried out. The low-temperature measurements in the antiferromagnetic regime show complex magnetic behavior. The Hall-effect cannot be explained by a superposition of anomalous and normal Hall-effect.

TT 9.7 Tue 13:30 P

Robust hybridization gap in the Kondo insulator YbB_{12} probed by femtosecond optical spectroscopy — •Amrit raj Pokharel[1], Steinn y. Agustsson[1], Viktor v. Kabanov[2], Fumitoshi Iga[3], Toshiro Takabatake[4], Hidekazu Okamura[5], and Jure Demsar[1] — [1]JGU Mainz, Mainz, Germany — [2]Jozef Stefan Institute, Ljubljana, Slovenia — [3]Ibaraki University, Mito, Japan — [4]Hiroshima University, Higashi-Hiroshima, Japan — [5]Tokushima University, Tokushima, Japan

Carrier relaxation dynamics is susceptible to subtle changes in the low energy electronic structure. In heavy fermions the dynamics is shown to be governed by the low energy indirect gap, E_g, resulting from interplay/hybridization between localized moments and conduction band electrons. Here, carrier relaxation dynamics in a prototype Kondo insulator YbB_{12} is studied over large temperature range and over three orders of magnitude in excitation density. We utilize the intrinsic nonlinearity of dynamics to quantitatively determine microscopic parameters, such as electron-hole recombination rate. The extracted value reveals that hybridization is accompanied by a strong charge transfer from localized 4f levels. Furthermore, results suggest hybridization gap to be present up to temperatures of the order of $E_g/k_B \approx 200$ K, and is extremely robust against electronic excitation. Finally, the results imply further changes in the low energy electronic structure below 20 K, attributed to short-range antiferromagnetic correlations between the localized levels [1].

[1] A. R. Pokharel, et. al., Phys. Rev. B 103, 115134 (2021)

TT 9.8 Tue 13:30 P

Floquet renormalization group approach to the periodically driven Kondo model — •Valentin Bruch[1], Mikhail Pletyukhov[1], Herbert Schoeller[1], and Dante Kennes[1,2] — [1]Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany and JARA-FIT, 52056 Aachen — [2]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany

We study the interplay of strong correlations and coherent driving by considering the Kondo model driven by a time-periodic bias voltage. By combining a recent nonequilibrium renormalization group method with Floquet theory, we find that the coherent dressing of the driving field leads to side-replicas of the Kondo resonance in the conductance, which are not completely washed out by the decoherence induced by the driving. We show that to accurately capture the interplay of driving and strong correlations one needs to go beyond simple phenomenological pictures, which underestimate decoherence, or adiabatic approximations, highlighting the relevance of memory effects. Within our method the differential conductance shows good quantitative agreement with experimental data in the full crossover regime from weak to strong driving. In the time-resolved current and differential conductance we identify nonlinear memory effects and time scales of the relaxation to the ground state.

TT 9.9 Tue 13:30 P

Quadrature Magnetoresistance from Impeded Cyclotron Motion — •Roemer Hinlopen[1], Stijn Hinlopen[2], Jake Ayres[1], and Nigel Hussey[1,3] — [1]University of Bristol, United Kingdom — [2]Fudura B.V., Netherlands — [3]High Field Magnet Laboratory (HFML-EMFL), Netherlands

Recently, quadratic to linear magnetoresistance (MR) as a function of magnetic field has emerged as a pervasive phenomenon among strange and quantum critical metals. Examples are the antiferromagnetic quantum critical metal $BaFe_2(As,P)_2$ (1), heavy fermion $(Yb,La)Rh_2Si_2$ (2) and optimally and overdoped cuprates (Nd-)LSCO (3,4), Tl-2201 and Bi-2201 (5) as well as electron doped LCCO (6). Given the variety of Fermi surface topologies, dominant interactions and energy scales in these systems, the striking similarity of their magnetic-field response suggests some universal, but as yet unidentified, organizing principle. Here, we propose a new, simple theory to explain this phenomenology based on impeded cyclotron motion. We reproduce the quadrature form and show a high level of robustness to scattering and correlation effects. The unsaturating nature of the MR is found even in the high field limit. We predict this model also explains the magnetoresistance observed in charge density wave systems such as the dichalcogenides.

[1] Nat. Phys. 12:916-919 (2016)
[2] Physica B: Cond. Matt. 378-380:72-73 (2006)
[3] Science 361:6401 (2018)
[4] G. Grissonnanche arXiv:2011.13054 (2020)
[5] J. Ayres et al. Nature (in press)
[6] Sci. Adv. 5:5, eaav6753 (2019)

TT 9.10 Tue 13:30 P

Possible superconductivity from incoherent carriers in overdoped cuprates — •Caitlin Duffy[1], Matija Čulo[1,2], Jake Ayres[1,3], Maarten Berben[1], Yu-Te Hsu[1], Roemer Hinlopen[3], Bence Bernáth[1], and Nigel Hussey[1,3] — [1]High Field Magnet Laboratory (HFML-EMFL), Netherlands — [2]Institut za fiziku, Zagreb, Croatia — [3]University of Bristol, United Kingdom

The non-superconducting normal state of the overdoped, hole-hoped cuprates is formed of two distinct charge sectors: one coherent with quasiparticle excitations, the other incoherent and governed by non-quasiparticle Planckian dissipation (1). From $p^* = 0.19$ to the end of the superconducting dome, a decrease in the superfluid carrier density $n_s(0)$ concurrent with an increase in the Hall (coherent) carrier density $n_H(0)$ from p to $1 + p$ is found; this striking anti-correlation contradicts the expectations of conventional BCS theory (2, 3). Here, we demonstrate that in two families of cuprates - $La_{2-x}Sr_xCuO_4$ and $Tl_2Ba_2CuO_{6+\delta}$ - the loss of carriers in the coherent sector is entirely compensated for by the growth in $n_s(0)$ with decreasing p. This implies that superconductivity in the overdoped cuprates stems from the sector that displays incoherent transport properties (4).

[1] J. Ayres *et al.*, *Nature*, (in press)
[2] I. Božović *et al.*, *Nature* **536**, 309*311 (2016)
[3] C. Putzke *et al.*, *Nat. Phys.* **17**, 826 (2021)
[4] M. Čulo, C. Duffy *et al.*, *SciPost Phys.* **11**, 012 (2021)

TT 9.11 Tue 13:30 P

Emergence of a fluctuating magnetic ground state in $Mn_{1-x}Fe_xSi$ — Andreas Bauer[1], Jonas Kindervater[1], •Johanna K. Jochum[2], Wolfgang Häussler[1,2], Nicolas Martin[3], Markus Garst[4], and Christian Pfleiderer[1] — [1]Physik Department, Technische Universität München, D-85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum, Technische Universität München, D85748 Garching, Germany — [3]Université Paris-Saclay, CNRS, CEA, Laboratoire Léon Brillouin, 91191 Gif-sur-Yvette, France — [4]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany

Substitutional doping of the cubic chiral magnet MnSi results in a suppression of magnetic order and quantum critical behavior that is masked by the influence of disorder. Combining measurements of the ac susceptibility and specific heat with elastic neutron scattering and neutron resonance spin-echo spectroscopy on single-crystal $Mn_{1-x}Fe_xSi$ in zero magnetic field, we show that up to $x = 0.10$ static helimagnetic order emerges through a Brazovskii-type fluctuation-induced first-order phasetransition. For $x = 0.12$, the signatures in the susceptibility are reminiscent of helimagnetic order, while the specific heat indicates the absence of a first-order transition and neutron spectroscopy unambiguously establishes the dynamic character down to temperatures of 50 mK, suggesting a magnetic ground state that is dominated by interacting chiral fluctuations.

TT 9.12 Tue 13:30 P

Orientation dependence of the transverse-field Ising transition in $LiHoF_4$ — •Andreas Wendl[1], Heike Eisenlohr[2], Felix Rucker[1], Christopher Duvinage[1], Markus Kleinhans[1], Matthias Vojta[2], and Christian Pfleiderer[1,3,4] — [1]Physik Department, TU München, Garching, Germany — [2]Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, Dresden, Germany — [3]Centre for QuantumEngineering (ZQE), TU München, Garching, Germany — [4]Munich Centre for Quantum Science and Technology (MCQST), TU München, Garching, Germany

The perhaps best understood example of a quantum critical point is the response of the dipolar Ising ferromagnet $LiHoF_4$ to a transverse field [1-3]. We report an investigation of the AC susceptibility of $LiHoF_4$ as a function of the magnetic field direction relative to the hard magnetic axis, deriving the evolution of the magnetic-phase-diagram as a function of field orientation. We discuss our findings in terms of a theoretical model taking quantiatively into account the non-Kramers nature of the Ho ions, the effects of hyperfine coupling and the presence of magnetic domains.

[1] D. Bitko et al., Phys. Rev. Lett. **77**, 940 (1996)
[2] H. M. Rønnow et al., Science **308**, 389 (2005)
[3] P. B. Chakraborty et al., Phys. Rev. B **70**, 144411 (2004)

TT 9.13 Tue 13:30 P

Pump-Probe AC Susceptibility of $LiHo_xY_{1-x}F_4$ (x = 4.5 %) — •Michael Lampl, Andreas Wendl, Markus Kleinhans, Laura Stapf, Marc A. Wilde, and Christian Pfleiderer — Physik-Department Technical University of Munich, Garching, Germany

$LiHoF_4$ under a transverse magnetic field exhibits one of the best understood examples of a quantum critical point. Substitutional doping of Ho with non-magnetic Yttrium may be used to study the effects of disorder [1]. In the highly diluted system $LiHo_xY_{1-x}F_4$ (x = 4.5 %), investigated in our study, the nature of the ground state is still unresolved [2]. To explore the ground state properties of this system, multiple studies employed so-called pump-probe susceptibility measurements [3-5]. We revisit this question and report a study of the pump-probe susceptibility as a function temperature and field orientation, covering a wide parameter range.

[1] J. P. Gingras and P. Henelius, J. Phys.: Conf. Ser. **320**, 012001 (2011).
[2] J. A. Quilliam *et al.*, Phys. Rev. Lett. **101**, 187204 (2008).
[3] S. Ghosh *et al.*, Science **296**, 2195 (2002)
[4] M. A. Schmidt *et al.*, Proc. Natl. Acad. Sci. USA **111**, 3689 (2014)
[5] D. M. Silevitch *et al.*, Nature Com. **10**, 4001 (2019)

TT 9.14 Tue 13:30 P

Gross-Neveu-Heisenberg criticality from competing nematic and antiferromagnetic orders in bilayer graphene — Shouryya Ray and •Lukas Janssen — TU Dresden, Germany

The nature of the ground state of Bernal-stacked bilayer graphene has received significant attention in the last ten years, but still represents an open problem both experimentally and theoretically. The two most promising scenarios feature nematic and antiferromagnetic orders. We have studied theoretically the competition between these two orders, revealing that they allow a coexistence phase characterized by both nematicity and antiferromagnetism. This leads to interesting quantum phase transitions, including weak first-order transitions and continuous Gross-Neveu-type transitions that feature emergent Lorentz invariance. Implications for experiments in bilayer graphene are discussed.

[1] S. Ray, L. Janssen, Phys. Rev. B 104, 045101 (2021)

TT 9.15 Tue 13:30 P

Terahertz conductivity of heavy-fermion systems from time-resolved spectroscopy — •Chia-Jung Yang[1], Shovon Pal[1], Farzaneh Zamani[2], Kristin Kliemt[3], Cornelius Krellner[3], Oliver Stockert[4], Hilbert v. Löhneysen[5], Johann Kroha[2], and Manfred Fiebig[1] — [1]ETH Zurich, Switzerland — [2]University of Bonn, Germany — [3]Goethe-University Frankfurt, Germany — [4]MPI CPfS Dresden, Germany — [5]KIT Karlsruhe, Germany

Ultrafast terahertz (THz) spectroscopy has recently been introduced as a novel tool to investigate the quasiparticle dynamics across the quantum phase transition in heavy-fermion compounds [1,2]. The incident THz pulse with a spectral range of 0.1–3 THz creates collective intraband excitations within the heavy band as well as resonant interband transitions between the hybridizing heavy and light parts of the conduction band. The former leaves the heavy quasiparticles intact, while the latter breaks the Kondo-singlet and leads to a time-delayed echo-like response [1,2]. In this contribution, we expand our investigations towards the individual transport properties of strongly and weakly correlated electrons. We utilize the time-resolved, phase-sensitive THz spectroscopy to separate two types of excitations and derive the associated optical conductivity. We find that the Kondo-singlet-breaking interband transitions do not create a conventional metallic Drude peak, while the Kondo-retaining intraband excitations yield the Drude response as expected [3].

[1] C. Wetli *et al.*, Nat. Phys. **14**, 1103 (2018)
[2] S. Pal *et al.*, PRL **122**, 096401 (2019)
[3] C.-J. Yang *et al.*, PRR **2**, 033296 (2020)

TT 9.16 Tue 13:30 P

Multifractality at the spin quantum Hall (class C) transition — •Martin Puschmann[1], Daniel Hernangómez-Pérez[2], Bruno Lang[3], Soumya Bera[4], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, D-93053 Regensburg, Germany — [2]Department of Molecular Chemistry and Material Science, Weizmann Institute of Science, Rehovot 7610001, Israel — [3]IMACM and Institute of Applied Computer Science, Bergische Universität Wuppertal, D-42119 Wuppertal, Germany — [4]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

Recent analytical work on the integer quantum Hall transition (class A) predicts a parabolic dependency of the exponents τ_q, that describe the system-size scaling of wavefunction moments $|\psi|^{2q}$. [1] The prediction has raised attention, since it contradicts numerical observations [2]. The arguments of [1] rely on conformal invariance and therefore are believed to carry over also to class C. Since in class C corrections to scaling are under control, it provides an excellent laboratory for testing the salient concepts numerically. Thus motivated, we investigate τ_q in class C and eliminate subleading powers guided by finite-size corrections of distribution functions. Thereby, we demonstrate unambiguously the presence of quartic terms in τ_q [3], inconsistent with the predicted parabolic shape but in agreement with [4].

[1] M. R. Zirnbauer, Nucl. Phys. B 941, 458 (2019)
[2] e.g. K. Slevin and T. Ohtsuki, Phys. Rev. B 80, 041304 (2009)
[3] M. Puschmann et al., Phys. Rev. B 103, 235167 (2021)
[4] J. Karcher et al., arXiv:2107.06414

TT 9.17 Tue 13:30 P

Spin-phonon interaction and tunnel splitting in single-molecule magnets — •Kilian Irländer[1], Jürgen Schnack[1], and Heinz-Jürgen Schmidt[2] — [1]Fakultät für Physik, Universität Bielefeld, Postfach 100131, Bielefeld D-33501, Germany — [2]Fachbereich Physik, Universität Osnabrück, Osnabrück D-49069, Germany

Quantum tunneling of the magnetization is a phenomenon that impedes the use of small anisotropic spin systems for storage purposes even at the lowest temperatures. Phonons, usually considered for temperature dependent relaxation of magnetization over the anisotropy barrier, also contribute to magnetization tunneling for integer spin quantum numbers. In this context, it is not viable to consider phonons perturbatively but to treat spins and phonons on the same footing by performing quantum calculations of a Hamiltonian where the single-ion anisotropy tensors are coupled to harmonic oscillators. We demonstrate the ability of phonons to induce a tunnel splitting of the ground doublet which then reduces the required bistability due to Landau-Zener tunneling of the magnetization [Phys. Rev. B 102, 054407]. We also present the unexpected observation that certain spin-phonon Hamiltonians are robust against the opening of a tunneling gap, even for strong spin-phonon coupling. The key to understanding this phenomenon is provided by an underlying supersymmetry that involves both spin and phonon degrees of freedom.

[1] Eur. Phys. J. B 94, 68

TT 9.18 Tue 13:30 P

NMR investigations of the 2D Heisenberg system CuPOF under pressure — •F. Bärtl[1,2], D. Opherden[1,2], C. P. Landee[3], S. Molatta[1,2], J. Wosnitza[1,2], M. Baenitz[4], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Department of Physics, Clark University, Worcester, Massachusetts, USA — [4]MPI for Chemical Physics of Solids, Dresden, Germany

The molecular-based material CuPOF ($[Cu(pz)_2(2\text{-}OHpy)_2](PF_6)_2$) is an excellent realization of a two-dimensional square-lattice quantum $S = 1/2$ Heisenberg antiferromagnet, with an intralayer exchange coupling $J/k_B = 6.8$ K and an interlayer coupling $J' \approx 10^{-4}J$. Previously reported nuclear magnetic resonance (NMR) data revealed a low-temperature transition to commensurate antiferromagnetic (AF) quasistatic long-range order (LRO), with a preceding crossover from isotropic Heisenberg to anisotropic XY behaviour. We present further NMR studies of the low-temperature correlations in magnetic fields up to 7 T and temperatures down to 0.3 K. The application of hydrostatic pressure up to 10 kbar leads to a change of the interlayer coupling and, therefore, the magnetic correlations in the critical regime. The transition regime is probed by ^1H and ^{31}P spectroscopy and relaxometry, revealing a non-monotonic change of T_N with increasing pressure. The commensurate AF LRO below T_N still persists at high pressures, as revealed by a splitting of the ^1H NMR lines, stemming from the broken symmetry of the local spin polarizations in the LRO regime.

TT 9.19 Tue 13:30 P

Magnetic heat transport and strong magneto-elastic coupling in the frustrated spin-chain mineral linarite — •Matthias Gillig[1,2], Xiaochen Hong[1,3], Piyush Sakrikar[4], Gaël Bastien[5], Anja Wolter[1], Leonie Heinze[6], Satoshi Nishimoto[1,2], Bernd Büchner[1,2], and Christian Hess[1,3] — [1]IFW Dresden, Germany — [2]TU Dresden, Germany — [3]Bergische Universität Wuppertal, Germany — [4]IISER Mohali, India — [5]Charles University, Prague, Czech Republic — [6]TU Braunschweig, Germany

Motivated by recent theoretical results predicting a finite thermal Drude weight in frustrated spin chains, we have studied the thermal conductivity of the mineral Linarite $PbCuSO_4(OH)_2$ at low temperature. In this well-studied material the Cu-ions form a s=1/2 spin chain with competing FM nearest-neighbor and AFM next-nearest-neighbor interactions, creating a magnetically frustrated system which orders below $T_N = 2.8$ K in an elliptical spiral ground state. In a magnetic field along the spin chain, other magnetically ordered phases can be induced. Our results reveal that the thermal conductivity κ in zero field is dominated by a phononic contribution. As a function of magnetic field κ shows a peculiar non-monotonic behavior. Whenever the magnetic field value approaches a critical field, κ is highly suppressed. This trend can be explained by magnetic fluctuations which are expected near a phase boundary and which reduce thermal conductivity due to strong phonon scattering. Furthermore, a magnon thermal transport channel was verified in the spiral phase.

TT 9.20 Tue 13:30 P

Vibrating-coil magnetometry of the magnetic phase diagram of $Gd_2Ga_5O_{12}$ — •Markus Kleinhans and Christian Pfleiderer — Physik-Department, Technische Universität München, D-85748 Garching, Germany

Magnetic frustration attracts great interest since it leads to exotic magnetic orders like spin liquids, spin glasses and spin ice all associated with the geometric frustration of magnetic spins. We report vibrating coil magnetometry down to mK temperatures [2] of the frustrated system $Gd_2Ga_5O_{12}$[1,3,4]. Based on the magnetization measured in a spherical sample for field along ⟨100⟩, ⟨110⟩, and ⟨111⟩ we track the magnetic phase diagram as a function of field orientation in great detail.

[1] P. P. Deen textitet al., PRB **91**, 014419 (2015)
[2] S. Legl *et al.*, RSI **81**, 043911 (2010)
[3] S. Hov. *et al.*, JMMM **455-456**, 15-18 (1980)
[4] P. Schiffer and A.P. Ramirez *et al.*, PRL **2500**, 73 (1994)

TT 9.21 Tue 13:30 P

Low-temperature investigation of thermodynamic properties on the spin-liquid candidate system $PbCuTe_2O_6$ in various finite fields. — •Paul Eibisch[1], Christian Thurn[1], Ulrich Tutsch[1], Arif Ata[1], Abanoub R. N. Hanna[2,3], A. T. M. Nazmul Islam[3], Shravani Chillal[3], Bella Lake[3], Bernd Wolf[1], and Michael Lang[1] — [1]PI Goethe-University Frankfurt — [2]IFKP, TU Berlin — [3]HZ Berlin

The quantum spin liquid is an exotic state of magnetic systems which shows no long-range order down to $T = 0$ K but instead exhibits persistent spin dynamics with highly entangled spins fluctuating between various degenerate configurations. A favourable route to realize this state is to use geometric frustrations for instance in 2D materials where the spins interact on top of a kagome lattice. In this study we present low-temperature thermodynamic measurements in various fields on the spin-liquid candidate system $PbCuTe_2O_6$ showing a Hyperkagome lattice, a 3D adaptation of the 2D kagome lattice. First investigations on polycrystalline samples supported the spin-liquid character [1], whereas more recent studies revealed an even more exotic behaviour i.e. a ferroelectric phase transition around $T = 1$ K together with a diverging thermal Grüneisen parameter, indicating proximity to a quantum critical point [2]. Here we show that the magnetic Grüneisen parameter diverges as well, supporting zero-field-quantum-critical behaviour. Further focus of our investigations lies on the field dependence of the ferroelectric transition.

[1] S.Chillal *et al.*, Nat. Commun. **11**, 2348 (2020)
[2] C.Thrun *et al.*, arXiv:2103.17175

TT 9.22 Tue 13:30 P

Nesting instability of gapless U(1) spin liquids with spinon Fermi pockets in two dimensions — •Wilhelm Krüger and Lukas Janssen — TU Dresden, 01062 Dresden, Germany

Quantum spin liquids are exotic states of matter that may be realized in frustrated quantum magnets and feature fractionalized excitations and emergent gauge fields. Here, we consider a gapless U(1) spin liquid with spinon Fermi pockets in two spatial dimensions. Such a state appears to be the most promising candidate to describe the exotic field-induced behavior observed in numerical simulations of the antiferromagnetic Kitaev honeycomb model. A similar such state may also be responsible for the recently-reported quantum oscillations of the thermal conductivity in the field-induced quantum paramagnetic phase of α-$RuCl_3$. We consider the regime close to a Lifshitz transition, at which the spinon Fermi pockets shrink to small circles around high-symmetry points in the Brillouin zone. By employing renormalization group and mean-field arguments, we demonstrate that interactions lead to a gap opening in the spinon spectrum at low temperatures, which can be understood as a nesting instability of the spinon Fermi surface. This leads to proliferation of monopole operators of the emergent U(1) gauge field and confinement of spinons. While signatures of fractionalization may be observable at finite temperatures, the gapless U(1) spin liquid state with nested spinon Fermi pockets is ultimately unstable at low temperatures towards a conventional long-range-ordered ground state, such as a valence bond solid. Implications for Kitaev materials in external magnetic fields are discussed.

TT 9.23 Tue 13:30 P

Magnetostriction in the J-K-Γ-model on the honeycomb lattice — •Alexander Schwenke and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany

Using the numerical linked cluster expansion (NLCE) [1], we investigate thermodynamic and magnetoelastic properties of the J-K-Γ spin-$\frac{1}{2}$ model on the honeycomb lattice in the presence of a magnetic field $\vec{B}$, for field orientations both in-plane and out-of-plane.

Apart from the specific heat and the magnetization, we focus in particular on the linear magnetostriction coefficient $\lambda(B,T)$. As a prime result and based on expansions up to order $\sim \mathcal{O}(11)$, we find clear indications for a field-induced transition in $\lambda(B,T)$.

Employing exchange parameters as proposed for $\alpha - RuCl_3$, our results are very similar to recently observed experimental data [2] on this proximate quantum spin-liquid candidate material.

[1] M. Rigol et al., Phys. Rev. Lett. 97, 187202 (2006)
[2] S. Gass et al., Phys. Rev. B 101, 245158 (2020)

TT 9.24 Tue 13:30 P

Glass-like transitions in the frustrated charge system θ-(BEDT-TTF)$_2$CsM(SCN)$_4$ (M = Cs and Co) revealed by thermal expansion measurements — •Yohei Saito[1], Tatjana Thomas[1], Steffi Hartmann[1], Tim Thyzel[1], Yassine Agarmani[1], Hungwei Sun[1], Jens Müller[1], Kenichiro Hashimoto[2], Takahiko Sasaki[2], Hiroshi Yamamoto[3], and Michael Lang[1] — [1]Institute of Physics, Goethe University Frankfurt, Frankfurt (M), Germany — [2]Institute for Materials Research, Tohoku University, Sendai, Japan — [3]Institute for Molecular Science, Okazaki, Japan

Geometrical frustration causes degenerate states, giving rise to intriguing quantum phenomena such as a spin liquid. In addition to a frustrated spin system, a frustrated charge system is proposed in organic conductors called θ-type BEDT-TTF salts. It is expected that charge ordering is suppressed and is possibly replaced by a charge glass state. In organic charge-ordered salts, the charge order transition accompanies a structural transition. Therefore, investigating their elastic properties is of fundamental interest. We performed thermal expansion measurements on θ-(BEDT-TTF)$_2$CsM(SCN)$_4$ (M = Cs and Co) that does not show charge ordering. The thermal expansion coefficient exhibited a glassy transition at 90-100 K. This behavior is reminiscent of the freezing of the terminal ethylene end-groups on the BEDT-TTF molecules. We also found another glassy transition at 120-130 K for both salts where the development of a superlattice structure was reported. These results point to the importance of the lattice degrees of freedom in the frustrated charge system.

TT 9.25 Tue 13:30 P

The one-dimensional Long-Range Falikov-Kimball Model: Thermal Phase Transition and Disorder-Free Localisation — •Thomas Hodson[1], Josef Willsher[2], and Johannes Knolle[2,3,1] — [1]Blackett Laboratory, Imperial College London, London SW72AZ, United Kingdom — [2]Department of Physics TQM, Technische Universit at Munchen,James-Franck-Strasse 1, D-85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Disorder or interactions can turn metals into insulators. One of the simplest settings to study this physics is given by the FK model, which describes itinerant fermions interacting with a classical Ising background field. Despite the translational invariance of the model, inhomogenous configurations of the background field give rise to effective disorder physics which lead to a rich phase diagram in two (or more) dimensions with finite temperature charge density wave (CDW) transitions and interaction-tuned Anderson versus Mott localized phases. Here, we propose a generalised FK model in one dimension with long-range interactions which shows a similarly rich phase diagram. We use an exact Markov Chain Monte Carlo method to map the phase diagram and compute the energy resolved localisation properties of the fermions. We compare the behaviour of this transitionally invariant model to an Anderson model of uncorrelated binary disorder about a background CDW field which confirms that the fermionic sector only fully localizes for very large system sizes.

TT 9.26 Tue 13:30 P

Anisotropic Magnetoresistance in LAO/STO nanostructures — •Mithun S Prasad[1] and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120 Halle, Germany — [2]Interdisziplinäres Zentrum für Meterialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Straße 4, D-06120 Halle, Germany

The high-mobility two-dimensional electron gas (2DEG) confined at the interface LaAlO3 (LAO) and SrTiO3 (STO) provides new opportunities to explore Nanoelectronic devices. In our group, we have developed an industry-compatible Nanopatterning technique [1] for the LAO/STO interface. Recent studies on this interface have revealed that at low temperature the current is confined to filaments which are linked to structural domain walls in the STO[2] with drastic consequences for example for the temperature dependence of local transport properties [3]. We have investigated magneto-transport in nanostructures having a different crystalline orientation with respect to the lattice. Our experiments show that not only the resistance but also the magnetoresistance varies with orientation. The magnetoresistance can even change sign strongly supporting the model of filamentary charge transport. The angle of orientation of the domain walls can lead to various localization effects on the application of magnetic fields which can explain the anisotropy found in our experiments.

[1] M. Z. Minhas et.al, AIP Advances 6, 035002 (2016)
[2] Kalisky et.al, Nat. Mat. 12, 1091-1095 (2013)
[3] M. Z. Minhas et.al, Sci. Rep. 7, 5215(2017)

TT 9.27 Tue 13:30 P

Anisotropic metamagnetism in trilayer ruthenate $Sr_4Ru_3O_{10}$ — •Izidor Benedičič[1], Masahiro Naritsuka[1], Luke C. Rhodes[1], Rosalba Fittipaldi[2], Veronica Granata[3], Christopher Trainer[1], Antonio Vecchione[2], and Peter Wahl[1] — [1]School of Physics and Astronomy, University of St Andrews, North Haugh. St Andrews, Fife KY16 9SS, United Kingdom — [2]CNR-SPIN, UOS Salerno, Via Giovanni Paolo II 132, I-84084, Fisciano, Italy — [3]Dipartimento di Fisica "E.R.Caianiello", Universita di Salerno, I-84084 Fisciano, Salerno,Italy

The ground state of metamagnetic materials can be precisely controlled by application of magnetic field, making them exciting candidates for spintronic applications. In itinerant metamagnets, such as trilayer ruthenate $Sr_4Ru_3O_{10}$, understanding their electronic structure is crucial for successful manipulation and tuning of their magnetic properties. I will show measurements using quasiparticle interference imaging in a low temperature scanning tunneling microscope to study the electronic structure of $Sr_4Ru_3O_{10}$ in magnetic field. We find a strongly anisotropic response to the in-plane field, suggesting an unusually strong effect of the orthorhombic distortion on the electronic structure. Using DFT calculations, we can model the QPI signal and find the Fermi surface dominated by bands of spin-minority character, putting constraints on theories for the origin of the metamagnetic transition.

TT 9.28 Tue 13:30 P

Real-space cluster dynamical mean-field theory: Center focused extrapolation on the one- and two particle level — Marcel Klett[1], •Nils Wentzell[2], Thomas Schaefer[1], Fedor Simkovic[3], Olivier Parcollet[2], Sabine Andergassen[4], and Philipp Hansmann[5] — [1]Theory of strongly correlated quantum matter, Max Planck Institute for Solid State Research, Stuttgart — [2]Center for Computational Quantum Physics, Flatiron institute, NYC — [3]College de France, Paris — [4]Institut fuer Theoretische Physik and Center for Quantum Science, University Tuebingen — [5]Institut für Theoretische Physik, Friedrich-Alexander-University Erlangen-Nuernberg

We revisit the cellular dynamical mean-field theory (CDMFT) for the single band Hubbard model on the square lattice at half filling, reaching real-space cluster sizes of up to 9 x 9 sites. Using benchmarks against direct lattice diagrammatic Monte Carlo at high temperature, we show that the self-energy obtained from a cluster center focused extrapolation converges faster with the cluster size than the periodization schemes previously introduced in the literature. The same benchmark also shows that the cluster spin susceptibility can be extrapolated to the exact result at large cluster size, even though its spatial extension is larger than the cluster size.

We acknowledge financial support from the Deutsche Forschungsgemeinschaft (DFG) through ZUK 63 and Project No. AN 815/6-1

TT 9.29 Tue 13:30 P

Spectral function of the Hubbard model using cluster perturbation theory — •Nicklas Enenkel[1], Peter Schmitteckert[2], and Markus Garst[1] — [1]Karlsruher Institut für Technologie, Karlsruhe, Deutschland — [2]HQS - Quantum Simulations, Karlsruhe, Deutschland

The spectral function of the single band Hubbard model is calculated as part of a benchmark study using cluster perturbation theory (CPT). Within the framework of CPT, the Green function of a certain cluster of sites is first calculated numerically exactly, and, in a second step, the hopping of electrons between the clusters is treated in perturbation theory. Practically, however, a numerically reliable determination of the cluster Green function poses a challenge, and we compare various numerical approaches involving exact diagonalization, Chebychev expansion and equation of motion techniques. Results for the full spectral function are presented and discussed for the one- and two-dimensional Hubbard model.

TT 9.30 Tue 13:30 P

Four-point functions on the real-frequency axis – A spectral representation and its numerical evaluation — •Fabian B. Kugler[1,2], Seung-Sup B. Lee[2], and Jan von Delft[2] — [1]Rutgers University, USA — [2]LMU Munich, Germany

We present spectral representations for multipoint correlation functions for each of three widely-used formalisms: the imaginary-frequency Matsubara formalism and the real-frequency zero-temperature as well as Keldysh formalisms. The spectral representations separate information on the system's dynamics, encoded in universal partial spectral functions, from the correlators' analytical properties, encoded in formalism-dependent convolution kernels [1]. We present numerical results for the four-point vertex of the Anderson impurity model, obtained by a novel numerical renormalization group scheme [2]. In the imaginary-frequency Matsubara formalism, our approach allows us to compute the vertex at arbitrarily low temperatures and to follow the complete crossover from strongly interacting particles to weakly interacting quasiparticles. In the real-frequency Keldysh formalism, we first benchmark our method against analytical results at weak and infinitely strong interaction. Then, we consider the dynamical mean-field solution of the Hubbard model to reveal the rich real-frequency structure of the vertex in the metal-insulator coexistence regime.

[1] F. B. Kugler, S.-S. B. Lee, J. von Delft, arXiv:2101.00707, accepted in PRX
[2] S.-S. B. Lee, F. B. Kugler, J. von Delft, arXiv:2101.00708, accepted in PRX

TT 9.31 Tue 13:30 P

Accuracy of the typicality approach using Chebyshev polynomials — Florian Gayk[1], Heinz-Jürgen Schmidt[2], Andreas Honecker[3], Jürgen Schnack[4], and •Henrik Schlüter[4] — [1]Fakultät für Physik, Universität Bielefeld, Postfach 100131, Bielefeld D-33501, Germany — [2]Fachbereich Physik, Universität Osnabrück, Osnabrück D-49069, Germany — [3]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, CY Cergy Paris Université, Cergy-Pontoise Cedex F-95302 — [4]Fakultät für Physik, Universität Bielefeld, Postfach 100131, Bielefeld D-33501, Germany

Trace estimators allow us to approximate thermodynamic equilibrium observables with astonishing accuracy. A prominent representative is the finite-temperature Lanczos method (FTLM) which relies on a Krylov space expansion of the exponential describing the Boltzmann weights. Here we report investigations of an alternative approach which employs Chebyshev polynomials [1]. This method turns out to be also very accurate in general, but shows systematic inaccuracies at low temper- atures that can be traced back to an improper behaviour of the approximated density of states with and without smoothing kernel. Applications to archetypical quantum spin systems are discussed as examples.

[1] H. Schlüter, F. Gayk, H.-J. Schmidt, A. Honecker and J. Schnack, Zeitschrift für Naturforschung A, 2021 https://doi.org/10.1515/zna-2021-0116

TT 9.32 Tue 13:30 P

Inhomogeneous mean-field approach to collective excitations near the superfluid–Mott glass transition — •Martin Puschmann[1,2], João C. Getelina[1,3], José A. Hoyos[3], and Thomas Vojta[1] — [1]Department of Physics, Missouri University of Science and Technology, Rolla, Missouri, 65409, USA — [2]Institute of Theoretical Physics, University of Regensburg, D-93040, Regensburg, Germany — [3]Instituto de Física de São Carlos, Universidade de São Paulo, C.P. 369, São Carlos, São Paulo, 13560-970, Brazil

We develop an inhomogeneous quantum mean-field approach to the behavior of collective excitations across the superfluid–Mott glass transition in two dimensions, complementing recent quantum Monte Carlo simulations [1,2]. In quadratic approximation, the Goldstone (phase) and Higgs (amplitude) modes completely decouple. Each is described by a disordered Bogoliubov Hamiltonian which can be solved by an inhomogeneous multi-mode Bogoliubov transformation. We find that the Higgs mode is spatially localized in both phases. The corresponding scalar spectral function shows a broad peak that is noncritical in the sense that its peak frequency does not soften but remains nonzero across the quantum phase transition. In contrast, the lowest-energy Goldstone mode delocalizes in the superfluid phase, leading to a zero-frequency spectral peak. We compare these findings to both the results of the quantum Monte Carlo simulations and the general knowledge on localization of bosonic excitations. We also show first results for three-dimensional systems.

[1] M. Puschmann et al., Phys. Rev. Lett. 125 (2020), 027002
[2] M. Puschmann et al., Ann. Phys. (2021), 168526

TT 9.33 Tue 13:30 P

Applications of real-space truncated unity functional RG — •Jonas B. Hauck[1], Carsten Honerkamp[2], and Dante M. Kennes[1,3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen, 52074 Aachen,Germany and JARA - Fundamentals of Future Information Technology — [2]Institute for Theoretical Solid State Physics, RWTH Aachen University, 52074 Aachen, Germany and JARA - Fundamentals of Future Information Technology — [3]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free Electron Laser Science, 22761 Hamburg, Germany

The discovery of superconductivity in a quasicrystalline material and its approximants lead to a plethora of theoretical predictions. Calculations in such systems are however computationally very heavy, rendering numerical verification of these hypotheses difficult. To resolve this issue we developed a real-space version of the truncated unity functional renormalization group. In this talk I will present this method and discuss its possible use when combining it with the momentum space TUfRG. I will give a short introduction into the derivation, the implementation and showcase the predictive power of the method by presenting our investigation of a penrose quasicrystal and the chiral edge modes in a $d + id$ superconductor.

TT 9.34 Tue 13:30 P

Tracking the footprints of spin fluctuations: a multi-method, multi-messenger study of the two-dimensional Hubbard model — •T. Schäfer[1], N. Wentzell[2], F. Šimkovic[3,4], Y.-Y. He[2], C. Hille[5], M. Klett[1], C. Eckhardt[6], B. Arzhang[7], V. Harkov[8], F.-M. Le Régent[4], A. Kirsch[4], Y. Wang[9], A. J. Kim[10], E. Kozik[10], E. A. Stepanov[8], A. Kauch[6], S. Andergassen[5], P. Hansmann[11], D. Rohe[12], Y. Vilk[9], J. P. F. LeBlanc[7], S. Zhang[2], A.-M. S. Tremblay[9], M. Ferrero[3,4], O. Parcollet[2], and A. Georges[2,3,4] — [1]MPI-FKF, Stuttgart — [2]CCQ, Flatiron Institute, New York — [3]Collège de France, Paris — [4]École Polytechnique, Palaiseau — [5]Universität Tübingen — [6]TU

Wien — [7]Memorial University of Newfoundland — [8]University of Hamburg — [9]Université de Sherbrooke — [10]King's College London — [11]University of Erlangen-Nuremberg — [12]Forschungszentrum Juelich GmbH

This work represents an extensive multi-method, multi-messenger assessment of the wealth of computational methods that have been developed in recent years to determine the physical properties of the Hubbard model, the most fundamental model for electronic correlations, in two spatial dimensions. These methods range from simple mean-field theory to cutting-edge quantum-field theoretical approaches as dynamical mean field theory and its extensions. Each of these methods is compared to two numerically exact benchmarks and the role of magnetic fluctuations as well as their implications on the theory of metallic materials with strong magnetic correlations are elucidated.

TT 9.35 Tue 13:30 P

Enhancement of paring in asymmetric Hubbard ladder model — •Anas Abdelwahab, Gökmen Polat, and Eric Jeckelmann — Leibniz Universität Hannover, Hannover, Germany

We investigate a ladder system with two inequivalent legs, namely two legs with two different Hubbard interaction and two different intra-leg hopping terms. We use exact diagonalization and the density matrix renormalization group method to determine ground-state properties of this system at half-filling and at various doping. We found strong enhancement of pairing correlations of dopped ladders at some ranges of model parameters. We discuss the behaviors of charge, spin and pairing correlations.

TT 9.36 Tue 13:30 P

Orientational order parameters for arbitrary quantum systems* — •Michael te Vrugt and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

The concept of quantum-mechanical nematic order, which is important in systems such as superconductors, is based on an analogy to classical liquid crystals, where order parameters are obtained through orientational expansions [1]. We generalize this method to quantum mechanics based on an expansion of Wigner functions [2]. This provides a systematic framework for the derivation of quantum order parameters, which unifies all known types of quantum orientational order into one framework and has a natural connection to the classical case. The formalism recovers the standard definitions for spin systems. For Fermi liquids, the formalism reveals the nonequivalence of various definitions of the order parameter used in the literature.

Funded by the Deutsche Forschungsgemeinschaft (DFG) - WI 4170/3-1

[1] M. te Vrugt, R. Wittkowski, AIP Adv. 10, 035106 (2020)
[2] M. te Vrugt, R. Wittkowski, Ann. Phys. (Berl.) 532, 2000266 (2020)

TT 9.37 Tue 13:30 P

Electronic transport in molecular junctions: The generalized Kadanoff-Baym ansatz with initial contact and correlations — •Riku Tuovinen[1], Robert van Leeuwen[2], Enrico Perfetto[3], and Gianluca Stefanucci[3] — [1]University of Helsinki, Finland — [2]University of Jyväskylä, Finland — [3]Università di Roma Tor Vergata, Italy

The generalized Kadanoff-Baym ansatz (GKBA) offers a computationally inexpensive approach to simulate out-of-equilibrium quantum systems within the framework of nonequilibrium Green's functions. For finite systems, the limitation of neglecting initial correlations in the conventional GKBA approach has recently been overcome [1]. However, in the context of quantum transport, the contacted nature of the initial state, i.e., a junction connected to bulk leads, requires a further extension of the GKBA approach. In this work, we lay down a GKBA scheme that includes initial correlations in a partition-free setting [2]. In practice, this means that the equilibration of the initially correlated and contacted molecular junction can be separated from the real-time evolution. The information about the contacted initial state is included in the out-of-equilibrium calculation via explicit evaluation of the memory integral for the embedding self-energy, which can be performed without affecting the computational scaling with the simulation time and system size. We demonstrate the developed method in carbon-based molecular junctions.

[1] D. Karlsson et al., Phys. Rev. B 98, 115148 (2018)
[2] R. Tuovinen et al., J. Chem. Phys. 154, 094104 (2021)

TT 9.38 Tue 13:30 P

Luttinger liquids with inhomogeneous interactions — Sebastian Huber[1] and •Marcus Kollar[2] — [1]Theoretical Solid State Physics, Ludwig-Maximilians-University, Munich, Germany; current address: Institute for Solid-State Physics, TU Wien, Austria — [2]Theoretical Physics III, University of Augsburg, Germany

We study a generalization of the two-flavor spinless Tomonaga-Luttinger model which includes inhomogeneous local interactions and scattering potentials [1]. For a wide range of parameters we obtain the spectrum and Green function exactly using Kronig identities with momentum transfer. While Green functions have a power-law form as in homogeneous Luttinger liquids, a sufficiently strong position dependence of the interaction breaks their translational invariance. Furthermore, the Luttinger-liquid interrelations between excitation velocities and Green function exponents are modified in such Luttinger droplets.

[1] S. Huber, M. Kollar, Phys. Rev. Research 2, 043336 (2020)

TT 9.39 Tue 13:30 P

RPA as exact high-density limit of 1D correlated electrons — •Klaus Morawetz[1,2], Vinod Ashokan[3], Renu Bala[4], and Kare Narain Pathak[5] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — [3]Department of Physics, Dr. B.R. Ambedkar NationalInstitute of Technology, Jalandhar (Punjab) - 144 011, India — [4]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India — [5]Department of Physics, MCM DAV College for Women, 160036 Chandigarh, India

It is shown that in d-dimensional systems, the vertex corrections beyond the random phase approximation (RPA) or GW approximation scales with the power $d-\beta-\alpha$ of the Fermi momentum if the relation between Fermi energy and Fermi momentum is $\epsilon_f \sim p_f^\beta$ and the interacting potential possesses a momentum-power-law of $\sim p^{-\alpha}$. The condition $d < \beta+\alpha$ specifies systems where RPA is exact in the high-density limit. The one-dimensional structure factor is calculated analytically and the ground-state energy is presented exactly in the high-density and Coulomb limit. The proposed high-density expansion agrees with diffusive Monte Carlo simulations which we performed for this purpose.

[1] Eur. Phys. J. B 91 (2018) 29
[2] Phys. Rev. B 97 (2018) 155147
[3] Phys. Rev. B 101 (2020) 075130

TT 9.40 Tue 13:30 P

Quantum friction in the hydrodynamic model — •Kunmin Wu, Thomas Schmidt, and María Farias — Campus Limpertsberg, University of Luxembourg Faculty of Science, Technology and Medicine 162 A, avenue de la Faïencerie L-1511 Luxembourg

We study the phenomenon of quantum friction in a system consisting of a polarizable atom moving at a constant speed parallel to a metallic plate. The plate is described using a charged hydrodynamic model for the electrons. This model featuring long-range, instantaneous interactions is appropriate for graphene or a clean metal in a temperature range where scattering due to Coulomb interactions dominates over the scattering of electron by impurities. We find that a quantum friction force between the atom and the metal surface exists even in the absence of intrinsic damping in the plate, but that it only starts once the velocity of the atom exceeds the effective speed of sound in the plate. We argue that this condition can be fulfilled most easily in metals with nearly empty or nearly filled bands. We make quantitative predictions for the friction force to the second and fourth order in the atomic polarizability, and show that the threshold behavior persists to all orders of the perturbation theory.

TT 9.41 Tue 13:30 P

Dicke transition in open many-body systems determined by fluctuation effects — •Alla Bezvershenko[1], Catalin-Mihai Halati[2], Ameneh Sheikhan[2], Corinna Kollath[2], and Achim Rosch[1] — [1]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [2]Physikalisches Institut, University of Bonn, Nussallee 12, 53115 Bonn, Germany

We develop an approach to describe the Dicke transition of interacting many-particle systems strongly coupled to the light of a lossy cavity. A mean-field approach is combined with a perturbative treatment of fluctuations beyond mean-field, which becomes exact in the thermodynamic limit. Fluctuations are crucial to determine the mixed state character of the transition and to unravel universal properties of the emerging self-organized states. A rate equation is used to calculate an effective temperature. We validate our results by comparing to time-dependent matrix-product-state calculations.

TT 9.42 Tue 13:30 P

Dynamical quantum phase transitions in a chiral p-wave superconductor upon chemical potential quenches — •Yuto Shibata[1,2], Chitra Ramasubramanian[2], and Aline Ramires[1] — [1]Condensed Matter Theory Group, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [2]Institute for Theoretical Physics, ETH Zürich, 8093 Zürich, Switzerland

Dynamical quantum phase transitions (DQPTs) have been shown useful to identify non-trivial topology of quantum systems [1,2]. However, most of the preceding works do not incorporate self-consistency conditions for order parameters, which leads to periodic DQPTs.

Here, we study the dynamics of a two-dimensional chiral p-wave superconductor upon a quantum quench in the sign of the chemical potential within the BCS weak-coupling limit. We solve the BdG equations using fourth-order Runge-Kutta methods self-consistently and observe the phase of order parameter persistently oscillates sinusoidally in time after the quench. Despite the imposition of self-consistent conditions, periodic DQPTs are observed. These are identified as cusps in Loschmidt echo and accompanied by simultaneous creation of topological defects in the Pancharatnam geometric phase over curves in momentum space. We also discuss the robustness of the persistent phase oscillation against deformation of the Fermi surface and introduction of asymmetry to the chemical potential quenches.

[1] M. Heyl, Rep. Prog. Phys. **81**, 054001 (2018).
[2] N. Fläschner *et al.*, Nature Physics **14**, 265-268 (2018).

TT 9.43 Tue 13:30 P

Localization dynamics in a centrally coupled system — •Sebastian Wenderoth[1], Nathan Ng[2], Michael Kolodrubetz[3], Eran Rabani[2], and Michael Thoss[1] — [1]University of Freiburg, Freiburg, Germany — [2]University of California, Berkeley, USA — [3]University of Texas, Dallas, USA

In recent years, locally interacting system with static disorder, such as e.g. a random-field Ising chain with nearest neighbor interactions, received much attention because they can exhibit many-body localization. Many-body localized systems fail to equilibrate locally under unitary time evolution due to the absence of transport and the emergence of quasi-local integrals of motions, and thus, retain information about the initial state in local observables.

In our work, we explore the dynamics of a spin chain with a local antiferromagnetic interaction, and non-local spin-flip interactions induced by coupling of the spins to a central d-level system (qudit). We employ the multilayer multi-configuration time-dependent Hartree approach [2,3] to simulate the dynamics of moderately large spin chains in a numerically exact way. Using this approach, we examine dynamical properties of the spin chain and the qudit, with particular focus on the question whether the system retains information about the initial state in local observables.

[1] A. Pal *et al.*, Phys. Rev. B **82**, 174411 (2010)
[2] H. Wang *et al.*, J. Chem. Phys. **119**, 1289 (2003)
[3] O. Vendrell *et al.*, J. Chem. Phys. **134**, 044135 (2011)

TT 10: Materials and devices for quantum technology (joint session HL/TT)

Time: Wednesday 10:00–12:45 Location: H4

See HL 14 for details of this session.

TT 11: Focus Session: Facets of Many-Body Quantum Chaos (organised by Markus Heyl and Klaus Richter) (joint session DY/TT)

This session covers the same topics as the TT-DY-MA symposium with the same name and five invited speakers on Tuesday, September 28th.

Time: Wednesday 10:00–13:00 Location: H6

See DY 7 for details of this session.

TT 12: New Experimental Techniques

Time: Wednesday 10:00–11:00 Location: H7

TT 12.1 Wed 10:00 H7

Chip-based magnetic levitation of superconducting microparticles for macroscopic quantum experiments — •Marti Gutierrez[1], Achintya Paradkar[1], Gerard Higgins[1,2], and Witlef Wieczorek[1] — [1]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Kemivagen 9, SE-412 96 Gothenburg, Sweden — [2]Vienna Center for Quantum Science and Technology (VCQ), Faculty of Physics, University of Vienna, Boltzmanngasse 5, Vienna, A-1090, Austria

In this work, we demonstrate chip-based magnetic levitation of superconducting microparticles. Magnetic levitation has been proposed as a platform to decouple the center-of-mass (COM) motion of a levitated mechanical resonators from the environment. As a result, this platform enables the development of novel, ultra-sensitive force and acceleration sensors, as well as performing quantum experiments with macroscopic objects of 10^13 atomic mass units. Our approach is based on an integrated magnetic trap consisting of a two-chip stack with micro-fabricated niobium superconducting coils. We further fabricate near spherical lead spheres of sub-100um diameter. A pair of integrated coils is used to generate the magnetic trapping field, while additional coils are used for SQUID-based detection and, independently, for feedback-based manipulation of the COM motion of the levitated particle. We show first trapping experiments, where we observe the motion of the levitated particle optically and via SQUID-based readout. In future experiments, we aim to couple the levitated particle to superconducting circuits, in order to perform quantum control over its COM motion.

TT 12.2 Wed 10:15 H7

Reaching the ultimate energy resolution of a quantum detector — •Bayan Karimi[1], Fredrik Brange[1,2], Danilo Nikolic[3], Joonas T. Peltonen[1], Peter Samuelsson[2], Wolfgang Belzig[3], and Jukka P. Pekola[1] — [1]QuESTech and QTF Centre of Excellence, Department of Applied Physics, Aalto University, Finland — [2]Department of Physics and NanoLund, Lund University, Sweden — [3]QuESTech and Fachbereich Physik, Universität Konstanz, Germany

We demonstrate experimentally detection of equilibrium fluctuations of temperature in a system of about 10^8 electrons exchanging energy with phonon bath at a fixed temperature [1]. In this experiment, we employ a radio-frequency thermometer, connected to a nanocalorimeter, based on a zero-bias anomaly of a tunnel junction between a superconductor and proximitized normal metal [2,3]. It features noninvasive detection and essentially uncompromised sensitivity down to the lowest temperatures of below 20 mK. We show theoretically that this detector is capable of observing single microwave photons in a continuous manner [4,5].

[1] B. Karimi, F. Brange, P. Samuelsson, J. P. Pekola, Nat. Commun. **11**, 367 (2020)
[2] B. Karimi and J. P. Pekola, Phys. Rev. Appl. **10**, 054048 (2018)
[3] B. Karimi, D. Nikolić, T. Tuukkanen, J. T. Peltonen, W. Belzig, J. P. Pekola, Phys. Rev. Applied **13**, 054001 (2020)
[4] B. Karimi and J. P. Pekola, Phys. Rev. Lett. **124**, 170601 (2020)
[5] J. P. Pekola and B. Karimi, arXiv:2010.11122 (2020)

TT 12.3 Wed 10:30 H7

Towards time domain phase diagram of metastable charge-ordered states — •Yaroslav Gerasimenko[1,2], Jan Ravnik[1,3], Jaka Vodeb[1], Michele Diego[1], Yevhenii Vaskivskyi[1], Viktor Kabanov[1], Igor Vaskivskyi[1], Tomaz Mertelj[1], and Dragan Mihailovic[1] — [1]Jozef Stefan Institute, Ljubljana, Slovenia — [2]University of Regensburg, Regensburg, Germany — [3]PSI, Villigen, Switzerland

Metastable self-organized electronic states in quantum materials are emergent states of matter[1] typically formed through phase transitions under non-equilibrium conditions. It is of fundamental importance to understand the process of their formation that can involve multiple mechanisms[1,2] spanning a large range of timescales.

Here we combine multiple techniques to map the evolution of metastable states in 1T-TaS_2, a prototypical charge-ordered quantum material, using the photon density and temperature as control parameters on timescales ranging from 10^{-12} to 10^3 s. The combination of STM and in situ ultrafast excitation allows us to observe explicitly both parametric stability and nanoscale relaxation of the light-induced metastable states on the scale of seconds, while time-resolved optical techniques and electrical measurements allow us to study the ordering and relaxation processes down to a few picoseconds. [3]

[1] Ya. A. Gerasimenko et al., Nat. Mater. 18, 1078-1083 (2019)
[2] Ya. A. Gerasimenko et al., npj Quantum Materials 4, 1-9 (2019)
[3] J. Ravnik et al., Nat. Comm. 12, 2323 (2021)

TT 12.4 Wed 10:45 H7

Advanced technique for probing critical elasticity in strongly coupled electron-phonon systems — •Yassine Agarmani, Jan Zimmermann, Steffi Hartmann, Bernd Wolf, and Michael Lang — Institute of Physics, Goethe University Frankfurt, Germany

The recently proposed phenomena of critical elasticity arises from a non-perturbative coupling between lattice and critical electronic degrees of freedom. As demonstrated for the Mott insulator κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl, tuning to the critical endpoint of the first order Mott transition cause a vanishing elastic modulus and a violation of Hooke's law of elasticity [1, 2]. Similar effects are expected to surround the critical region of the valence transition in $EuPd_2Si_2$. Measurements of relative length changes under control of temperature and pressure have proven a most sensitive tool for investigating this phenomenon of critical elasticity. In order to develope a deeper understanding of critical elasticity, an expansion of the setup used in Ref. [2] has been designed and realized. It consists of two identical capacitive dilatometer systems, the temperature of which can be controlled individually, and which are connected to a He-gas pressure reservoir. We discuss the new possibilities this system offers for performing high-resolution measurements of relative length changes over wide ranges of temperature and pressure.

[1] Zacharias *et al.*, Eur. Phys. J. Spec. Top. 224, 1021-1040 (2015)
[2] Gati *et al.*, Sci. Adv. 2, e1601646 (2016)

TT 13: Quantum Computing (joint session TT/DY)

Time: Wednesday 11:15–13:00 Location: H7

TT 13.1 Wed 11:15 H7

Probing the critical current coupling of defects in Josephson junctions — •Alexander Konstantin Neumann[1], Benedikt Berlitz[1], Alexey V. Ustinov[1,2,3], and Jürgen Lisenfeld[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]National University of Science and Technology MISIS, Moscow 119049, Russia — [3]Russian Quantum Center, Skolkovo, Moscow 143025, Russia

Material defects form a major source of decoherence in state of the art superconducting quantum bits. It has been a long standing question whether defects residing in the tunnel barrier of Josephson junctions modify their critical current. We investigate this with spectroscopic measurements and QuTiP simulations on individual defects strongly coupled to a transmon qubit. By observing avoided level crossings at driving amplitudes allowing for multi-photon transitions, we quantify the strength of the critical current coupling. Moreover, we find an effective direct interaction between the defect and the qubit's readout resonator, providing an additional decoherence channel.

TT 13.2 Wed 11:30 H7

Cavity mediated quantum gate between distant charge qubits — •Florian Kayatz, Jonas Mielke, and Guido Burkard — Department of Phyiscs, University of Konstanz, Konstanz, Germany

Gate based quantum computers require high fidelity single-qubit and two-qubit gates to allow for arbitrary multi-qubit operations that are needed to perform a quantum algorithm. Ideally, one has "all-to-all" connectivity, i.e. an architecture with two-qubit gates between any desired pair of qubits. Notably, short-ranged interactions such as capacitive coupling and the exchange interaction cannot be harnessed to implement two-qubit gates between distant qubits. We investigate whether a high-fidelity iSWAP gate between distant charge qubits can be implemented by using a microwave resonator as an intermediate system mediating the interaction. In particular, we consider charge qubits formed by a single electron confined in a Si double quantum dot that are coupled to a microwave resonator via electric dipole coupling. We theoretically demonstrate that, in the dispersive regime, the photons can mediate an iSWAP gate. We then calculate the gate fidelity in the presence of the dominant noise sources, quasi-static charge noise, resonator damping and phonon induced charge relaxation, and find a very limited gate fidelity.

TT 13.3 Wed 11:45 H7

Crosstalk analysis for single-qubit and two-qubit gates in spin qubit arrays — •Irina Heinz and Guido Burkard — University of Konstanz, Konstanz, Germany

Scaling up spin qubit systems requires high-fidelity single-qubit and two-qubit gates. Gate fidelities exceeding 98% were already demonstrated in silicon based single and double quantum dots, whereas for the realization of larger qubit arrays crosstalk effects on neighboring qubits must be taken into account. We analyze qubit fidelities impacted by crosstalk when performing single-qubit and two-qubit operations on neighbor qubits with a simple Heisenberg model. Furthermore we propose conditions for driving fields to robustly synchronize Rabi oscillations and avoid crosstalk effects. In our analysis we also consider next to nearest neighbor crosstalk and show that double synchronization leads to a restricted choice for the driving field strength, exchange interaction, and thus gate time. Considering realistic experimental conditions we propose a set of parameter values to perform a nearly crosstalk-free CNOT gate and so open up the pathway to scalable quantum computing devices.

TT 13.4 Wed 12:00 H7

Spin shuttling in a silicon double quantum dot — •Florian Ginzel[1], Adam R. Mills[2], Jason R. Petta[2], and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

The transport of quantum information between different nodes of the device is crucial for a quantum processor. In the context of spin qubits, this can be realized by coherent electron spin shuttling between quantum dots. Here we theoretically study a minimal version of spin shuttling between two quantum dots (QDs) occupied by one electron [1]. We analyze the possibilities and limitations of spin transport during a detuning sweep in a silicon double QD. This research is motivated by recent experimental progress [2,3]. Spin-orbit interaction and an inhomogeneous magnetic field play an important role for spin shuttling and are included in our model. Interactions that couple the position, spin and valley degrees of freedom open avoided crossings in the spectrum allowing for diabatic transitions and interfering paths. The outcomes of single and repeated spin shuttling protocols are explored by means of numerical simulations and an approximate analytic model based on the Landau-Zener model. We find that fast high-fidelity spin-shuttling is feasible for optimal choices of parameters or protected by constructive interference.

[1] Ginzel et al., Phys. Rev. B 102, 195418 (2020)
[2] T. Fujita et al., npj Quantum Information 3, 22 (2017)
[3] A. R. Mills et al., Nat. Comm. 10, 1063 (2019)

TT 13.5 Wed 12:15 H7

Simulating hydrodynamics on NISQ devices with random circuits — •Jonas Richter and Arijeet Pal — Department of Physics and Astronomy, University College London, UK

We show that pseudorandom circuits, recently implemented in Google's seminal "quantum supremacy" experiment, are not just abstract tools to outperform classical computers, but in fact form tailor-made building blocks to simulate certain aspects of quantum many-body systems on noisy intermediate-scale quantum computers. Specifically, we propose an algorithm consisting of a random circuit followed by a trotterized Hamiltonian time evolution to study transport properties in the linear response regime, which we numerically exemplify for one- and two-dimensional quantum spin systems. While the algorithm operates without an overhead of bath or ancilla qubits for initial-state preparation and measurement, our numerics further suggest that it is comparatively robust against systematic Trotter errors and noisy gates.

[1] J. Richter and A. Pal, Phys. Rev. Lett. 126, 230501 (2021)

TT 13.6 Wed 12:30 H7

Adaptive variational NISQ quantum algorithms for dynamics and excited states preparation — Yongxin Yao[1,2], Niladri Gomes[1,2], Feng Zhang[1,2], Cai-Zhuang Wang[1,2], Kai-Ming Ho[1,2], Thomas Iadecola[1,2], and •Peter P. Orth[1,2] — [1]Ames Laboratory, Ames, Iowa, USA — [2]Iowa State University, Ames, Iowa, USA

Simulating quantum dynamics of interacting many-body systems is one of the main potential applications of quantum computing, since the growth of entanglement makes such simulations exponentially hard on classical devices. The shallow circuit requirement of current QPUs limits algorithms based on Trotter product formulas to simulate early time dynamics. Here, we present an adaptive approach to construct a variational wave function ansatz for accurate quantum dynamics simulations based on McLachlan's variational principle [1]. The key idea is to dynamically expand the variational ansatz along the time-evolution path such that the McLachlan distance, which is a measure of the simulation accuracy, remains below a set threshold. We apply this adaptive variational quantum dynamics simulation approach (non)integrable quantum spin models and find the circuits to contain up to two orders of magnitude fewer CNOT gates than those obtained from first-order Trotter expansion. We also present results on development of an adaptive VQE-X algorithm for preparation of highly excited states in many-body models [2].

[1] Yao et al., PRX Quantum 2, 030307 (2021)
[2] Zhang et al., arXiv:2104.12636 (2021)

TT 13.7 Wed 12:45 H7

Simulating a discrete time crystal over 57 qubits on a quantum computer — •Philipp Frey and Stephan Rachel — School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

We simulate the dynamics of a spin-1/2 chain with nearest neighbor Ising interactions, quenched disorder and periodic driving over 57 qubits on a current quantum computer. Based on the dynamics of local spin depolarisation we observe discrete time crystalline (DTC) behaviour due to many body localisation (MBL). We probe random initial states along with fully polarised states and compare the cases of vanishing and finite disorder to distinguish MBL from prethermal dynamics. In order to extract the signal from the noisy data produced by current quantum computer devices, we develop a strategy for error mitigation and show that the results are robust under variations of the parameters introduced in this scheme. A transition between DTC and a thermal phase is observed via critical fluctuations in the sub-harmonic frequency response of the system, as well as a significant speed-up of spin depolarisation. Our findings are consistent with previous numerical simulations, but represent the realization of a DTC with largest system size to date.

TT 14: Many-Body Quantum Dynamics I (joint session DY/TT)

Time: Wednesday 13:30–14:45 Location: H6

See DY 9 for details of this session.

TT 15: Many-Body Quantum Dynamics II (joint session DY/TT)

Time: Thursday 10:00–11:30 Location: H2

See DY 11 for details of this session.

TT 16: PhD Focus Session: Symposium on Strange Bedfellows - Magnetism Meets Superconductivity" (joint session MA/AKjDPG) (joint session MA/TT)

At first sight, it seems that the phenomena of magnetism and superconductivity do not go along, as indicated by the Meissner effect, when a magnetic field is completely expelled from the interior of a conventional superconductor. However, the synergy of these two manifestations of nature in condensed matter does occur and can be rather interesting! Theoretical works have predicted the existence of exotic states at the interface between a superconductor and a magnet, such as the sought-after Majorana fermions and spin-triplet superconductivity. The first have been predicted to route an efficient way to implement quantum computers (currently a European scientific flagship), while the latter allows the creation of spin-polarized supercurrents, opening up fundamentally new possibilities for spintronics. Therefore, our symposium aims at putting together experts to provide a fundamental and practical understanding of the subject to discuss most recent developments from the theoretical and experimental sides, and to show perspectives for applications.

Organizers: Annika Stellhorn, Flaviano José dos Santos, Markus Hoffmann (Forschungszentrum Jülich and Peter Grünberg Institut)

Time: Thursday 10:00–12:45 Location: H5

See MA 13 for details of this session.

TT 17: Charge Density Wave Materials

Time: Thursday 10:00–11:00 Location: H6

TT 17.1 Thu 10:00 H6

Condensation signatures of photogenerated interlayer excitons in a van der Waals heterostack — •Johannes Figueiredo[1], Lukas Sigl[1], Florian Sigger[1], Jonas Kiemle[2], Ursula Wurstbauer[1], and Alexander Holleitner[1] — [1]Walter Schottky Institut, Technical University of Munich — [2]Institute of Physics, Westfälische Wilhelms-Universität Münster

Due to large exciton binding energies and long lifetimes, atomistic van der Waals heterostacks of TMDCs present an ideal platform for studying high-temperature condensation of excitons. At cryogenic temperatures, optically generated interlayer excitons in such heterostructures yield several signatures regarding the condensation of the photogenerated excitons. The transition into this state is consistent with the predicted critical condensation temperature above 10K. Our studies provide a first phase-diagram of the achieved quantum degenerate interlayer exciton ensemble. [1]

[1] L. Sigl *et. al*, Phys. Rev. Research 2, 042044(R) (2020)

TT 17.2 Thu 10:15 H6

Doping fingerprints of spin and lattice fluctuations in moiré superlattice systems — •Niklas Witt[1], José Pizarro[1], Takuya Nomoto[2], Ryotaro Arita[2], and Tim Wehling[1] — [1]Universität Bremen — [2]University of Tokyo

Twisted van der Waals materials open up novel avenues to control electronic correlation and topological effects. These systems contain the unprecedented possibility to precisely tune strong correlations, topology, magnetism, nematicity, and superconductivity with an external non-invasive electrostatic doping. By doing so, rich phase diagrams featuring an interplay of different states of correlated quantum matter can be unveiled. The nature of the superconducting order presents a recurring overarching open question in this context.

In this work, we quantitatively assess the case of spin-fluctuation-mediated pairing for Γ-valley twisted transition metal dichalcogenide homobilayers. We construct a low-energy honeycomb model on which basis we self-consistently and dynamically calculate a doping dependent phase diagram for the superconducting transition temperature T_c. A superconducting dome emerges with a maximal $T_c \approx 0.1$-1 K depending on twist angle. We qualitatively compare our results with conventional phonon-mediated superconductivity and discern clear fingerprints which are detectable in doping-dependent measurements of the superconducting transition temperature, providing direct access to probing the superconducting pairing mechanism in twisted Van der Waals materials.

TT 17.3 Thu 10:30 H6

Electronic transformations in the semi-metallic transitional oxide Mo_8O_{23} — Venera Nasretdinova[1], •Yaroslav Gerasimenko[2,3], Jernej Mravlje[3], Gianmarco Gatti[4], Petra Sutar[3], Damjan Svetin[3], Anton Meden[5], Viktor Kabanov[3], Alexander Kuntsevich[6,7], Marco Grioni[4], and Dragan Mihailovic[1,3,5] — [1]CENN Nanocenter, Ljubljana, Slovenia — [2]University of Regensburg, Germany — [3]JSI, Ljubljana, Slovenia — [4]EPFL, Lausanne, Switzerland — [5]University of Ljubljana, Slovenia — [6]LPI RAS, Moscow, Russia — [7]HSE, Moscow, Russia

Mo_8O_{23} is a low-dimensional stoichiometric transitional metal oxide from MoO_{3-x} family. Its room-temperature phase associated with charge density wave (CDW) is accompanied by non-monotonic resistivity at low temperatures well below structural transitions. Using tunneling and angle-resolved spectroscopy, transport measurements and density functional calculations we reveal electronic transformations leading to a multi-band correlated ground state [1,2]. We observe the metal-to-insulator transition at 343K in resistivity, consistent with CDW onset. At low temperatures, the picture with the only CDW order parameter is broken by the onset of the correlated ground state visible both in transport and spectroscopic probes. Spatially-resolved tunneling spectroscopy studies reveal the emergent electronic texture. We discuss the possible origins of the electronic order that emerge in the absence of any structural or magnetic transitions [3].

[1] V. Nasretdinova et al. PRB 99, 085101
[2] V. Nasretdinova et al., Sci.Rep. 9, 15959 (2019)
[3] V. Nasretdinova et al., in preparation

TT 17.4 Thu 10:45 H6

Field tuning beyond the heat death of a charge-density-wave chain — •Manuel Weber[1,2] and James Freericks[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Department of Physics, Georgetown University, Washington, DC 20057, USA

Time-dependent driving of quantum systems has emerged as a powerful tool to engineer exotic phases far from thermal equilibrium; when the drive is periodic this is called Floquet engineering. The presence of many-body interactions can lead to runaway heating, so that generic systems are believed to heat up until they reach a featureless infinite-temperature state. Finding mechanisms to slow down or even avoid this heat death is a major goal—one such mechanism is to drive toward an even distribution of electrons in momentum space. Here we show how such a mechanism avoids the heat death for a charge-density-wave chain in a strong dc electric field; minibands with nontrivial distribution functions develop as the current is prematurely driven to zero. We also show how the field strength tunes between positive, negative, or close-to-infinite effective temperatures for each miniband. These results suggest that nontrivial metastable distribution functions should be realized in the prethermal regime of quantum systems coupled to slow bosonic modes.

TT 18: Frustrated Magnets

Time: Thursday 10:00–12:45 Location: H7

TT 18.1 Thu 10:00 H7

Magnon Crystallization in the Kagome Lattice Antiferromagnet — •Jürgen Schnack[1], Jörg Schulenburg[2], Andreas Honecker[3], and Johannes Richter[4] — [1]Fakultät für Physik, Universität Bielefeld, Postfach 100131, D-33501 Bielefeld, Germany — [2]Universitätsrechenzentrum, Universität Magdeburg, D-39016 Magdeburg, Germany — [3]Laboratoire de Physique Theorique et Modelisation, CNRS UMR 8089, CY Cergy Paris Universite, F-95302 Cergy-Pontoise Cedex, France — [4]Institut für Physik, Universität Magdeburg, P.O. Box 4120, D-39016 Magdeburg, Germany & Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany

We present numerical evidence for the crystallization of magnons below the saturation field at nonzero temperatures for the highly frustrated spin-half kagome Heisenberg antiferromagnet [Phys. Rev. Lett. 125, 117207 (2020)]. This phenomenon can be traced back to the existence of independent localized magnons or, equivalently, flatband multimagnon states. We present a loop-gas description of these localized magnons and a phase diagram of this transition, thus providing information for which magnetic fields and temperatures magnon crystallization can be observed experimentally. The emergence of a finite-temperature continuous transition to a magnon crystal is expected to be generic for spin models in dimension D > 1 where flatband multimagnon ground states break translational symmetry.

TT 18.2 Thu 10:15 H7

Coexistence of static and dynamic spins in the new Kitaev iridate β-ZnIrO$_3$ — •Aleksandr Zubtsovskii and Alexander A. Tsirlin — EP VI, EKM, University of Augsburg, Germany

The three-dimensional Kitaev iridate β-Li_2IrO_3 shows complex magnetic behavior caused by the exchange anisotropy and frustration, and serves as a suitable ground to seek new materials with spin-liquid physics. Here, we report the detailed study of magnetic properties in the new Kitaev compound, β-$ZnIrO_3$, prepared by the low-temperature topotactic ion exchange reaction. The crystal structure characterized by x-ray and neutron diffraction as well as high-resolution electron microscopy exhibits symmetry lowering with respect to the parent β-Li_2IrO_3, but no structural disorder. Magnetic behavior is studied using magnetization and heat capacity measurements as well as μSR. The results indicate spin freezing below $T_f \sim 5$ K and a broad fluctuating regime that extends up to 40 K.

TT 18.3 Thu 10:30 H7

Spin-orbit coupled Mott insulator, Sr_2IrO_4: spin and charge orders — •Mehdi Biderang[1], Alireza Akbari[2], and Jesko Sirker[1] — [1]Department of Physics and Astronomy, University of Manitoba, Winnipeg, Manitoba, Canada R3T 2N2 — [2]Max Planck Institute for the Chemical Physics of Solids, D-01187 Dresden, Germany

An antisymmetric spin-orbit coupling of a two-dimensional single-band Hubbard Hamiltonian is investigated. We propose that this is the most basic paradigm for understanding the electrical characteristics of locally noncentrosymmetric transition metal (TM) oxides like Sr_2IrO_4. Based on exact diagonalizations of small clusters and the random-phase approximation, we study the correlation effects on charge and magnetic order as a function of doping and of the TM-oxygen-TM bond angle. We see dominating commensurate in-plane antiferromagnetic fluctuations for low doping and small angles, whereas ferromagnetic fluctuations dominate for larger angles. Moderately strong nearest-neighbor Hubbard interactions can also stabilize a charge density wave order. We find good qualitative agreement between the dispersion of magnetic excitations in the hole-doped scenario and resonant inelastic x-ray scattering measurements.

TT 18.4 Thu 10:45 H7

Two-triplon excitations in frustrated bilayer systems — •Erik Wagner and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Braunschweig, Germany

We study the magnetism of frustrated bilayer spin models. Starting from the limit of decoupled dimers we use the perturbative continuous unitary transformation (pCUT), based on the flow equation method, to perform series expansion in order to analyze the spectrum, up to the two-triplon excitations. First we apply this method to the Kitaev-Heisenberg bilayer, consisting of two honeycomb Kitaev spin-models with anisotropic intralayer Ising-exchange $J_{x,y,z}$, coupled by additional interlayer Heisenberg exchange J. We evaluate the groundstate energy and the one particle dispersion up to 9th order in $J_{x,y,z}$ as well as the two-particle interactions and spectrum up to 6th order [1]. We detail the presence of (anti-)bound two-particle states and analyze their wavefunctions. Additionally we discuss the impact of two-particle interactions on the magnetic Raman response of the Kitaev-Heisenberg bilayer. Extensions of our approach to other frustrated bilayers will be considered, focusing on the $SU(2)$ invariant J-J_1-J_2-Heisenberg square-lattice bilayer and including calculations up to 7th and 4th order in $J_{1,2}$ for one- and two-particle matrix elements.

[1] E. Wagner, W. Brenig, arXiv:2103.13402

15 min. break.

TT 18.5 Thu 11:15 H7

Anisotropy of the magnetoelastic coupling investigated in the Kitaev material $RuCl_3$ — •Vilmos Kocsis[1], David A. S. Kaib[2], Kira Riedl[2], Sebastian Gass[1], Paula Lampen-Kelley[3,4], David G. Mandrus[3,4], Stephen E. Nagler[4], Nicolas P. Rodriguez[1], Kornelius Nielsch[1], Roser Valenti[2], Bernd Büchner[1], and Anja U. B. Wolter[1] — [1]IFW-Dresden, Dresden, Germany — [2]Goethe-Universität Frankfurt, Frankfurt, Germany — [3]University of Tennessee, Knoxville, USA — [4]Oak Ridge National Laboratory, Oak Ridge, USA

The Kitaev material α-$RuCl_3$ is among the most promising candidates to host a quantum spin-liquid state. Recent investigations have revealed the importance of the magnetoelastic coupling and the magnetic anisotropy in α-$RuCl_3$. In this combined theoretical and experimental research we investigate the anisotropic magnetic and magnetoelastic properties for magnetic fields applied along the main crystallographic axes as well as for fields canted out of the honeycomb plane. We found that the magnetostriction anisotropy is unusually large compared to the anisotropy of the magnetization, which is related to the strong magnetoelastic Γ'-type coupling in our *ab-initio* derived model. We observed large, non-symmetric anisotropy in the magnetic and magnetoelastic properties for magnetic fields canted out of the honeycomb *ab*-plane in opposite directions, namely for fields canted towards the $+c^*$ or $-c^*$ axes, respectively). The observed directional anisotropy is related to the uniformly aligned Cl_6 octahedra around the magnetic ion Ru^{3+}.

TT 18.6 Thu 11:30 H7

Evidence for kagome intrinsic excitations in the thermal conductivity of herbertsmithite — •Ralf Claus[1], Jan Bruin[1], Yosuke Matsumoto[1], Masahiko Isobe[1], Jürgen Nuss[1], and Hidenori Takagi[1,2,3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [2]Department of Physics, The University of Tokyo, Bunkyo-ku,Tokyo 133-0022, Japan — [3]Institute for Functional Matter and Quantum Technologies,University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Quantum spin liquids (QSLs) are a novel state of matter that may host exotic excitations like itinerant charge-neutral spin-1/2 quasiparticles (spinons). One prominent candidate for a QSL ground state is the spin-1/2 Heisenberg antiferromagnet on the kagome lattice. Herbertsmithite ($ZnCu_3(OH)_6C_{l2}$) provides a perfect realization of this model. However, despite intense theoretical and experimental efforts the nature of its ground state remains under debate. An important open question concerns the existence of an excitation gap.

To address this issue, we performed thermal transport measurements on herbertsmithite single crystals down to 80 mK. Thermal conductivity (k) only captures mobile excitations in the material and is therefore a powerful tool to detect low-lying (gapless) spinons. In our measurements, we confirmed the absence of a finite k/T (spinon Fermi surface) term but additionally observed an unusual field dependence. By carefully comparing in- and out-of-plane heat flow, we were able to identify kagome intrinsic excitations down to lowest temperature.

TT 18.7 Thu 11:45 H7

Interplay of magnetism and dimerization in pressurized Kitaev compound β-Li_2IrO_3 — •Bin Shen, Anton Jesche, Maximilian Seidler, Friedrich Freund, Philipp Gegenwart, and Alexander A. Tsirlin — EP VI, EKM, University of Augsburg, Germany

Quantum spin liquids in a Kitaev honeycomb model, characterized by their quantum entanglement and fractionalized spin excitations, are subject to extensive studies recently. Here, we present magnetization measurements under pressure for β-Li_2IrO_3, the Kitaev material with the putative pressure-induced spin-liquid state, and construct the temperature-pressure phase diagram. A delicate interplay between magnetism and dimerization is revealed. β-Li_2IrO_3 undergoes incommensurate magnetic ordering at $T_N = 38$ K at ambient pressure. Upon applying hydrostatic pressure, T_N is almost pressure-independent before the transition abruptly disappears at around 1.5 GPa. At around 1.4 GPa, a signature of structural dimerization seen as a small step in the magnetic susceptibility appears at $T_d \approx 120$ K and shifts to higher temperatures upon further compression. Intriguingly, a low-temperature Curie-like upturn with the effective moment of about 0.7 μ_B is still observed. Using ab initio calculations, we interpret these results as the formation of a partially dimerized state that evades long-range magnetic order but features a fraction of magnetic Ir^{4+} sites.

Work supported by the German Research Foundation through the Sino-German Cooperation Group on Emergent Correlated Matter.

TT 18.8 Thu 12:00 H7

Thermal Transport of a Co-based candidate Kitaev quantum spin liquid (kQSL) material $Na_2Co_2TeO_6$ — •Xiaochen Hong[1,2], Matthias Gillig[1], Richard Hentrich[1], Weiliang Yao[3], Vilmos Kocsis[1], Arthur Witte[1,4], Tino Schreiner[1], Danny Baumann[1], Nicolás Pérez[1], Anja Wolter[1], Yuan Li[3], Bernd Büchner[1,4], and Christian Hess[1,2] — [1]IFW-Dresden, Germany — [2]Bergische Universität Wuppertal, Germany — [3]Peking University, China — [4]TU Dresden, Germany

Motivated by recent theoretical predications that kQSL states can be realized in certain $3d$ transition metal based materials, we studied the thermal transport properties of $Na_2Co_2TeO_6$ single crystals in a wide field-temperature parameter space, up to 16 T and down to 50 mK. We found that phonons, which are strongly scattered by magnetic excitations, are responsible for thermal transport in $Na_2Co_2TeO_6$. By analyzing the field-temperature dependence of the magneto-phonon scattering, we found major similarities between $Na_2Co_2TeO_6$ and the leading kQSL candidate α-$RuCl_3$, supporting theoretical proposals. Besides, we discovered highly anisotropic field effect, signatures of multiple field-induced transitions, and novel oscillation-like thermal transport features. Our findings encourage more studies on $Na_2Co_2TeO_6$, as a promising kQSL material and an exotic quantum magnet.

TT 18.9 Thu 12:15 H7

Spin liquid and ferroelectricity close to a quantum critical point in $PbCuTe_2O_6$ — •Christian Thurn[1], Paul Eibisch[1], Arif Ata[1], Maximilian Winkler[2], Peter Lunkenheimer[2], István Kézsmárki[2], Ulrich Tutsch[1], Yohei Saito[1], Steffi Hartmann[1], Jan Zimmermann[1], Abanoub R. N. Hanna[3,4], A. T. M. Nazmul Islam[4], Shravani Chillal[4], Bella Lake[3,4], Bernd Wolf[1], and Michael Lang[1] — [1]PI, Goethe University Frankfurt — [2]EP V, University Augsburg — [3]IFKP, TU Berlin — [4]HZ Berlin

Geometrical frustration among interacting spins combined with strong quantum fluctuations destabilize long-range magnetic order in favor of more exotic states such as spin liquids (SL). While in quasi-two-dimensional (quasi-2D) systems a number of SL candidates were found, in 3D the situation is less favorable due to reduced quantum fluctuations and more relevant competing states. Here we report studies of thermodynamic, magnetic and dielectric properties on single crystalline and pressed-powder samples of $PbCuTe_2O_6$, a candidate for a 3D frustrated quantum spin liquid (QSL) [1-3] featuring a hyperkagome lattice. Whereas the low-T properties of the powder are consistent with the proposed QSL state [1-3], a more exotic behaviour is found for the single crystals: they show ferroelectric order at $T_{FE} \approx 1$ K, accompanied by strong lattice distortions, and a modified magnetic response – still consistent with a QSL – but with clear indications for quantum critical behaviour.

[1] Koteswararao *et al.*, PRB **90**, 035141 (2014)
[2] Khuntia *et al.*, PRL **116**, 107203 (2016)
[3] Chillal *et al.*, Nat. Commun. **11**, 2348 (2020)

TT 18.10 Thu 12:30 H7

NMR and magnetization investigations of the field-induced order in the frustrated triangular-lattice compound $NaYbSe_2$ — •S. Luther[1,2], K. M. Ranjith[3], T. Reimann[1], Ph. Schlender[4], B. Schmidt[3], J. Sichelschmidt[3], H. Yasuoka[3], J. Wosnitza[1,2], T. Doert[4], M. Baenitz[3], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]MPI for Chemical Physics of Solids, Dresden, Germany — [4]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany

The Yb-based delafossite $NaYbSe_2$ is a triangular-lattice antiferromagnet with space group $R\bar{3}m$. In this compound, spin-orbit coupling leads to a pronounced magnetic anisotropy. The absence of magnetic long-range order at zero field is suggestive for a quantum spin-liquid ground state. From specific-heat and magnetization experiments, magnetically ordered states were observed for $H \perp c$ and $H \parallel c$ exceeding 2 and 9 T, respectively. ^{23}Na ($I = 3/2$) NMR probes the microscopic details of the field-induced magnetic structure. Measurements of the $1/T_1$-relaxation rate are consistent with the specific-heat data. At $H \perp c = 5$ T, the magnetization indicates an up-up-down spin arrangement with according asymmetric broadening of the NMR spectra. At $H \parallel c = 16$ T, an umbrella-type configuration of the magnetic moments is predicted, in agreement with a symmetric broadening of the NMR spectra. Low-field measurements reveal a continuous increase of the $1/T_1$-relaxation rate and spectral broadening without any signature of long-range order down to 0.3 K.

TT 19: Unconventional Superconductors

Time: Thursday 11:15–12:45 Location: H6

TT 19.1 Thu 11:15 H6

Characterization and spectroscopy of a new non-centrosymmetric superconductor — •Alfredo Spuri, Angelo Di Bernardo, and Elke Scheer — Universität Konstanz

Superconductor with a lack of inversion symmetry in their crystal structure have recently been proposed as systems hosting an unconventional and other topologically nontrivial superconducting states, which could pave their application for the fabrication of novel devices for superconducting spintronics and quantum computing. Moved by these motivations, we have investigated the transport and spectroscopic properties of the non-centrosymmetric superconductor Nb0.18Re0.82 down to the 2D limit. Hall transport measurements in the normal state and tunnelling spectroscopic experiments reveal the emergence of a complex physical behaviour, which suggests the existence of a superconducting order parameter with unconventional properties.

TT 19.2 Thu 11:30 H6

Spatially intertwined superconductivity and charge order in 1T-TaSSe revealed by scanning tunnelling spectroscopy — •Yaroslav Gerasimenko[1,2], Marion van Midden[2], Erik Zupanic[2], Petra Sutar[2], Zvonko Jaglicic[3], and Dragan Mihailovic[2,3] — [1]University of Regensubrg, Regensburg, Germany — [2]Jozef Stefan Institute, Ljubljana, Slovenia — [3]Univeristy of Ljubljana, Ljubljana, Slovenia

The interplay of different emergent phenomena - superconductivity (SC) and domain formation - appearing on different spatial and energy scales are investigated using high-resolution scanning tunnelling spectroscopy in the prototypical transition metal dichalcogenide superconductor 1T-TaSSe single crystals ($T_{SC} = 3.5$ K) at temperatures from 1 to 20 K. Our major observation is that while the SC gap size smoothly varies on the scale of $\lesssim 10$ nm, its spatial distribution is not correlated to the domain structure. On the other hand, there is statistically significant correlation of the SC gap Δ_{SC} with spectral weight of the narrow band at the Fermi level formed from the same Ta $5d$ orbitals as the Mott-Hubbard band. We show that the narrow band follows the evolution of Hubbard bands in space, proving unambiguously its relation to the charge order. The correlations between the two suggest a non-trivial link between rapidly spatially varying charge order and superconductivity common in many quantum materials, and high-temperature superconductors in particular.

TT 19.3 Thu 11:45 H6

Angular dependence of the superconductivity in $CeRh_2As_2$ — •Javier Landaeta[1], Pavlo Khanenko[1], Jacinta Banda[1], Ilya Sheikin[2], Sanu Mishra[2], Seunghyun Khim[1], Manuel Brando[1], Christoph Geibel[1], and Elena Hassinger[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Univ. Grenoble Alpes, CNRS, LNCMI EMFL, F-38042 Grenoble, France

$CeRh_2As_2$ is an unconventional superconductor with multiple superconducting phases. When $\mu_0 H \parallel c$, this material shows a field-induced transition from a low-field superconducting state SC1 to a high-field SC2 with critical field H_{c2} = 14 T and T_c = 0.26 K. For $\mu_0 H \parallel ab$, only the SC1 with H_{c2} = 2 T is observed. The phase-diagrams and their anisotropy might be explained by the influence of Rashba-spin-orbit coupling at the Ce sites where the inversion symmetry is broken locally. Above T_c, a possibly quadrupolar phase is present at $T_0 \approx 0.4$ K, whose influence on the superconducting state remains unknown. Here, we present a comprehensive study of the angular dependence of the upper critical fields and T_0 using low temperature magnetic ac susceptibility, specific heat and torque in single crystalline $CeRh_2As_2$. The SC2 state is strongly suppressed when rotating the magnetic field away from the c-axis and disappears for an angle of 35°. We find that the H_{c2} of SC2 for angles departing from the c axis is attained when the in-plane component of the field reaches the in-plane Pauli limit. This result corroborates idea that the field-induced state SC2 is an odd-parity state with a d-vector in the plane in $CeRh_2As_2$.

TT 19.4 Thu 12:00 H6

Twisted Superconductivity in the high magnetic field phase of $CeRh_2As_2$ — •Aline Ramires[1] and David Möckli[2] — [1]Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [2]Instituto de Física, Universidade Federal do Rio Grande do Sul, 91501-970 Porto Alegre, Brazil

$CeRh_2As_2$, a locally noncentrosymmetric heavy fermion material, was recently reported to host a remarkable magnetic field versus temperature phase diagram with two superconducting phases and upper critical fields much above the Pauli limit [1]. In this material, the two inequivalent Ce sites per unit cell, related by inversion symmetry, introduce a sublattice structure corresponding to an extra internal degree of freedom. In this talk, I briefly review some mechanisms that allow for Pauli limit violation and discuss what properties of the normal state are key for the development of a superconducting state robust against magnetic fields. I discuss intra-sublattice and inter-sublattice pairing scenarios and how we can construct superconducting states that violate the Pauli limit by twisting the most stable superconducting state with respect to the internal sublattice degree of freedom [2]. I will also comment on ongoing work that highlights the role of normal state electronic structure parameters, as well as effects of impurities, and subleading instabilities in the phase diagram of this material [3].

[1] S. Khim *et al.*, arXiv:2101.09522 (2021)
[2] D. Möckli and A. Ramires, Phys. Rev. Research **3**, 023204 (2021)
[3] D. Möckli and A. Ramires, arXiv:2107.09723 (2021)

TT 19.5 Thu 12:15 H6

Nematicity and checkerboard order in the surface layer of Sr_2RuO_4 — •Carolina A. Marques[1], Luke C. Rhodes[1], Rosalba Fittipaldi[2], Veronica Granata[3], Chi Ming Yim[1], Renato Buzio[2], Andrea Gerbi[2], Antonio Vecchione[2], Andreas W. Rost[1,4], and Peter Wahl[1] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, UK. — [2]CNR-SPIN, Italy. — [3]Dipartimento di Fisica, Università di Salerno, Italy. — [4]Max-Planck-Institute for Solid State Research, Stuttgart, Germany.

Superconductivity in strongly correlated systems is often found near exotic electronic phases, such as antiferromagnetism and electronic nematicity. These phases can be highly sensitive to minor changes in the crystal structure, induced by doping or strain. In the unconventional superconductor Sr_2RuO_4, a 6° rotation of the RuO_6 octahedra at the surface seems to suppress its superconducting state and pushes a van Hove singularity below the Fermi energy. Using ultra-low temperature Scanning tunnelling microscopy, we study the low energy electronic properties of the reconstructed surface of Sr_2RuO_4[1]. Our measurements show clear signatures of C_4 symmetry breaking, together with the appearance of a checkerboard order, associated with a peak in the tunnelling spectrum, which splits in a magnetic field, revealing a charge nature. Tight binding calculations show that a nematic order parameter coexisting with a charge modulation reproduces the observed low energy density of states. Understanding the underlying physics at this surface provides a new platform to study the strongly correlated phases of Ruthenate materials.

[1] Adv. Mat. 2100593 (2021)

TT 19.6 Thu 12:30 H6

Quasiparticle Interference of the van-Hove singularity in Sr_2RuO_4 — •Andreas Kreisel[1], Carolina A. Marques[2], Luke C. Rhodes[2], Xiangru Kong[3], Tom Berlijn[3], Rosalba Fittipaldi[4], Veronica Granata[5], Antonio Vecchione[4], Peter Wahl[2], and Peter J. Hirschfeld[6] — [1]Institut für Theoretische Physik, Universität Leipzig — [2]SUPA, University of St Andrews,UK — [3]CNMS, Oak Ridge National Laboratory, USA — [4]CNR-SPIN, UOS Salerno, Italy — [5]Dipartimento di Fisica, Università di Salerno, Italy — [6]Department of Physics, University of Florida, USA

The single-layered ruthenate Sr_2RuO_4 is one of the most enigmatic unconventional superconductors. While for many years it was thought to be the best candidate for a chiral p-wave superconducting ground state, desirable for topological quantum computations, recent experiments suggest a singlet state, ruling out the original p-wave scenario. The superconductivity as well as the properties of the multi-layered compounds of the ruthenate perovskites are strongly influenced by a van Hove singularity in proximity of the Fermi energy. Tiny structural distortions move the van Hove singularity across the Fermi energy with dramatic consequences for the physical properties. Here, we determine the electronic structure of the van Hove singularity in the surface layer of Sr_2RuO_4 by quasiparticle interference imaging. We trace its dispersion and demonstrate from a model calculation accounting for the full vacuum overlap of the wave functions that its detection is facilitated through the octahedral rotations in the surface layer.

TT 20: Quantum Dots and Wires (joint session HL/TT)

Time: Thursday 13:30–16:30 Location: H4

See HL 18 for details of this session.

TT 21: Focus Session: Topological Kagome Metals

The peculiar nature of the kagome lattice known to give rise exotic quantum states. When mixed with the itinerant character of the carriers, theoretically, it is predicted to host dispersionless electronic flat bands along with the linearly dispersing Dirac bands allowing one to bring together the topologically nontrivial states and the electronic correlations that lie at the center of condensed matter physics due to their roles in variety of novel quantum phenomena, such as unconventional superconductivity, heavy-fermion physics, Mott insulator states, etc. Recently, the experimental efforts caught with the predictions and several compounds are proposed as promising kagome metals, where one can realize the peculiar kagome physics in the real-world environment.

Organizers: Ece Uykur and Martin Dressel (Stuttgart University)

Time: Thursday 13:30–16:00 Location: H7

Invited Talk TT 21.1 Thu 13:30 H7

A new class of charge density wave superconductors in the topological kagome metals AV_3Sb_5 (A=K, Rb, Cs) — •Stephen Wilson — Materials Department, University of California Santa Barbara

Kagome metals are compelling materials platforms for hosting electronic states that feature an interplay between topologically nontrivial electronic states and correlated electron phenomena. These two features can, for instance, arise from the Dirac points, flatbands, and saddle-points endemic to the kagome lattice type in simple tight-binding models. Recently in this field, the discovery of a new class of kagome metals of the form AV_3Sb_5 with A=K, Cs, or Rb has provided a unique setting for exploring the interplay between Z_2 electronic topology and intertwined charge density wave and superconducting orders. These metals realize a kagome lattice of nonmagnetic vanadium ions with an electron-filling that populates saddle-points and their corresponding van Hove singularities in the electronic density of states near the Fermi level. Nesting effects in this setting are predicted to stabilize a variety of unusual states, ranging from charge density wave order that breaks time reversal symmetry to unconventional superconductivity. Here I will present some of our recent work exploring the phase transitions and broken symmetries in these materials. Particular attention will be given to the nature of the charge density wave instability.

TT 21.2 Thu 14:00 H7

Kagome metals — •Ronny Thomale — Theoretische Physik I, Julius-Maximilians-Universität Würzburg

The recent discovery of AV_3Sb_5 (A=K,Rb,Cs) has uncovered an intriguing arena for exotic Fermi surface instabilities in kagome metals. Aside from charge density wave order, a multi-dome superconducting phase is found, with strong indications to be of unconventional origin. We find that the sublattice interference mechanism is necessary and sufficient to uncover the nature of unconventional particle-hole and particle-particle pairing in the V net kagome metals. We predict a Peierls-type charge density wave with finite relative angular momentum and orbital current formation. With regard to the possible nature of unconventional pairing, we find a rich phase diagram depending on the range of the screened electronic interactions, the multi-orbital content, and the location of multiple van Hove singularities with respect to the Fermi level. Combined, kagome metals open a new domain of unconventional electronic order, unfolding a plethora of fascinating experimental and theoretical investigations.

TT 21.3 Thu 14:15 H7

Kagome and non-kagome physics of AV_3Sb_5 — •Alexander A. Tsirlin — EP VI, EKM, University of Augsburg, Germany

Layered compounds AV_3Sb_5 (A = K, Rb, Cs) are non-magnetic kagome metals with an intricate coexistence of and competition between superconducting and charge-density-wave (CDW) instabilities. In this talk, I will present our recent study of these compounds via x-ray diffraction, density-functional calculations, and broadband optical spectroscopy, with a focus on delineating between the roles of vanadium kagome planes and Sb atoms that encompass these planes. The following aspects will be addressed: i) band saddle points in the vicinity of the Fermi level and their positions depending on the A atom; ii) possible structures of the CDW state; iii) electronic and structural mechanisms of stabilizing the CDW; iv) evolution of crystal and electronic structures under pressure where re-entrant superconductivity has been observed. I will argue that both CDW formation in and pressure evolution of AV_3Sb_5 are strongly influenced by the Sb atoms that should be deemed an integral part of these kagome metals.

15. min. break

TT 21.4 Thu 14:45 H7

Study on the Magnetic Weyl Semimetal Phase in Kagome Lattice, $Co_3Sn_2S_2$ — •Defa Liu — Max Planck Insititute of Microstructure Physics

Materials with kagome lattice attract lots of investigations recently as they can realize many exotic phases and properties, such as the existence of flat band,superconductivity, CDW order, topological Dirac semimetal and Weyl semimetal phases, which can provide an ideal platform to study the interplay between them. Among the kagome materials, the ferromagnetic $Co_3Sn_2S_2$ has many exotic physical properties, such as the large anomalous Hall effect (AHE) and the anomalous Nernst effect (ANE). And also $Co_3Sn_2S_2$ is the first experimentally confirmed magnetic Weyl semimetal. In this talk, I will introduce how to use the angle-resolved photoemission spectroscopy (ARPES) to confirm the magnetic Weyl semimetal phase in $Co_3Sn_2S_2$, including the observation of the surface Fermi arcs and bulk Weyl point [1], the observation of the spin-orbit coupling (SOC) effect [2], and the observation of the topological phase transition in $Co_3Sn_2S_2$ [3]. These results not only can help to understand the formation mechanism of the Weyl semiemtal phase and the large anomalous Hall effect (AHE) and the anomalous Nernst effect (ANE) in $Co_3Sn_2S_2$, but also provide insights into the interplay between the magnetism and the topology.

[1] D.F. Liu et al., Science 365, 1282-1285 (2019)
[2] D.F. Liu et al., arXiv: 2103.08113
[3] D.F. Liu et al., arXiv: 2106.03229

TT 21.5 Thu 15:15 H7

Optical investigations of *Re*Mn_6Sn_6 kagome metals — •Maxim Wenzel[1], Olga Iakutkina[1], Hechang Lei[2], Martin Dressel[1], and Ece Uykur[1] — [1]1. Physikalisches Institut, Universität Stuttgart, D-70569 Stuttgart, Germany — [2]Department of Physics, Renmin University of China, 100872 Beijing, China

Magnetic kagome metals became model compounds for exploring the interplay between strong electronic correlations and magnetism along with topologically non-trivial states. Consisting of magnetic kagome planes along with the itinerant carriers, they ought to possess Dirac Fermions, flat bands and saddle points in the vicinity of the Fermi energy, E_F. The rare earth kagome metal series, $ReMn_6Sn_6$ (Re = Gd, Tb, Y) opens a new way for further investigations of the influence of magnetism on the electronic properties. While the crystal structure does not differ significantly, the underlying magnetic structure strongly depends on the rare earth element separating the Mn-kagome layers. Here, we report temperature-dependent optical spectroscopy study on series of $ReMn_6Sn_6$ compounds in a broad frequency range of 50 - 18000 cm^{-1} down to $T = 10$ K. The optical signatures of the strongly correlated flat bands and the Dirac fermions are comparatively discussed.

TT 21.6 Thu 15:30 H7

Polarization dependent localization in layered kagome metal FeSn — •Ananya Biswas[1], Frederik Bolle[1], Olga Iakutkina[1], Hechang Lei[2], Yoshichika Onukio[3], Martin Dressel[1], and Ece Uykur[1] — [1]1. Physikalisches Institut, Universität Stuttgart, D-70569 Stuttgart, Germany — [2]Department of Physics, Renmin University of China, 100872 Beijing, China — [3]Faculty of Science, University of Ryukyus, Japan

The roots of coexistence of Dirac bands and flat bands (from extended Hubbard Model) in kagome metals holds immense significance to study correlated electron systems. Antiferromagnetic FeSn is an ideal 2D kagome lattice having its Néel temperature T_N=370K. Moments of Fe atoms are ferromagnetically ordered within the Fe-Sn kagome planes, which are separated by Sn layers along c direction where each layer is coupled antiferromagtically to the adjacent kagome planes. Thus, FeSn provides ideal platform of polarization dependent investigation based on isolated and spatially decoupled kagome planes of 2D kagome network in bulk crystals. We investigated polarization effect of low energy dynamics in FeSn through infrared spectroscopy down to 10K. Results show two distinct carriers along kagome plane, which can be realized by Drude like free carrier contribution and a pronounced localization peak. Furthermore, a more coherent transport across kagome plane is reflected in our polarization dependent optical studies.

TT 21.7 Thu 15:45 H7

Nature of unconventional pairing in the kagome superconductors AV_3Sb_5 — •Xianxin Wu[1], Tilman Schwemmer[2], Tobias Müller[2], Armando Consiglio[2], Giorgio Sangiovanni[2], Domenico Di Sante[3], Yasir Iqbal[4], Werner Hanke[2], Andreas P. Schnyder[1], M. Michael Denner[5], Mark H. Fischer[5], Titus Neupert[5], and Ronny Thomale[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]University of Würzburg, Würzburg, Germany — [3]University of Bologna, Bologna, Italy — [4]Indian Institute of Technology Madras, Chennai, India — [5]University of Zurich, Zurich, Switzerland

The recent discovery of AV_3Sb_5 (A=K,Rb,Cs) has uncovered an intriguing arena for exotic Fermi surface instabilities in a kagome metal. Among them, superconductivity is found in the vicinity of multiple van Hove singularities, exhibiting indications of unconventional pairing. We show that the sublattice interference mechanism is central to understanding the formation of superconductivity in a kagome metal. Starting from an appropriately chosen minimal tight-binding model with multiple van Hove singularities close to the Fermi level for AV_3Sb_5, we provide a random phase approximation analysis of superconducting instabilities. Non-local Coulomb repulsion, the sublattice profile of the van Hove bands, and the interaction strength turn out to be the crucial parameters to determine the preferred pairing symmetry. Implications for potentially topological surface states are discussed, along with a proposal for additional measurements to pin down the nature of superconductivity in AV_3Sb_5.

TT 22: Poster Session: Disordered and Granular Superconductors: Fundamentals and Applications in Quantum Technology

Time: Thursday 13:30–15:30 Location: P

TT 22.1 Thu 13:30 P

Superinsulators: "localization" and granularity without disorder — •cristina diamantini[1] and carlo trugenberger[2] — [1]Department of Physics and Geology, University of Perugia, via Pascoli snc, Perugia, Italy — [2]SwissScientific Technologies SA, rue du Rhone 59, Geneva, Switzerland

It is often believed that suppression of transport in condensed matter systems requires many-body localization (MBL) by strong disorder. There is by now, however a vast body of literature showing that this is not the case: MBL-like phenomena can arise in absence of disorder by confinement, the phenomenon preventing quarks to "exit" from protons. I will discuss the example of the superinsulators, a new state of matter where condensation of magnetic monopole instantons generates an "endogenous emergent disorder" leading to an infinite resistance (even at finite temperatures) by the confinement of electric charge, Cooper pairs playing the role of quarks. The granularity of these materials around the superconductor-to-superinsulator transition is also emergent, due to the competition of two quantum phase transitions and is not due to disorder. I will present recent experimental evidence that rules out disorder-driven MBL as a cause of the infinite resistance, while confirming its endogenous instanton origin.

TT 22.2 Thu 13:30 P

Collective excitations in weakly-coupled disordered superconductors — •Bo Fan[1], Abhisek Samanta[2], and Antonio Miguel Garcia-Garcia[1] — [1]Shanghai Center for Complex Physics, School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China — [2]Physics Department, Technion, Haifa 32000, Israel

Isolated islands in two-dimensional strongly-disordered and strongly-coupled superconductors become optically active inducing sub-gap collective excitations in the ac conductivity. Here, we investigate the fate of these excitations as a function of the disorder strength in the experimentally relevant case of weak electron-phonon coupling. An explicit calculation of the ac conductivity, that includes vertex corrections to restore gauge symmetry, reveals the existence of collective sub-gap excitations, related to phase fluctuations and therefore identified as the Goldstone modes, for intermediate to strong disorder. As disorder increases, the shape of the sub-gap excitation transits from peaked close to the spectral gap to a broader distribution reaching much smaller frequencies. Phase-coherence still holds in part of this disorder regime. The requirement to observe sub-gap excitations is not the existence of isolated islands acting as nano-antennas but rather the combination of a sufficiently inhomogeneous order parameter with a phase fluctuation correlation length smaller than the system size. Our results indicate that, by tuning disorder, the Goldstone mode may be observed experimentally in metallic superconductors based for instance on Al, Sn, Pb or Nb.

TT 22.3 Thu 13:30 P

Andreev bound states in disordered superconductors — •Idan Tamir — FU Berlin

At strong enough disorder, superconductivity losses its uniformity and exhibits local gap variations. These are considered a precursor for the eventual breakdown of superconductivity. Using high resolution tunneling spectroscopy to locally study amorphous superconducting films, we observe an abundance of sharp in-gap excitations. We relate these excitations to Andreev bound states induced by either large superconducting gap variations or the interaction with native magnetic impurities. Both possibilities are not accommodated in current theoretical models.

TT 22.4 Thu 13:30 P

Dielectric properties of amorphous indium oxide on the insulating side of the superconductor-insulator transition — Nikolaj Ebensperger[1], Paul Kugler[1], •Anastasia Bauernfeind[1], Martin Dressel[1], Benjamin Sacépé[2], Mikhail Feigel'man[3], and Marc Scheffler[1] — [1]1. Physikalisches Institut, University of Stuttgart, Stuttgart, Germany — [2]Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, Grenoble, France — [3]L.D. Landau Institute for Theoretical Physics, Chernogolovka, Russia

Amorphous indium oxide (a:InO) plays a prominent role in the study of strongly disordered superconductors. In particular, the disorder-driven transition (SIT) between superconducting and insulating states can be realized. Compared to the superconducting side of the SIT, the insulating side has been explored much less experimentally due to the lack of appropriate experimental means. Here we present dielectric measurements on insulating a:InO, performed at GHz frequencies and at temperatures down to the mK regime, on a set of samples with varying disorder. We obtain the real and imaginary parts of the dielectric function (corresponding to frequency-dependent conductivity) as function of disorder, temperature, and frequency. We analyse these data based on theory for hopping in disordered systems, and we trace the evolution of the dielectric function, e.g. the increase of its real part upon approaching the SIT.

TT 22.5 Thu 13:30 P

Decoupling of superconducting layers in $[(SnSe)_{1+\delta}]_n[NbSe2]_m$ ferecrystals — •O. Chiatti[1], K. Mihov[1], M. Trahms[1], T. Griffin[1], C. Grosse[1], D. Hamann[2], K. Hite[2], M. B. Alemayehu[2], D. C. Johnson[2], and S. F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Solid State Chemistry, University of Oregon, Eugene, OR, USA

Van-der-Waals superlattices with two-dimensional (2D) superconducting layers of a transition-metal dichalchogenide (TMD) embedded between other materials have recently received a lot of attention [1]. Embedding the TMD layers protects them from exposure to air and makes it possible to observe 2D superconductivity. Here, we examine $[(SnSe)_{1+\delta}]_n[NbSe2]_m$ ferecrystals [2] with $n = 1$ and varying m. The ferecrystals are stacks of polycrystalline layers grown with atomic layer precision, but without an epitaxial relationship between the layers [2]. For $m \leq 9$ we observe a superconducting phase below a critical temperature, which decreases with increasing distance between the $NbSe_2$ monolayers. For $m \geq 9$ an insulating behavior is observed. The Ginzburg-Landau (GL) coherence lengths are determined from the upper critical magnetic fields. The perpendicular GL coherence length decreases with increasing distance between the $NbSe_2$ monolayers, indicating a decoupling of the superconducting layers [3].

[1] A. Devarakonda *et al.*, Science **370**, 231 (2020)
[2] C. Grosse *et al.*, Sci. Rep. **6**, 33457 (2016)
[3] M. Trahms *et al.*, Supercond. Sci. Technol. **31**, 065006 (2018)

TT 22.6 Thu 13:30 P

Resonant microwave spectroscopy close to the superconductor to insulator transition — •Maximilian Kristen[1,2], Jan Nicolas Voss[2], Micha Wildermuth[2], Yannick Schön[2], Andre Schneider[2], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2,3,4] — [1]Institut für QuantenMaterialien und Technologien (IQMT), Karlsruher Institut für Technologie — [2]Physikalisches Institut, Karlsruher Institut für Technologie — [3]Russian Quantum Center, Skolkovo, Moscow, Russia — [4]National University of Science and Technology MISIS, Moscow, Russia

High kinetic inductance circuits in the vicinity of the superconductor to insulator transition (SIT) are an interesting research topic not only for applications like quantum circuits or detectors, where the SIT poses a limit on the maximum available kinetic inductance of a wire, but also as a tool to study fundamental aspects of superconductor physics.

We perform microwave measurements on resonators made from highly resistive films. As a material of choice, we use granular aluminum at high oxide levels, due to the low intrinsic loss and the possibility to approach the SIT from the superconducting side. We focus on the low frequency noise behavior of these resonators and present the latest experimental results

TT 22.7 Thu 13:30 P

Growth of superconducting granular aluminum films on cryogenically cooled substrates — •Aniruddha Deshpande, Jan Pusskeiler, Martin Dressel, and Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany

Granular aluminum (grAl) consisting of nanometer-sized aluminum grains separated by aluminum oxide has peculiar superconducting properties. The critical temperature can be substantially enhanced compared to pure bulk aluminum up to 3.7K and the low superfluid density of grAl is promising for applications in quantum circuits. The material properties of grAl can be tuned during thin-film growth by parameters such as oxygen pressure and substrate temperature. Here we use thermal evaporation of aluminum and deposition in low-pressure oxygen environment onto cryogenically cooled substrates to reduce the grain size compared to room-temperature growth, and we characterize the grAl films for their temperature-dependent sheet resistance and their superconducting critical temperature.

TT 22.8 Thu 13:30 P

Modified properties of disordered superconducting films with amorphous and granular structure — •Mariia Sidorova[1,2], Alexej Semenov[1], Stephan Steinhauer[3], Samuel Gyger[3], Val Zwiller[3], Xiaofu Zhang[4], Andreas Schilling[4], and Heinz-Wilhelm Hübers[1,2] — [1]DLR, Institute of Optical Sensor Systems, Berlin, Germany — [2]Humboldt-Universität zu Berlin, Berlin, Germany — [3]KTH Royal Institute of Technology, Stockholm, Swede — [4]University of Zürich, Zürich, Switzerland

Thin disordered superconducting films are intensively exploited in various superconducting devices, for instance, superconducting single-photon detectors (SSPDs) and hot-electron bolometers (HEBs). The dimensionality of such films usually duffers with respect to various physical phenomena, for instance, it is two-dimensional (2d) to superconductivity and weak localization, three-dimensional (3d) to normal conduction, and approach a 2d-3d crossover with respect to phonons. Properties of low-dimensional systems differ from bulk materials and their either theoretical or empirical description remains very limited.

We have studied several superconducting films with thicknesses below 10 nm and different morphology: amorphous WSi and polycrystalline granular NbN and NbTiN. Employing magnetoconductance and calorimetric measurements, we derived an electron-phonon scattering rate and determined sound velocities and phonon heat capacities. Our results indicate a systematic reduction of the sound velocity in all films as compared to the corresponding bulk crystalline material, and a significant impact of the film morphology on the phonon heat capacity.

TT 22.9 Thu 13:30 P

Multifractal correlations of the local density of states in dirty superconducting films — •Matthias Stosiek — Sophia University, Physics Division, Tokyo, Japan

Mesoscopic fluctuations of the local density of states encode multifractal correlations in disordered electron systems. We study fluctuations of the local density of states in a superconducting state of weakly disordered films. We perform numerical computations in the framework of the disordered attractive Hubbard model on two-dimensional square lattices. Interactions are taken into account within mean-field approximation. Our numerical results are explained by an analytical theory. The numerical data and the theory together form a coherent picture of multifractal correlations of the local density of states in weakly disordered superconducting films. [1]

[1] M. Stosiek, F. Evers, I. S. Burmistrov, arXiv:2107.06728 (2021)

TT 23: Poster Session: Emerging Phenomena in Superconducting Low Dimensional Hybrid Systems

Time: Thursday 13:30–15:30 Location: P

TT 23.1 Thu 13:30 P

Electronic structure and charge density wave order in monolayer NbS_2 — •Timo Knispel[1], Jeison A. Fischer[1], Jan Berges[2], Arne Schobert[2], Erik van Loon[2,3], Wouter Jolie[1], Daniela Mohrenstecher[1], Tim Wehling[2], and Thomas Michely[1] — [1]Institute of Physics II, University of Cologne, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Institut für Theoretische Physik, Bremen Center for Computational Materials Science and MAPEX Center for Materials and Processes, Otto-Hahn-Allee 1, University of Bremen, 28359 Bremen, Germany — [3]Department of Physics, Lund University, Professorsgatan 1, 223 63, Lund, Sweden

We investigated monolayer 1H-NbS_2 grown in-situ on graphene/Ir(111) by high-resolution scanning tunneling microscopy and spectroscopy at temperatures down to 0.4K. The characteristic 3x3 CDW pattern is present only in the monolayer, but absent in the bilayer. We analyze the CDW gap, contrast inversion in the dI/dV maps towards both sides of the gap and the suppression of the CDW pattern in the gap. Furthermore, quasiparticle interference is observed at island edges and defects and enables us to measure the dispersion of the hole-like pocket around the Γ-point. Density of states, dispersion around the Γ-point and the properties of the CDW are compared to density functional theory calculations.

Support from the Deutsche Forschungsgemeinschaft, CRC 1238 (project number 277146847, subprojects A01 and B06) is gratefully acknowledged.

TT 23.2 Thu 13:30 P

Dynamics of collective modes in an unconventional charge density wave system $BaNi_2As_2$ — •Amrit raj Pokharel[1], Vladimir Grigorev[1], Arjan Mejas[2], Amir a. Haghighirad[3], Rolf Heid[3], Yi Yao[3], Michael Merz[3], Matthieu Le tacon[3], and Jure Demsar[1] — [1]Institute of Physics, JGU Mainz, Mainz, Germany — [2]Institute of Solid State Physics, TU Wein, Vienna, Austria — [3]Institute of Quantum Materials and Technologies, KIT, Karlsruhe, Germany

$BaNi_2As_2$ is a non-magnetic analogue of $BaFe_2As_2$, the parent compound of a prototype pnictide high temperature superconductor displaying superconductivity already at ambient pressure. Recent diffraction studies demonstrated the existence of two types of periodic lattice distortions above and below the triclinic phase transition, suggesting the existence of an unconventional charge-density-wave (CDW) order. Upon doping, CDW order is suppressed, resulting in a six-fold increase of the superconducting transition temperature and enhanced nematic fluctuations. Here, we apply time-resolved optical spectroscopy to investigate collective response of the CDWs in $BaNi_2As_2$. By performing temperature and excitation density dependent studies we demonstrate the existence of collective modes of the CDW order. The smooth evolution of these modes through the structural phase transition implies the CDW order in the triclinic phase evolves from the unidirectional CDW in the tetragonal phase and may indeed trigger the structural phase transition.

[1] V. Grigorev, et. al., arXiv:2102.09926 (2021)

TT 23.3 Thu 13:30 P

Electronic phase diagram of the excitonic insulator candidates $Ta_2Ni(Se_{1-x}S_x)_5$ — •Pavel Volkov[1], Mai Ye[1], Himanshu Lohani[2], Irena Feldman[2], Amit Kanigel[2], and Girsh Blumberg[1,3] — [1]Rutgers University — [2]Technion — [3]NICPB, Tallin

Excitonic insulator is a phase driven by Coulomb attraction between electrons and holes leading to a proliferation of particle-hole pairs. However, excitonic insulators break lattice symmetries, raising the question of whether a particular transition is excitonic or structural. I will demonstrate that electronic Raman scattering can be used to elucidate the transition origin in the $Ta_2Ni(Se_{1-x}S_x)_5$ family of candidate materials. In particular, at low x the transition is excitonic-driven and shows deviations from mean-field predictions indicating strong correlations. At large sulfur content, the contribution of excitons diminishes and the transition becomes purely structural. The study reveals a quantum phase transition of an excitonic insulator masked by a preemptive structural order.

TT 24: Poster Session: Transport

Time: Thursday 13:30–16:00 Location: P

TT 24.1 Thu 13:30 P

Efficient steady-state solver for the hierarchical equations of motion approach: formulation and application to charge transport through nanosystems — •Christoph Kaspar and Michael Thoss — University of Freiburg

We present an iterative algorithm [1] to efficiently solve the hierarchical equations of motion (HEOM) [2,3] for the steady-state of open quantum systems. The approach reduces the computational resources required by traditional steady-state solvers, in particular for larger systems or the low temperature regime. It uses the method of matrix equations in combination with a efficient preconditioning technique and a hierarchy truncation scheme. We illustrate the numerical performance of the method by applications to models of charge transport in single-molecule junctions.

[1] Kaspar *et al.*, J. Phys. Chem. A **125**, 23, 5190-5200 (2021)
[2] Jin *et al.*, J. Chem. Phys. **128**, 234703 (2008)
[3] Tanimura, J. Chem. Phys. **153**, 020901 (2020)

TT 24.2 Thu 13:30 P

Spin-orbit interaction induces charge beatings in a lightwave-STM – single molecule junction — •Moritz Frankerl and Andrea Donarini — Institute for Theoretical Physics, University of Regensburg, 93049 Regensburg, Germany

Experiments based on lightwave-STM have shown how to obtain both space and time resolution of single molecule vibrations on their intrinsic length and time scales [1]. We investigate theoretically the electronic dynamics of a copper-phthalocynanine in a lightwave-STM by simulating the full pump-probe cycle [2]. Beatings in the transferred charge reveal the intertwined spin and orbital dynamics, modulated by a tip induced exchange field [3]. We study the dynamics directly in the time domain within a generalized master equation approach. A deeper understanding of our numerical results is obtained via coupled Bloch like equations for the molecular spin and pseudospin [4].

[1] T. L. Cocker et al., Nature 539, 263-267 (2016)
[2] M. Frankerl et al, Phys. Rev. B 103, 085420 (2021)
[3] M. Braun et al., Phys. Rev. B 70, 195345 (2004)
[4] M. Maurer et al., Phys. Rev. Research 2, 033440 (2020)

TT 24.3 Thu 13:30 P

Pseudospin resonances reveal synthetic spin-orbit interaction — •Christoph Rohrmeier and Andrea Donarini — Institute of Theoretical Physics University of Regensburg, Regensburg, Germany

The interplay between interference and interaction produces several effects in degenerate quantum systems, including spin torques [1], dark states formation [2] and multilevel coherences [3]. In this context, a spin resonance without spin splitting has been first predicted for a single quantum dot spin valve [4]. We investigate a spinful double quantum dot coupled to leads in a pseudospin valve configuration. We predict in the stability diagram a rich variety of current resonances which are modulated by the system parameters [5]. In the presence of ferromagnetic leads and pseudospin anisotropy, those resonances split, turn into dips, and acquire a Fano shape, thus revealing a synthetic spin-orbit interaction induced on the double quantum dot. A set of rate equations derived for a minimal model captures those features. The model accurately matches the numerical results obtained for the full system in the framework of a generalized master equation and calculated within the next to leading order approximation.

[1] M. Braun et al., Phys. Rev. B 70, 195345 (2004)
[2] A. Donarini et al., Nature Comm. 10, 381 (2019)
[3] M. Maurer et al., Phys. Rev. Research 2, 033440 (2020)
[4] M. Hell et al., Phys. Rev. B 91, 195404 (2015)
[5] C. Rohrmeier et al., Phys. Rev. B 103, 205420 (2021)

TT 24.4 Thu 13:30 P

Feynman-Vernon influence functional approach to quantum transport in interacting nanojunctions: An analytical hierarchical study — •Luca Magazzu and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We present a nonperturbative and formally exact approach for the charge transport in interacting nanojunctions based on the Feynman-Vernon influence functional. By borrowing the nomenclature of the famous spin-boson model, we parametrize the two-state dynamics of each single-particle fermionic degree of freedom, in the occupation number representation, in terms of blips and sojourns. We apply our formalism to the exactly solvable resonant level model (RLM) and to the single-impurity Anderson model (SIAM), the latter being a prototype system for studying strong correlations. For both systems, we demonstrate a hierarchical diagrammatic structure. While the hierarchy closes at the second-tier for the RLM, this is not the case for the interacting SIAM. Upon inspection of the current kernel, known results from various perturbative and nonperturbative approximation schemes to quantum transport in the SIAM are recovered. Finally, a novel noncrossing approximation for the hierarchical kernel is developed, which enables us to systematically decrease temperature at each next level of the approximation.

[1] arXiv:2104.14497 (2021)

TT 24.5 Thu 13:30 P

An Atomistic Study of the Thermoelectric Signatures of CNT Peapods — •Alvaro Gaspar Rodriguez Mendez[1,2], Leonardo Medrano Sandonas[3], Arezoo Dianat[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Tu Dresden, 01062 Dresden, Germany. — [2]Max Planck Institute for Complex Systems, 01187 Dresden, Germany. — [3]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg.

Carbon-based nanomaterials have a great potential for the development of high performance thermoelectric (TE) materials because of their low-cost and for being environmentally friendly. Carbon nanotubes have, however, high electrical and thermal conductivities so that further nanoscale engineering is required to exploit them as TE materials. We investigate electron and phonon transport in CNT peapods to elucidate their potential advantage over pristine CNTs. We show their transport properties are sensitively modified by C60 encapsulation, when the CNT-C60 intermolecular interaction is strong enough to produce a periodic buckling of the CNT walls. Moreover, the phonon transmission is strongly suppressed at low and high frequencies, leading to a reduction of the phonon contribution to the overall thermal conductance, similar effect observed in recently proposed phononic metamaterials. We obtain in general a larger TE figure of merit over a broad temperature range for the CNT peapod when compared with the pristine CNT. Our findings show an alternative route for the enhancement of the TE performance of CNT-based devices.

TT 24.6 Thu 13:30 P

Evolution of Molecular Binding in Mechanically Controlled Break-Junctions — •Lokamani Lokamani[1,3], Florian Günther[2], Filip Kilibarda[3], Jeffrey Kelling[1], Guido Juckeland[1], Artur Erbe[3], and Sibylle Gemming[4] — [1]Department of Information Services and Computing, HZDR, Dresden, Germany — [2]Instituto de Física de São Carlos, Universidade de São Paulo, Brazil — [3]Department of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [4]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany

Electrical properties of single molecules can be investigated with extreme precision using atomically sharp metallic electrodes in mechanically controllable break junctions (MCBJs). The current-voltage (IV) characteristics in such junctions are considerably affected by the binding positions of the anchoring groups on the tip-facets and the configuration of the molecule. Hence, characterizing the electronic transport properties during a single tip-tip opening provides interesting insights into the tip-molecule interaction.

Here, we present a novel high-throughput approach to reproduce the time evolution of the electronic transport characteristics. We performed transport calculations using the self-consistent charge scheme of the density-functional-based tight binding approach and the Green's function formalism. In particular, we evaluated the energy level and the coupling of the dominating transport channel using the single level model. In contrast to standard approaches, we consider many thermodynamically relevant configurations.

TT 24.7 Thu 13:30 P

Revealing channel polarization of atomic contacts of ferromagnets and strong paramagnets by shot-noise measurements — Martin Prestel, •Marcel Strohmeier, Wolfgang Belzig, and Elke Scheer — University of Konstanz, 78457 Konstanz, Germany

We report measurements of the shot noise of atomic contacts using the mechanically controllable break junction (MCBJ) technique at low temperatures. In accordance with theoretical predictions [1, 2] single-atom contacts of the ferromagnets Co and Gd with conductance smaller than the conductance quantum show reduced noise compared to the expectation for the spin-degenerate single-channel transport. Additionally we focus on the strong paramagnets Pt [3], Pd [4], and Ir [5], where a nonmonotonic magnetotransport has been reported for atomic contacts, interpreted as emerging magnetic ordering in small dimension, which is expected due to the Stoner instability [6, 7]. Our recent measurements on Pd, Pt, and Ir reveal noise levels which are above, but close to the threshold to the spin-degenerate single-channel situation. An anticorrelation between the minimum noise and the bulk Stoner parameter of these elements is observed. We discuss by how far this might indicate that spin polarization is reflected in the noise signal.

[1] Olivera et al., PRB 95, 075409 (2017)
[2] Häfner et al., PRB 77, 104409 (2008)
[3] Strigl et al., Nature Comm. 6, 6172 (2015)
[4] Strigl et al., PRB 94, 144431 (2016)
[5] Prestel et al., PRB 100, 214439 (2019)
[6] Delin et al., PRL 92, 057201 (2004)
[7] Delin et al., PRB 68, 144434 (2003)

TT 24.8 Thu 13:30 P

Theory of coherent phonon mode excitation in metal nanoparticles — •Robert Salzwedel[1], Dominik Hoeing[2], Yannic Staechelin[2], Florian Schulz[2], Holger Lange[2], Andreas Knorr[1], and Malte Selig[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut für Physikalische Chemie, Universität Hamburg, 20146 Hamburg, Germany

Metal nanoparticles perform radial breathing mode oscillation upon excitation by a light pulse. Typically, these oscillations are assumed to be driven by the thermalization of hot electrons that impulsively heat the lattice [1,2].

Here we present a hydrodynamic theory based on the Heisenberg equation of motion formalism for the optical excitation of the electron gas in metal nanoparticles and the related electron-phonon interaction.

Our analysis reveals that spatial gradients of the electron density which are induced by the optical pump already drive coherent phonon oscillations whereas thermalization is found to be of reduced importance.

[1] Hodak, J. H. et al. (1999), *JOCP*, **111**(18)
[2] Ng, M. Y. et al. (2011), *JOCP*, **134**(9), 094116

TT 24.9 Thu 13:30 P

Direct current from AC driving of Dirac Fermions — •Adrian Seith, Jakob Schlosser, Jan Wilhelm, and Ferdinand Evers — Institut für Theoretische Physik, Universy of Regensburg, Germany

Recent developments in systems driven by an ultra-short laser pulse demonstrate the high-order harmonic generation in topological systems with a Dirac-type (surface) bandstructure [1]. We investigate the current-density that results from the laser pulse close to the surface. Simulations based on the Semiconductor Bloch equations as implemented in the CUED code [2] indicate the emergence of a DC-like current with a lifetime by far exceeding the pulse duration. An analytical solution within a model system of Dirac Fermions is possible explaining the effect rigorously together with the observed dependence on the carrier envelope phase (CEP). Consequences for experiments with realistic band structures are discussed, as well as applications to light-wave-electronics.

[1] Schmid et. al., Nature 593, 385 (2021)
[2] Wilhelm et. al., Phys. Rev. B 103, 125419 (2021)

TT 24.10 Thu 13:30 P

Laser-waveform control of high-harmonic emission - a theoretical analysis — •Jan Wilhelm, Maximilian Graml, Maximilian Nitsch, Patrick Grössing, and Ferdinand Evers — Institute of Theoretical Physics, University of Regensburg

When irradiating solids with a short, i.e. subcycle, laser pulse, the corresponding electric field initiates ultrafast electron dynamics in the material. Fingerprints of it are encoded in the emission spectrum that features high-harmonic generation. High-harmonic emission from a topological insulator has been observed recently in experiment [1] opening a platform to explore topology and quasi-relativistic quantum physics using strong laser fields. Strikingly, the high-harmonic orders can be shifted to non-integer multiples of the driving frequency by varying the carrier-envelope phase (CEP) of the driving field. We theoretically analyze the mechanisms leading to CEP shifts using semiconductor Bloch equations [2-4] finding that an interplay of chirp and CEP of the laser pulse lead to arbitrary CEP shifts.

[1] C. P. Schmid, et al., Nature 593, 385-390 (2021)
[2] W. Schäfer, M. Wegener, Semiconductor Optics and Transport Phenomena, Springer, Berlin (2002)
[3] M. Kira, S. W. Koch, Semiconductor Quantum Optics, Cambridge University Press (2011)
[4] J. Wilhelm, P. Grössing, A. Seith, J. Crewse, M. Nitsch, L. Weigl, C. Schmid, F. Evers, Phys. Rev. B 103, 125419 (2021)

TT 24.11 Thu 13:30 P

High-harmonic geneneration in topological insulator surface states — •Vanessa Junk[1], Cosimo Gorini[1,2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, Germany — [2]Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

High-order harmonics are typically generated when matter is interacting with strong-field light. In most materials efficient scattering and dephasing destroy coherences in the emitted spectra. In topological insulator (TI) surface states however, scattering is strongly suppressed. This opens up the possibility to observe signatures of coherent transport.

We present how Berry curvature effects imprint into the dynamics of strong-field light driven electrons in TI surface states. In the semiclassical framework, a non-zero Berry curvature leads to the emergence of a velocity component perpendicular to the external driving. Here, we compare the semiclassical predic-

tions with a full quantum mechanical simulation. The high harmonics spectra we calculate from the dynamics show an alternating polarization as has recently also been observed in experiment [1].
[1] C. Schmid, L. Weigl, P. Grössing, V. Junk, C. Gorini, S. Schlauderer, S. Ito, M. Meierhofer, N. Hofmann, D. Afanasiev, J. Crewse, K. Kokh, O. Tereshchenko, J. Güdde, F. Evers, J. Wilhelm, K. Richter, U. Höfer and R. Huber, Nature **593**, 385-390 (2021)

TT 25: Poster Session: Topology

Time: Thursday 13:30–16:00 Location: P

TT 25.1 Thu 13:30 P

Boosting the surface conduction in a topological insulator — •Mathieu Taupin[1], Gaku Eguchi[1], Monika Budnovski[1], Andreas Steiger-Thirsfeld[2], Yukiaki Ichida[3], Kenta Kuroda[3,4], Shik Shin[3], Akio Kimura[4], and Silke Paschen[1] — [1]Institute of Solid State Physics, TU Wien, Austria — [2]USTEM, TU Wien, Austria — [3]ISSP, The University of Tokyo, Japan — [4]Graduate School of Advanced Science and Engineering, Hiroshima University, Japan

Despite the intense research on topological insulators, manipulating the surface states by the application of external stimuli is surprisingly only little explored. For instance, some topological insulators have been shown to have an anomalous response when exposed to light, i.e. slow with non-exponential behaviour. These results hint on the tunability of the Dirac states with illumination, but the lack of consensus of the microscopic mechanism impedes progress.

Our work provides an understanding of these effects. We demonstrate that under external excitation (such as thermal radiation, light illumination and current driving), excited electrons will migrate to the surface states and remain there "permanently" due to the intrinsic Schottky barrier and space-charge separation between the surface and bulk carriers. This leads to a significant boost of the surface conduction, even in a bulk sample, which can be adjusted with the amplitude of the external excitation. We find striking similarities between our results and previous spectroscopic studies and propose a common mechanism, which is in principle applicable in any topological insulators.

TT 25.2 Thu 13:30 P

Dirac-like particles in a box in shaped topological insulator nanowires — •Maximilian Fürst, Michael Barth, Cosimo Gorini, and Klaus Richter — Universität Regensburg

Topological insulator nanowires exhibit strong spin-orbit coupling with surface states which are well-protected against backscattering [1]. Due to their Dirac-like dispersion they are intersting materials for studying emergent relativistic effects in condensed matter. We show how TI nanowires can be used to generate Dirac-like particles in a box by exploiting geometrical properties of the wires and applying an external coaxial magnetic field. These quantized energy levels can be probed by conductance calculations. In order to do that, we employ the numerical Python package kwant [2] and implement a shaped 3D topological insulator nanowire with a 3D bulk model as well as an effective 2D surface model. Quantized and flux dependent conductance lines exhibit strong constraints on the physical state of the trapped electrons what makes a practical application as a magnetically tunable momentum filter possible.
[1] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011)
[2] Ch. W. Groth et al., New J. Phys. 16, 063065 (2014)

TT 25.3 Thu 13:30 P

Anisotropic Nodal-Line-Derived Large Anomalous Hall Conductivity in ZrMnP and HfMnP — •Sukriti Singh, Jonathan Noky, Shaileyee Bhattacharya, Praveen Vir, Yan Sun, Nitesh Kumar, Claudia Felser, and Chandra Shekhar — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The nontrivial band structure of semimetals has attracted substantial research attention in condensed matter physics and materials science in recent years owing to its intriguing physical properties. Within this class, a group of non-trivial materials known as nodal-line semimetals is particularly important. Nodal-line semimetals exhibit the potential effects of electronic correlation in nonmagnetic materials, whereas they enhance the contribution of the Berry curvature in magnetic materials, resulting in high anomalous Hall conductivity (AHC). In this study, two ferromagnetic compounds, namely ZrMnP and HfMnP, are selected, wherein the abundance of mirror planes in the crystal structure ensures gapped nodal lines at the Fermi energy. These nodal lines result in one of the largest AHC values of 2840 ohm-1cm-1, with a high anomalous Hall angle of 13.6% in these compounds. First-principles calculations provide a clear and detailed understanding of nodal line-enhanced AHC. Our finding suggests a guideline for searching large AHC compounds.

TT 25.4 Thu 13:30 P

Observation of symmetry-enforced topological nodal planes in CoSi — Nico Huber[1], •Kirill Alpin[2], Grace L. Causer[1], Lukas Worch[1], Andreas Bauer[1], Georg Benka[1], Moritz M. Hirschmann[2], Andreas P. Schnyder[2], Christian Pfleiderer[1,3,4], and Marc A. Wilde[1] — [1]Physik Department, Technische Universität München, Garching, Germany — [2]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [3]MCQST, Technische Universität München, Garching, Germany — [4]Centre for Quantum Engineering (ZQE), Technische Universität München, Garching, Germany

In this work, we present a complete topological classification of CoSi, whose bandstructure features a plethora of Weyl points, topologically charged multifold crossings, and symmetry-enforced nodal planes. The latter are forced to have nonzero charges in the presence of SOC, which we show both theoretically for a general case and computationally via DFT calculations for CoSi, using an adaptive mesh of Wilson loops. The total charge is found to be consistent with the fermion doubling theorem. Resulting topological protectorates, intersections of the Fermi surface with topological nodal planes, are detected via measurements of Shubnikov-de Haas oscillations.

TT 25.5 Thu 13:30 P

Kerr effect in tilted nodal loop semimetals — Johan Ekström[1], Eddwi H. Hasdeo[1,2], Maria Belén Farias[1], and •Thomas L. Schmidt[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg — [2]Research Center for Physics, Indonesian Institute of Sciences, South Tangerang, Indonesia

We investigate the optical activity of tilted nodal loop semimetals. We calculate the full conductivity matrix for a band structure containing a nodal loop with possible tilt in the $x - y$ plane, which allows us to study the Kerr rotation and ellipticity both for a thin film and a bulk material. We find signatures in the Kerr signal that give direct information about the tilt velocity and direction, the radius of the nodal loop and the internal chemical potential of the system. These findings should serve as a guide to understanding optical measurements of nodal loop semimetals and as an additional tool to characterize them.

TT 25.6 Thu 13:30 P

Impurity-induced bound states and resonances in lattice Dirac-Weyl semimetals — •João P. Santos Pires[1], Bruno Amorim[2], and João M. Viana Parente Lopes[1] — [1]Centro de Física das Universidades do Minho e Porto, University of Porto, 4169-007 Porto, Portugal — [2]Centro de Física das Universidades do Minho e Porto, University of Minho, 4710-057 Braga, Portugal

The discovery of gapless 3D semimetals turned Dirac-Weyl electrons into a hot topic in condensed matter. The possibility of a putative impurity- or disorder-driven quantum phase transition that turns a semi-metallic phase (with vanishing DoS at the Fermi level) into a diffusive metallic phase have attracted particular interest. Despite the vast number of recent work addressing this problem, the picture remains unclear and seemingly dependent on the precise type of disorder considered.

In this work, we use a projected Green function method to study a four-band gapless Dirac Hamiltonian discretised in a simple cubic lattice, and in the presence of impurities composed of spherical clusters with on-site energy U. With this method, we evaluate the correction to the total and local density of states induced by the impurity. For cluster of radius larger than one lattice spacing, we found that eigenstates bound to the impurity cluster are formed, at fine-tuned values of U that depart from the predictions from the continuum theory. As this radius is increased, the lattice results progress towards the continuum theory predictions.

TT 25.7 Thu 13:30 P

Artificial event horizons in Weyl semimetal heterostructures and their non-equilibrium signatures — •Christophe De Beule[1], Solofo Groenendijk[1], Tobias Meng[2], and Thomas L. Schmidt[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg — [2]Institute for Theoretical Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01069 Dresden, Germany

We investigate transport in type-I/type-II Weyl semimetal heterostructures that realize effective black- or white-hole event horizons. We provide an exact solution to the scattering problem at normal incidence and low energies, both for a sharp and a slowly-varying Weyl cone tilt profile. In the latter case, we find two channels with transmission amplitudes analogue to those of Hawking radiation. Whereas the Hawking-like signatures of these two channels cancel in equilibrium, we demonstrate that one can favor the contribution of either channel using a non-equilibrium state, either by irradiating the type-II region or by coupling it to a magnetic lead. This in turn gives rise to a peak in the two-terminal differential conductance which can serve as an experimental indicator of the artificial event horizon.

TT 25.8 Thu 13:30 P

Crossed Andreev reflection in topological insulator nanowire T-junctions — •Jacob Fuchs[1], Michael Barth[1], Cosimo Gorini[1,2], Inanc Adagideli[3,4], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France — [3]Faculty of Engineering and Natural Sciences, Sabanci University, 34956 Orhanli-Tuzla, Turkey — [4]Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

We numerically study crossed Andreev reflection (CAR) in a topological insulator nanowire T-junction where one lead is proximitized by a superconductor. We find that CAR should be clearly observable in a wide parameter range, including perfect CAR in a somewhat more restricted range. Furthermore, it can be controlled by a magnetic field and is robust to disorder.

TT 25.9 Thu 13:30 P

Improving topological superconductivity in two- and three-dimensional Josephson junctions — •Aidan Wastiaux[1] and Falko Pientka[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Institute of Theoretical Physics, Goethe University, Frankfurt am Main

As opposed to the numerous theoretical developments in the field of topological heterostructures hosting robust quasiparticles, difficulties are piling up for experimentalists on their way to building realistic and tunable setups with usable topological states. We address this widespread issue in a specific platform involving a planar Josephson junction made of a semiconductor with strong spin-orbit coupling by proposing easy-to-reach regimes of parameters with enhanced stability of the Majorana end states. Moreover, the extension of those findings to a three-dimensional model provides henceforth a new flexible platform for realizing chiral Majorana edge states. Possible setups using Van der Waals heterostructures are suggested.

TT 25.10 Thu 13:30 P

Weyl systems: anomalous transport normally explained — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

The anomalous term $\sim \vec{E}\vec{B}$ in the balance of the chiral density can be rewritten as quantum current in the classical balance of density. This term is derived from the quantum kinetic equations for systems with SU(2) structure within a completely conserving approach and it is suggested that the term is of kinetic origin instead of anomaly. Regularization-free density and pseudospin currents are calculated in Graphene and Weyl-systems realized as the infinite-mass limit of electrons with quadratic dispersion and a proper spin-orbit coupling. The intraband and interband conductivities are discussed. The optical conductivity agrees well with the experimental values using screened impurity scattering and an effective Zeeman field. The universal value of Hall conductivity is shown to be modified due to the Zeeman field.

[1] Eur. Phys. J. B 92 (2019) 176
Phys. Lett. A 383 (2019) 1362
[2] Phys. Rev. B 94 (2016) 165415
[3] Phys. Rev. B 92 (2015) 245425
[4] errata: Phys. Rev. B93 (2016) 239904(E)
[5] Phys. Rev. B 92 (2015) 245426

TT 25.11 Thu 13:30 P

Current correlations of Cooper-pair tunneling into a quantum Hall system — Andreas Michelsen[1,2], Thomas Schmidt[1], and •Edvin Idrisov[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg — [2]SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews KY16 9SS, United Kingdom

We study Cooper-pair transport through a quantum point contact between a superconductor and a quantum Hall edge state at integer and fractional filling factors. We calculate the tunneling current and its finite-frequency noise to the leading order in the tunneling amplitude for dc and ac bias voltage in the limit of low temperatures. At zero temperature and in the case of tunneling into a single edge channel both the conductance and differential shot noise vanish as a result of the Pauli exclusion principle. In contrast, in the presence of two edge channels, this Pauli blockade is softened and a nonzero conductance and shot noise are revealed.

TT 25.12 Thu 13:30 P

Universal Hall conductance scaling in non-Hermitian Chern insulators — •Solofo Groenendijk[1], Thomas Schmidt[1], and Tobias Meng[2] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg — [2]Institute for Theoretical Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01069 Dresden, Germany

We investigate the Hall conductance of a two-dimensional Chern insulator coupled to an environment causing gain and loss. Introducing a biorthogonal linear response theory, we show that sufficiently strong gain and loss lead to a characteristic nonanalytical contribution to the Hall conductance. Near its onset, this contribution exhibits a universal power law with a power 3/2 as a function of Dirac mass, chemical potential, and gain strength. Our results pave the way for the study of non-Hermitian topology in fermionic transport experiments.

TT 25.13 Thu 13:30 P

Origin of the quasi-quantized Hall effect in $ZrTe_5$ — •Stanislaw Galeski and Johannes Gooth — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The quantum Hall effect (QHE) is traditionally considered to be a purely two-dimensional (2D) phenomenon. Recently, however, a three-dimensional (3D) version of the QHE was reported in the Dirac semimetal $ZrTe_5$. It was proposed to arise from a magnetic-field-driven Fermi surface instability, transforming the original 3D electron system into a stack of 2D sheets. Here, we report thermodynamic, spectroscopic, thermoelectric and charge transport measurements on such $ZrTe_5$ samples. The measured properties: magnetization, ultrasound propagation, scanning tunneling spectroscopy, and Raman spectroscopy, show no signatures of a Fermi surface instability, consistent with in-field single crystal X-ray diffraction. Instead, a direct comparison of the experimental data with linear response calculations based on an effective 3D Dirac Hamiltonian suggests that the quasi-quantization of the observed Hall response emerges from the interplay of the intrinsic properties of the $ZrTe_5$ electronic structure and its Dirac-type semi-metallic character.

TT 25.14 Thu 13:30 P

Generalized Chern numbers based on open system Green's functions — Maria Belén Farias, •Solofo Groenendijk, and Thomas Schmidt — Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

We present an alternative approach to studying topology in open quantum systems, relying directly on Green's functions and avoiding the need to construct an effective non-Hermitian (nH) Hamiltonian. We define an energy-dependent Chern number based on the eigenstates of the inverse Green's function matrix of the system which contains, within the self-energy, all the information about the influence of the environment, interactions, gain or losses. We explicitly calculate this topological invariant for a system consisting of a single 2D Dirac cone and find that it is half-integer quantized when certain assumptions about the self-energy are made. Away from these conditions, which cannot or are not usually considered within the formalism of nH Hamiltonians, we find that such a quantization is usually lost and the Chern number vanishes, and that in special cases, it can change to integer quantization.

TT 25.15 Thu 13:30 P

Geometrical Rabi oscillations in non-Abelian systems — •Hannes Weisbrich[1], Gianluca Rastelli[2], and Wolfgang Belzig[1] — [1]Universität Konstanz — [2]Universita di Trento

Topological phases of matter became a new standard to classify quantum systems in many cases, yet key quantities like the quantum geometric tensor providing local information about topological properties are still experimentally hard to access, especially in non-Abelian systems [1] when states are degenerate and the quantum geometric tensor has a non-Abelian form. We propose protocols to determine the quantum geometric tensor in non-Abelian quantum systems. We show theoretically that for a weak resonant driving of the local parameters the coherent Rabi oscillations and their frequencies are related to the non-Abelian quantum geometric tensor [2]. Our schemes suggest also a way to prepare eigenstates of the quantum metric, a task that is difficult otherwise in a degenerate subspace.

[1] H. Weisbrich, R. L. Klees, G. Rastellli, and W. Belzig, PRX Quantum 2, 010310 (2021)
[2] H. Weisbrich, G. Rastellli, and W. Belzig, arXiv:2105.02689 (2021); accepted in Phys. Rev. Research (2021)

TT 25.16 Thu 13:30 P

Non-Hermitian band topology from momentum-dependent relaxation in two dimensional metals with spiral magnetism — •Johannes Mitscherling and Walter Metzner — Max Planck Institute for Solid State Research, Stuttgart, Germany

We present the emergence of non-Hermitian band topology in a two dimensional metal with planar spiral magnetism due to a momentum-dependent relaxation rate. A sufficiently strong momentum dependence of the relaxation rate leads to exceptional points in the Brillouin zone, where the Hamiltonian is non-diagonalizable. The exceptional points appear in pairs with opposite topological charges and are connected by arc-shaped branch cuts. We show that exceptional points inside hole and electron pockets, which are generally present in a spiral magnetic state with a small magnetic gap, can cause a drastic change of the Fermi surface topology by merging those pockets at isolated points in the Brillouin zone. The spectral function observed in photoemission exhibits Fermi arcs. Its momentum dependence is smooth - despite of the non-analyticities in the complex quasiparticle band structure.

TT 25.17 Thu 13:30 P

On the origin of the corner modes of the breathing kagome lattice — •Miguel Angel Jimenez Herrera[1,2], María Blanco de Paz[2], Aitzol García Etxarri[2,3], and Dario Bercioux[2,3] — [1]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, 20018 Donostia-San Sebastián, Basque Country, Spain — [2]Donostia International Physics Center, 20018 Donostia-San Sebastián, Spain — [3]IKERBASQUE, Basque Foundation for Science, Euskadi Plaza, 5, 48009 Bilbao, Spain

Quantum simulating techniques conform a perfect laboratory to study low-dimensional systems, such as the Su-Schrieffer-Heeger model, in 1D, or the breathing kagome model, in 2D [1]. Here, we address the realization of latter model using the muffin tin method, a first-principles-like technique based on planar wave expansion of the Bloch wave function. We study the standard kagome model and the two breathing phases using topological and symmetry markers. We claim that such breathing phases are both atomic limits: one shows zero bulk polarization, while the other, also called obstructed atomic limit, displays a finite value. We have performed a topological quantum chemistry [2] analysis and we have obtained the same result, supporting our results.

[1] Kempkes *et al.*, Nat. Mater. **18**, 1292 (2019)
[2] Bradlyn *et al.*, Nature **547**, 298 (2017)

TT 25.18 Thu 13:30 P

Carrier transitions in gapped Dirac systems induced by strong light pulses — •Mario Ebner[1], Vanessa Junk[1], Cosimo Gorini[1,2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, Germany — [2]Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

In order to understand the interesting consequences of matter interacting with strong light pulses, such as higher harmonics generation, it is necessary to investigate how the light field influences the occupation of the energy bands in the system.

We theoretically study this redistribution of carriers in a Dirac system, such as graphene, in the presence of a mass gap. This is done in two ways: Firstly, we model the behaviour of electrons in the system by a wave packet propagating under the influence of the electric field pulse. Secondly, we want to emphasize another approach similar to [1], which essentially breaks down to solving the time-dependent Schrödinger equation for a single $\boldsymbol{k}$-mode. This gives a complementary view of the physical processes involved. In particular, we discuss the interplay between the motion in reciprocal space due to the electric field and the dipole matrix element between valence and conduction band which determines the observed populations.

As an outlook, we sketch how to deduce the resulting current which can be split in intra- and interband contributions and which can be used for computing higher harmonics spectra.

[1] S. A. O. Motlagh *et al*, J. Phys.: Condens. Matter **32**, 065305 (2020)

TT 26: Annual General Meeting of the Low Temperature Physics Division

Time: Thursday 18:00–19:30 Location: MVTT

Bericht, Wahl, Verschiedenes

TT 27: Topological Insulators and Semimetals (joint session TT/KFM)

Time: Friday 10:00–12:45 Location: H7

TT 27.1 Fri 10:00 H7

Wave-particle duality of electrons with spin-momentum locking — •Dario Bercioux[1,2], Tineke van den Berg[1], Dario Ferrero[3,4,5], Jerome Rech[4], Thibaut Jonckheere[4], and Thierry Martin[4] — [1]Donostia International Physics Center (DIPC), Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Basque Country, Spain — [3]Aix Marseille Univ, Université de Toulon, CNRS, CPT, Marseille, France — [4]Dipartimento di Fisica, Università di Genova, Via Dodecaneso 33, 16146, Genova, Italy — [5]SPIN-CNR, Via Dodecaneso 33, 16146 Genova, Italy

We investigate the effects of spin-momentum locking on the interference and diffraction pattern of electrons in a double- or single-slit Gedankenexperiment. We show that the inclusion of the spin degree-of-freedom when coupled to the carrier's motion direction — a typical situation occurring in systems with spin-orbit interaction — leads to modify the interference and diffraction patterns depending on the geometrical parameters system.

[1] Bercioux *et al.*, Eur. Phys. J. Plus **135**, 811 (2020)

TT 27.2 Fri 10:15 H7

Volkov-Pankratov states in topological graphene nanoribbons — Tineke L. van den Berg[1], •Alessandro De Martino[2], M. Reyes Calvo[3], and Dario Bercioux[1,4] — [1]Donostia International Physics Center, Donostia-San Sebastián, Spain — [2]Department of Mathematics, City, University of London, London, United Kingdom — [3]Departamento de Fisica Aplicada, Universidad de Alicante, Alicante, Spain — [4]IKERBASQUE, Basque Foundation of Science, Bilbao, Spain

In topological systems a smooth modulation of the gap at the interfaces between topologically distinct phases can lead to the appearance of massive edge states, as first described by Volkov and Pankratov in 1985. In this contribution I will show that, in the presence of intrinsic spin-orbit coupling smoothly modulated near the edges, graphene nanoribbons host Volkov-Pankratov states in addition to the topologically protected helical states. This result is obtained by means of two complementary methods, one based on the effective low-energy Dirac equation description and the other on a fully numerical tight-binding approach, with excellent agreement between the two. I will then briefly discuss how transport measurements might reveal the presence of Volkov-Pankratov states, and possible graphene-like structures in which such states might be observed.

TT 27.3 Fri 10:30 H7

Symmetry-enforced topological nodal planes — Marc A. Wilde[1,2], Matthias Dodenhöft[1], Arthur Niedermayr[1], Andreas Bauer[1,2], •Moritz M. Hirschmann[3], Kirill Alpin[3], Andreas P. Schnyder[3], and Christian Pfleiderer[1,2,4] — [1]Physik Department, Technische Universität München, Garching, Germany. — [2]Centre for QuantumEngineering (ZQE), Technische Universität München, Garching, Germany. — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany. — [4]MCQST, Technische Universität München, Garching, Germany.

Topological semimetals and metals may contain nodal points or lines, i.e., zero- or one-dimensional crossings in the energy bands. In the present work we discuss an extension to two-dimensional nodal features. These nodal planes are enforced in crystals with certain nonsymmorphic space groups. We specify the necessary conditions for the existence of nodal planes and consider in the process paramagnetic as well as magnetic space groups. Based on an analysis of symmetry eigenvalues we identify space groups that lead to nodal planes with a non-zero Chern number. Our arguments are supported by minimal models and explicit calculation of the topological invariants. Furthermore, we have identified a number of materials with topological nodal planes. Among them is the ferromagnetic phase of MnSi, for which we show that the symmetry-enforced topological nodal planes exist, using de Haas-van Alphen spectroscopy and density functional theory calculations.

[1] M.A. Wilde et al., Nature 594, 374-379 (2021)

TT 27.4 Fri 10:45 H7

Network of topological nodal planes and point degeneracies in CoSi — •Nico Huber[1], Kirill Alpin[2], Grace L. Causer[1], Lukas Worch[1], Andreas Bauer[1], Georg Benka[1], Moritz M. Hirschmann[2], Andreas P. Schnyder[2], Christian Pfleiderer[1], and Marc A. Wilde[1] — [1]Physik Department, Technische Universität München, D-85748 Garching, Germany — [2]Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

We report the experimental identification of symmetry-enforced topological nodal planes in CoSi which together with multifold point degeneracies and Weyl points form a network of band crossings satisfying the fermion doubling theorem. For this, we have combined measurements of Shubnikov-de Haas oscillations in CoSi with material-specific electronic structure calculations and a symmetry analysis [1]. The observation of two nearly dispersionless Shubnikov-de Haas frequency branches is shown to provide clear evidence of four distinct Fermi surface sheets at the R point of the Brillouin zone and of the symmetry-enforced orthogonality of the wave functions at the intersections with the nodal planes. These results highlight that CoSi features six- and fourfold crossings at R and Γ and that a comprehensive account of all topological charges in the network going beyond point degeneracies is needed.

[1] Huber et al., arXiv:2107.02820

15 min. break.

TT 27.5 Fri 11:15 H7

Twisted and chiral photon states scattered on chiral molecular liquids
— Silvia Müllner[1], Florian Büscher[1], Dirk Wulferding[2], Yurii G. Pashkevich[1,3], Vladimir Gnezdilov[1,4], Anton A. Pechkov[5], Andrey Surzhykov[5], and •Peter Lemmens[1] — [1]IPKM, TU Braunschweig, Germany — [2]CCES, Inst. for Basic Science, Seoul, Republic of Korea — [3]O.O. Galkin Donetsk Inst. for PaE, NASU, Kyiv - Kharkiv, Ukraine — [4]B. Verkin Inst. for Low Temp. Phys and Eng., NASU, Kharkiv, Ukraine — [5]Inst. Math. Phys., TU Braunschweig and PTB, Braunschweig, Germany

Twisted or structured light [1] has been recognized as a novel probe of chiral states of matter. The respective light matter coupling is still discussed controversially. Using resonant light-matter coupling of twisted and chiral photon states [1] to chiral molecular liquids we study their inelastic response. For this instance, quasi-elastic Raman scattering (QES) is investigated in isotropic, nematic and chiral nematic phases of liquid crystals. The response is diffusive and dominated by a narrow distribution or single relaxation rate.

We acknowledge important discussions with G. Napoli (Univ. del Salento, Lecce). This research was funded by the DFG Excellence Cluster QuantumFrontiers, EXC 2123, DFG Le967/16-1, DFG-RTG 1952/1, and the Quantum- and Nano-Metrology (QUANOMET) initiative of Lower Saxony within project NL-4.

[1] H. Rubinsztein-Dunlop, et al., Journ. Opt. 19, 013001 (2017)

TT 27.6 Fri 11:30 H7

Berry curvature-induced local spin polarisation in gated graphene/WTe_2 heterostructures
— •Jonas Kiemle[1,2], Lukas Powalla[3,4], Elio J. König[3], Andreas P. Schnyder[3], Johannes Knolle[2,5], Klaus Kern[3,4], Alexander Holleitner[1,2], Christoph Kastl[1,2], and Marko Burghard[3] — [1]Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, Garching — [2]MCQST, Schellingstrasse 4, München — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, Stuttgart — [4]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, Lausanne — [5]Department of Physics TQM, Technical University of Munich, James-Frank-Strasse 1, Garching

Experimental control of local spin-charge interconversion is of primary interest for spintronics. Van der Waals heterostructures combining graphene with a strongly spin-orbit coupled two-dimensional (2D) material enable such functionality by design. Here, we probe the gate-tunable local spin polarisation in current-driven graphene/WTe_2 heterostructures through magneto-optical Kerr microscopy. We observe, that even for a nominal in-plane transport, substantial out-of-plane spin accumulation is induced by a corresponding out-of-plane current flow [1]. Our findings unravel the potential of 2D heterostructure engineering for harnessing topological phenomena for spintronics, and constitute an important step toward nanoscale, electrical spin control.

[1] L. Powalla, J. Kiemle et al., arXiv:2106.15509 (2021)

TT 27.7 Fri 11:45 H7

Impact of domain disorder on optoelectronic properties of semimetal $MoTe_2$
— •Maanwinder Partap Singh[1,2], Jonas Kiemle[1,2], Philipp Zimmermann[1,2], Marko Burghard[3], Christoph Kastl[1,2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany. — [2]Munich Center of Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany. — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany.

$MoTe_2$, one of the candidates to realize the topological type-II Weyl semimetal, crystallizes in several structures. At room temperature, $Mote_2$ can have either a semiconducting (2H) or a metallic phase (1T'). Upon cooling, the monoclinic phase undergoes a transition at ~ 240 K into an orthorhombic phase (T_d), which breaks the inversion symmetry. We investigate the optoelectronic properties of $MoTe_2$ as a function of temperature using photocurrent spectroscopy in combination with Raman and transient reflection spectroscopy. We elucidate the impact of phase disorder on the generation of local photocurrents especially with respect to ultrafast photogalvanic currents [1].

[1] Singh et al. (submitted)(2021)

TT 27.8 Fri 12:00 H7

2D-Berry-curvature-driven large anomalous Hall effect in layered topological nodal-line MnAlGe
— •Satya N. Guin and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Topological magnets comprising two-dimensional (2D) magnetic layers with Curie temperatures (TC) exceeding room temperature are key for dissipationless quantum transport devices. However, the identification of a material with 2D ferromagnetic planes that exhibits an out-of-plane-magnetization remains a challenge. We report a ferromagnetic, topological, nodal-line, and semimetal MnAlGe composed of square-net Mn layers that are separated by nonmagnetic Al-Ge spacers. The 2D ferromagnetic Mn-layers exhibit an out-of-plane magnetization below TC 503 K. Density functional calculations demonstrate that 2D arrays of Mn atoms control the electrical, magnetic, and therefore topological properties in MnAlGe. The unique 2D distribution of the Berry curvature resembles the 2D Fermi surface of the bands that formed the topological nodal line near the Fermi energy. A large anomalous Hall conductivity (AHC) of 700 S/cm is obtained at 2 K and related to this nodal line-induced 2D Berry curvature distribution. The high transition temperature, large anisotropic out-of-plane magnetism, and natural hetero-structure-type atomic arrangements consisting of magnetic Mn and non-magnetic Al/Ge elements render nodal-line MnAlGe one of the few, unique, and layered topological ferromagnets that have ever been observed.

[1] S. N. Guin et al., Adv. Mater. 2021, 33 (21), 2006301

TT 27.9 Fri 12:15 H7

A quantum oscillation study in the Dirac nodal-line semimetal HfSiS
— •Claudius Müller[1], Jasper Linnartz[1], Leslie Schoop[2], Nigel Hussey[1,3], and Steffen Wiedmann[1] — [1]High Field Magnet Laboratory (HFML-EMFL), IMM, Radboud University, Nijmegen, the Netherlands — [2]Department of Chemistry, Princeton University, Princeton, New Jersey, USA — [3]H. H. Wills Physics Laboratory, University of Bristol, Bristol, UK

We have performed a de Haas - van Alphen (dHvA) quantum oscillation study of HfSiS in high magnetic fields up to 31 T. For parallel alignment of the magnetic field and the c-axis, we observe quantum oscillations originating from individual electron and hole pockets, as well as oscillations caused by magnetic breakdown (MB) between these pockets. The MB orbits come in a wide variety, ranging from a so-called 'figure-of-eight' orbit to orbits enclosing large areas in the Brillouin zone (BZ). These MB orbits can be seen as a manifestation of Klein tunneling in momentum space [1], although in a regime of partial transmission due to the finite separation between adjacent pockets. Our experimental observation, the strong dependence of the oscillation amplitude on the field angle and the cyclotron masses of the MB orbits, is in good agreement with the theoretical predictions for this novel tunneling phenomenon.

[1] M. van Delft et al., Phys. Rev. Lett. 121, 256602 (2018)

TT 27.10 Fri 12:30 H7

Magnetic breakdown and open orbits in $LaIn_3$
— •Jasper Linnartz[1], Davide Pizzirani[1], Claudius Müller[1], Sam Teicher[2], Ratnadwip Singha[3], Sebastiaan Klemenz[3], Leslie Schoop[3], and Steffen Wiedmann[1] — [1]High Field Magnet Laboratory (HFML-EMFL), IMM, Radboud University, Nijmegen, the Netherlands — [2]Materials Department and California Nanosystems Institute, University of California Santa Barbara, Santa Barbara, USA — [3]Department of Chemistry, Princeton University, Princeton, USA

$LaIn_3$ which crystalizes in the $AuCu_3$ structure provides is a highly tunable system for emergent phenomena in condensed matter such as a monotonic increase of its critical temperature upon Sn doping. It is also considered as a model system for the heavy fermion systems $CeIn_3$ and $PrIn_3$.

We present a systematic de Haas-van Alphen quantum oscillations study on $LaIn_3$ up to 30 T. By measuring the temperature and angle dependence, the Fermi surface and the charge carrier properties such as the effective cyclotron masses are determined. While the finding of some pockets of the complex Fermi surface is in agreement with theoretical predictions, the observation of various high-frequency oscillations at specific angles points towards field-induced magnetic breakdown that can be described in a two-dimensional network of open orbits.

TT 28: Transport (joint session TT/DY)

Time: Friday 13:30–15:00 Location: H6

TT 28.1 Fri 13:30 H6

Spin-relaxation in superconducting graphene systems — •Michael Barth, Jacob Fuchs, Andreas Costa, Klaus Richter, Jaroslav Fabian, and Denis Kochan — Universität Regensburg

The spin-relaxation time τ_s is a fundamental quantity as it determines how long spins can propagate before they relax. For quasi-particles in s-wave superconductors that scatter off magnetic impurities this quantity is expected to decrease by lowering the temperature, known as the Hebel-Slichter-effect [1]. We have shown that this decrease of the spin-relaxation time does not happen generally in all superconductors [2]. A completely opposite behavior can be observed, if Yu-Shiba-Rusinov (YSR) states develop deeply inside the superconducting gap, since then the magnetic moments energetically decouple from the coherence peaks what in turn weakens an exchange interaction with quasi-particles. By employing analytical and numerical methods we have shown that such deep lying in-gap YSR states are formed if a system with magnetic impurities is doped to resonances. As an explicit example we will present results for graphene and bilayer graphene decorated with light magnetic impurities as hydrogen and fluorine.

[1] L. C. Hebel and C. P. Slichter, Phys. Rev. 113, 1504 (1959)
[2] D. Kochan, M. Barth, A. Costa, K. Richter, J. Fabian, Phys. Rev. Lett. 125, 087001 (2020)

TT 28.2 Fri 13:45 H6

Aharonov-Bohm Oscillations in Minimally Twisted Bilayer Graphene — Christophe De Beule[1], Fernando Dominguez[2], and •Patrik Recher[2,3] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg — [2]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [3]Laboratory for Emerging Nanometrology, 38106 Braunschweig, Germany

We investigate transport in the network of valley Hall states that emerges in minimally twisted bilayer graphene under interlayer bias. To this aim, we construct a scattering theory that captures the network physics. In the absence of forward scattering, symmetries constrain the network model to a single parameter that interpolates between one-dimensional chiral zigzag modes and pseudo-Landau levels. Moreover, we show how the coupling of zigzag modes affects magnetotransport. In particular, we find that scattering between parallel zigzag channels gives rise to Aharonov-Bohm oscillations that are robust against temperature, while coupling between zigzag modes propagating in different directions leads to Shubnikov-de Haas oscillations that are smeared out at finite temperature.

TT 28.3 Fri 14:00 H6

Spin interference effects in quantum rings in the presence of SU(2) fields — Alberto Hijano[1,2,3], Tineke van den Berg[3], Diego Frustaglia[4], and •Dario Bercioux[3,5] — [1]University of the Basque Country, UPV/EHU, Bilbao, Spain — [2]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain — [3]Donostia International Physics Center, Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [4]Departamento de Física Aplicada II, Universidad de Sevilla, E-41012 Sevilla, Spain — [5]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain

We present a theory of conducting quantum networks that accounts for Abelian and non-Abelian fields acting on spin carriers [1]. We apply this approach to model the conductance of mesoscopic spin interferometers of different geometry (such as squares and rings), reproducing recent experimental findings in nanostructured InAsGa quantum wells subject to Rashba spin-orbit and Zeeman fields [2,3] (as, e.g., the manipulation of Aharonov-Casher interference patterns by geometric means). Moreover, by introducing an additional field-texture engineering, we manage to single out a previously unnoticed spin-phase suppression mechanism. Our approach can also be used for the study of complex networks and the spectral properties of closed systems.

[1] Hijano *et al.*, Phys. Rev. B **103**, 155419 (2021)
[2] Nagasawa, *et al.*, Nat. Commun. **4**, 2526 (2013)
[3] Wang *et al.*, Phys. Rev. Lett. **123**, 266804 (2019)

TT 28.4 Fri 14:15 H6

Length dependent symmetry in narrow chevron-like graphene nanoribbons — •Koen Houtsma[1], Mihaela Enache[1], Remco Havenith[1,2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, 9747AG Groningen, the Netherlands — [2]Stratingh Institute for Chemistry, University of Groningen, 9747AG Groningen, the Netherlands

Graphene nanoribbons (GNRs) are an exciting material due to their excellent and tunable electronic properties. For instance, GNRs with armchair edges possess a width-dependent band gap, whereas zigzag GNRs are expected to host spin-polarized edge states and be semimetallic [1]. Previously, narrow chevron-like GNRs, which host a combination of zigzag and armchair edge terminations, were fabricated on a Au(111) substrate from the prochiral precursor 6,12-dibromochrysene through a combination of Ullmann-type coupling and cyclodehydrogenation [2]. Depending on the number of monomer units the ribbons are made of, an even and an odd number lead to a mirror and a point symmetric ribbon, respectively. Using scanning tunneling spectroscopy we investigated the potential effect of this length dependent symmetry on the electronic properties. In addition, bends are formed in these ribbons through a common coupling defect. We characterized these bends using a combination of high-resolution scanning tunneling microscopy and spectroscopy. The bends are based on the formation of both a five- and six-membered ring and their electronic properties are altered.

[1] K. Nakada et al., Phys. Rev. B 54, 17954 (1996)
[2] T.A. Pham et al., Small 13, 1603675 (2017)

TT 28.5 Fri 14:30 H6

Thermal fluctuations of two-dimensional crystalline membranes: a scale-invariant but nonconformal field theory — •Achille Mauri and Mikhail I. Katsnelson — Radboud University, Institute for Molecules and Materials, Nijmegen, The Netherlands

Statistical fluctuations of two-dimensional membranes have been the subject of extensive investigations, from string theories to biological and condensed matter systems such as graphene and other atomically-thin 2D materials. In the case of solid layers subject to vanishing external tension, the interplay of thermal fluctuations and anharmonic phonon-phonon interactions gives rise to a crucial renormalization of the elastic constants: as a result, the long-wavelength behavior of phonon fluctuations is scale-invariant and it is controlled by an interacting fixed point of the renormalization group (RG). In this contribution, we argue that, in contrast with several other field-theories, the emergent dilatation symmetry is not enhanced to the full conformal invariance. We analyze in particular, the structure of the energy-momentum tensor $T_{\mu\nu}$ within an ϵ-expansion, after extension of the problem from the physical dimension $D = 2$ to a non-integer dimensionality $D = 4 - \epsilon$. The trace $T_{\mu\mu}$ reduces, at the fixed point, to the total divergence of a non-trivial virial current, implying the absence conformal invariance.

TT 28.6 Fri 14:45 H6

Viscous, elastic and ballistic shear response of electron fluids probed through optical spectroscopy — •Davide Valentinis[1,2], Jan Zaanen[3], Dirk van der Marel[4], and Joerg Schmalian[1,2] — [1]Institut für Quantenmaterialien und Technologien, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstra{\ss}e 1, D-70569 Stuttgart (DE) — [3]Department of Quantum Matter Physics, University of Geneva, 24 Quai Ernest-Ansermet, 1211 Geneva 4, Switzerland — [4]Institute-Lorentz for Theoretical Physics, Leiden University, PO Box 9506, NL-2300 RA Leiden, The Netherlands

Can optical spectroscopy provide complementary and unambiguous fingerprints of spatial nonlocality in bulk and layered materials, and under which conditions? To answer these questions, we investigate the nonlocal current response of 3D charged Fermi liquids, and 2D isotropic and anisotropic metals, taking into account momentum-conserving collisions and momentum-relaxing scattering in kinetic-theory approaches. In strongly interacting Fermi liquids, a propagating shear mode of Fermi-surface deformation, analogous to transverse sound in liquid helium, determines characteristic oscillating patterns of the thin-film transmission as a function of radiation frequency. We develop a kinetic theory for the distribution function of 2D Fermi gases with arbitrary electronic dispersion relation, using a collision operator formalism. The skin depth and surface impedance are shown to qualitatively depend on the shape and orientation of the polygonal Fermi surface.

TT 29: Topological Superconductors

Time: Friday 13:30–15:00 Location: H7

TT 29.1 Fri 13:30 H7

Doping a topological insulator: a promising strategy to find topological superconductors? — Sebastian Wolf, Tylor Gardener, and •Stephan Rachel — School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

The search for topological superconductors is one of the most pressing and challenging questions in condensed matter and material research. Despite some early suggestions that doping a topological insulator might be a successful recipe to find topological superconductors, until today there is no general understanding of the relationship of the topology of the superconductor and the topology of its underlying normal state system. One of the major obstacles is the strong effect of the Fermi surface and its subsequent pairing tendencies, usually preventing a detailed comparison between different topological superconducting systems. Here we present an analysis of various doped insulators-topological and trivial–for which the differences of the Fermi surfaces have been removed. Our approach allows us to analyze and compare superconducting instabilities of different insulating normal state systems with identical Fermi surfaces and to present rigorous results on how beneficial it might be to dope a topological insulator.

TT 29.2 Fri 13:45 H7

Accidental Two-Component Order Parameter in UTe_2 — •Florian Theuss[1], Gael Grissonnanche[1], Nicholas Butch[2,3], Johnpierre Paglione[3], Sheng Ran[4], Kelly Nygren[5], Peter Ko[5], and Brad Ramshaw[1] — [1]Cornell University, Ithaca, NY, USA — [2]NIST, College Park, MD, USA — [3]University of Maryland, College Park, MD, USA — [4]Washington University, St. Louis, MO, USA — [5]CHESS, Ithaca, NY, USA

The recently discovered unconventional superconductor UTe_2 is a promising candidate to host time-reversal symmetry breaking (TRSB) in the ordered state, below about 1.6 K. TRSB, indicated by a field trainable Kerr effect, would require a two-component order parameter. Due to the orthorhombic crystal symmetry of UTe_2, a two-component order parameter is expected to be accidental, resulting in two successive superconducting phase transitions. We address this question with Resonant Ultrasound Spectroscopy, where we measure mechanical resonance frequencies of the sample and can resolve two jumps in their temperature dependence with close to part per million resolution. This gives us information about the possibility of a two-component order parameter and constrains its symmetry. Additionally, we perform near-field/far-field high-energy X-ray diffraction experiments to investigate sample homogeneity.

This work is supported by the Office of Basic Energy Sciences of the United States Department of Energy under award no. DE-SC0020143 and partially based upon research conducted at the Materials Solutions Network at CHESS (MSN-C) which is supported by the Air Force Research Laboratory under award FA8650-19-2-5220.

TT 29.3 Fri 14:00 H7

Sub-gap and supra-gap transport characteristics of the finite Kitaev chain — •Nico Leumer[1], Milena Grifoni[1], Bhaskaran Muralidharan[2], and Magdalena Marganska[1] — [1]Institute for Theoretical Physics, University of Regensburg, Germany — [2]Department of Electrical Engineering, Indian Institute of Technology Bombay, India

We investigate the nonlinear transport in a normal - Kitaev chain- normal (N-K-N) junction. Using exact analytical results for the spectrum and Green's function of the Kitaev chain in the whole regime of parameters, an exact expression for the linear conductance is provided, and insight into the complex interplay of crossings and anticrossings in the supra-gap region is obtained. In particular, we discuss how the ratio of the direct charge transfer and the local Andreev reflection relates to the spatial profile of the lowest lying state. Also, we demonstrate that the supra-gap transport shows stable and strong contributions from the local Andreev reflection which yields the same contribution as the direct processes at the anti-crossing [1].

[1] N. Leumer, M. Grifoni, B. Muralidharan, M. Marganska, Phys. Rev. B, **103**, 165432 (2021)

TT 29.4 Fri 14:15 H7

2π Domain Walls for Tunable Majorana Devices — •Daniel Hauck[1], Stefan Rex[2,3], and Markus Garst[1] — [1]Karlsruhe Institute of Technology, Institute for Theoretical Solid State Physics, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe — [2]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [3]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe

Superconductor-magnet hybrid structures provide a platform for investigating topological phases with localized Majorana states. Such states have previously been predicted for elongated Skyrmions in the magnetic layer. Here we consider 2π domain walls that can be easily controlled experimentally. Depending on the boundary conditions, we demonstrate that localized Majorana states can be found at both ends of such walls. This establishes 2π domain walls as tunable elements for the realization of Majorana devices.

TT 29.5 Fri 14:30 H7

Majorana Bound States Induced by Antiferromagnetic Skyrmion Textures — •Sebastián A. Díaz[1,2], Jelena Klinovaja[2], Daniel Loss[2], and Silas Hoffman[3,2] — [1]Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany — [2]Department of Physics, University of Basel, Basel, Switzerland — [3]Department of Physics, University of Florida, Gainesville, USA

Majorana bound states are zero-energy states predicted to emerge in topological superconductors and intense efforts seeking a definitive proof of their observation are still ongoing. A standard route to realize them involves antagonistic orders: a superconductor in proximity to a ferromagnet. Here, we show that this issue can be resolved using antiferromagnetic rather than ferromagnetic order. We propose to use a chain of antiferromagnetic skyrmions, in an otherwise collinear antiferromagnet, coupled to a bulk conventional superconductor as a novel platform capable of supporting Majorana bound states that are robust against disorder. Crucially, the collinear antiferromagnetic region neither suppresses superconductivity nor induces topological superconductivity, thus allowing for Majorana bound states localized at the ends of the chain. Our model introduces a new class of systems where topological superconductivity can be induced by editing antiferromagnetic textures rather than locally tuning material parameters, opening avenues for the conclusive observation of Majorana bound states.

[1] S. A. Díaz, J. Klinovaja, D. Loss, S. Hoffman, arXiv:2102.03423

TT 29.6 Fri 14:45 H7

Interaction-Stabilized Topological Magnon Insulator in Ferromagnets — •Alexander Mook, Kirill Plekhanov, Jelena Klinovaja, and Daniel Loss — University of Basel, Basel, Switzerland

Condensed matter systems admit topological collective excitations above a trivial ground state, an example being Chern insulators formed by Dirac bosons with a gap at finite energies. However, in contrast to electrons, there is no particle-number conservation law for collective excitations, which gives rise to particle-number-nonconserving many-body interactions whose influence on single-particle topology is an open issue of fundamental interest in the field of topological quantum materials.

Taking magnons in ferromagnets as an example, we uncover topological magnon insulators that are stabilized by interactions through opening Chern-insulating gaps in the magnon spectrum. This finding can be traced back to the fact that the particle-number nonconserving interactions break the effective time-reversal symmetry of the harmonic theory. Hence, magnon-magnon interactions are a source of topology that can introduce chiral edge states. Importantly, interactions do not necessarily cause detrimental damping but can give rise to topological magnons with exceptionally long lifetimes. Our results demonstrate that particle-number-nonconserving many-body interactions play an important role in generating nontrivial single-particle topology.

[1] A. Mook, K. Plekhanov, J. Klinovaja, D. Loss, Phys. Rev. X 11, 021061 (2021)

Vacuum Science and Technology Division
Fachverband Vakuumphysik und Vakuumtechnik (VA)

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Overview of Invited Talks and Sessions

(Lecture hall H2)

Invited Talks

VA 1.1	Mon	10:00–10:30	H2	**Deterministic and stochastic numerical approaches in Rarefied Gas Dynamics** — •Stylianos Varoutis, Christos Tantos
VA 1.2	Mon	10:30–11:00	H2	**Deterministic modeling of neutral gas flows of tokamak nuclear fusion devices** — •Christos Tantos, Stylianos Varoutis
VA 1.3	Mon	11:00–11:30	H2	**Stochastic Simulation of Mercury Diffusion Pumps Using Direct Simulation Monte Carlo** — •Tim Teichmann, Christian Day, Thomas Giegerich
VA 2.1	Mon	11:45–12:15	H2	**IFMIF-DONES gas flow modelling using Test Particle Monte-Carlo Simulations** — •Volker Hauer
VA 2.2	Mon	12:15–12:45	H2	**Current design status and outgassing considerations for the vacuum system of the Einstein Telescope** — •Katharina Battes, Christian Day, Stefan Hanke

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Sessions

VA 1.1–1.3	Mon	10:00–11:30	H2	**Rarefied gas flows and novel approaches for particle simulation**
VA 2.1–2.2	Mon	11:45–12:45	H2	**Vacuum technology: New developments and applications**
VA 3	Mon	14:00–15:00	MVVA	**Annual General Meeting**

Annual General Meeting of the Vacuum Science and Technology Division

Monday 14:00–15:00 MVVA

- Bericht
- Wahl
- Verschiedenes

Sessions

VA 1: Rarefied gas flows and novel approaches for particle simulation

Time: Monday 10:00–11:30 Location: H2

Invited Talk VA 1.1 Mon 10:00 H2
Deterministic and stochastic numerical approaches in Rarefied Gas Dynamics — •Stylianos Varoutis and Christos Tantos — Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany
During the last decade research in the field of rarefied gas dynamics has attracted a lot of attention. This refreshed interest is due to applications in the emerging field of nano- and micro-fluidics, as well as to the more traditional fields of vacuum technology and high altitude aerodynamics. Some of these applications may include important phenomena such as those related to polyatomic gases, chemical reactions, evaporation and condensation. The gas rarefaction is specified by the Knudsen number (Kn), which is defined as the ratio of the mean free path over a characteristic length of the problem. In general, when the flow is considered as far from local equilibrium, then the well-known Navier-Stokes equations are not valid anymore. In this case, two main numerical approaches can be implemented. The first approach is based on the kinetic theory of gases as expressed by the Boltzmann equation or its associated kinetic models, in which a deterministic numerical solution is performed. The second approach is the Direct Simulation Monte Carlo (DSMC) method. Within the above framework, the first part of this talk will be devoted to the presentation of the aforementioned numerical approaches, while the second part will be devoted to the presentation of illustrative examples, as for instance, the modelling of the particle exhaust of a nuclear fusion reactor and the numerical modelling of a cryopump.

Invited Talk VA 1.2 Mon 10:30 H2
Deterministic modeling of neutral gas flows of tokamak nuclear fusion devices — •Christos Tantos and Stylianos Varoutis — Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany
Over the last few years much effort has been invested in modeling transport phenomena appearing in the complex geometry of the divertor region in tokamak fusion devices. Depending on the upstream plasma conditions, the flow reference Knudsen number, defined as the ratio of the mean free path over a characteristic length, may vary over a wide range. The rarefied flow behavior in these systems cannot be properly captured by the typical Navier-Stokes-Fourier approach and must be described by the integro-differential Boltzmann equation or reliable kinetic model equations. The Discrete Velocity Method (DVM) has developed into one of the most common techniques for solving the Boltzmann equation and the kinetic models. As it is well known simulating multidimensional rarefied gas problems based on the Boltzmann equation is computationally time consuming. Therefore, successful implementation of reliable kinetic models in such problems is important. In the present work, the Boltzmann equation is approximated by the well-known Bhatnagar Gross Krook (BGK) and Shakhov kinetic models supplemented with the deterministic discrete velocity method. Results are presented for He and D2 covering a wide range of the involved parameters. Extended comparisons between the deterministic approach and the stochastic Direct Simulation Monte Carlo (DSMC) method are presented.

Invited Talk VA 1.3 Mon 11:00 H2
Stochastic Simulation of Mercury Diffusion Pumps Using Direct Simulation Monte Carlo — •Tim Teichmann, Christian Day, and Thomas Giegerich — Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen
Currently, a continuously working pump train for DEMO (the European demonstration fusion power plant) is under active development. Mercury driven diffusion pumps have been chosen as possible candidates for the high vacuum pumping of the exhaust gases. In order to design and optimize diffusion pumps for DEMO, a reliable numerical simulation method is required.

The numerical simulation of the DEMO diffusion pumps is a complex challenge as the gas flow in the pump spans a wide Knudsen number range. Typical inlet pressures of the diffusion pumps for DEMO are expected to be in the order of 10^{-3} Pa during dwell and up to 1 Pa during burn respectively. This is equivalent to estimated Knudsen numbers in the range of 10 to 0.01. As the Navier-Stokes equations lose their validity at $Kn > 0.1$, classic continuum solvers cannot be applied to the problem at hand. Therefore, the Boltzmann equation has to be solved to describe this flow regime. In this case the Direct Simulation Monte Carlo (DSMC) method was chosen to solve the Boltzmann equation. This presentation focuses on the application of DSMC on the simulation of diffusion pumps.

VA 2: Vacuum technology: New developments and applications

Time: Monday 11:45–12:45 Location: H2

Invited Talk VA 2.1 Mon 11:45 H2
IFMIF-DONES gas flow modelling using Test Particle Monte-Carlo Simulations — •Volker Hauer — Karlsruhe Institute of Technology, Institute for Technical Physics, Karlsruhe, Germany
IFMIF, the International Fusion Materials Irradiation Facility, is a test facility for materials foreseen in fusion reactors. High neutron fluxes are generated with an energy spectrum and intensity similar to the conditions at the burn phase inside a fusion reactor. The high energy neutrons result from accelerating deuterons onto a lithium target. Simulations of the gas flow inside the IFMIF-DONES vacuum system were performed with the Test Particle Monte-Carlo code Molflow+. The IFMIF-DONES model is based on the latest design and of the LIPAc accelerator, which is being built for testing IFMIF accelerator components. Both, LIPAc and IFMIF-DONES share the same type of accelerator subsystems. The model was prepared for simulation by adding different sets of boundary conditions for the pumping of deuterium and hydrogen originating from beam losses and outgassing, respectively. The simulations of the gas pumping show pressure profiles which are mainly determined by the beam losses in this subsystem except for the Linac modules where the beam losses are very low. As LIPAc and IFMIF-DONES share most sections the pressure profiles are very similar.

Invited Talk VA 2.2 Mon 12:15 H2
Current design status and outgassing considerations for the vacuum system of the Einstein Telescope — •Katharina Battes, Christian Day, and Stefan Hanke — Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen
As third-generation, underground gravitational-wave observatory the Einstein Telescope is currently being planned in Europe. In order to enhance sensitivity compared to the current detectors as well as to expand the frequency band to lower frequencies, the length of the vacuum pipe arms will be increased to 10 km and the main optics will partly be cooled to cryogenic temperatures below 20 K.

Designed as an equilateral triangle, the Einstein Telescope will consist of six laser interferometers, which require high to ultra-high vacuum conditions. As especially residual gases like water can cryosorb as frost on the cryogenic mirror surfaces and thus degrade its optical performance, this frost formation has to be mitigated by properly designing the cryostat and additional pumping as well as considering the outgassing characteristics of the room temperature parts.

Therefore, potentially relevant materials are investigated at the Outgassing Measurement Apparatus, which uses a modified throughput method. As a result, besides total outgassing rates, information on the outgassing species are determined by a mass spectrometer.

This paper describes the current design of the Einstein Telescope vacuum system and evaluates materials and possible pre-treatments with respect to their potential application based on optimized outgassing characteristics.

VA 3: Annual General Meeting

Time: Monday 14:00–15:00 Location: MVVA

Working Group on Equal Opportunities
Arbeitskreis Chancengleichheit (AKC)

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Overview of Invited Talks and Sessions

(Lecture halls H1 and H5)

Invited Talks and Discussions

AKC 1.1	Mon	15:15–15:45	H1	**Gender and Diversity Studies as a Tool to Overcome Social Inequalities in Physics** — •Helene Götschel
AKC 1.2	Mon	15:45–16:15	H1	**Diversity in Physics?** — •Andrea B. Bossmann, Franziska Kaiser, Helene Götschel
AKC 2.1	Tue	12:00–13:00	H5	**The time after: How COVID-19 crisis redefined the R&I leadership** — •Jeanne Rubner, Burghilde Wieneke-Toutaoui, Kees Van der Beek, Sara Pirrone, Sunny Xin Wang

Sessions

AKC 1.1–1.2	Mon	15:15–16:15	H1	**Diversity in Physics**
AKC 2.1–2.1	Tue	12:00–13:00	H5	**The time after: How COVID-19 crisis redefined the R&I leadership**

Sessions

– Invited Talks and Discussions –

AKC 1: Diversity in Physics

Time: Monday 15:15–16:15 Location: H1

Invited Talk AKC 1.1 Mon 15:15 H1

Gender and Diversity Studies as a Tool to Overcome Social Inequalities in Physics — •Helene Götschel — Technische Universität Darmstadt

When we teach natural science to future scientists and engineers we are teaching more than facts, methods and concepts. We teach the 'hidden curriculum'. Teaching physics e.g. means that we transmit representations and norms of physical talent, technological competence, heroes in the history of physics, presumptions of heterosexual normativity, and hegemonic masculinity to the students. In doing so, we encourage some (male, white, middle class) students and erect barriers for others (female, students of colour, working class).

Gender and Diversity Studies is a framework to reflect on the reproduction of social inequalities. It can be understood as an eye opener for the gendered, classed and raced politics of knowledge-producing processes. In my talk I will offer some examples from my recent teaching practice and exploratory research as a physics professor to offer an inviting, open, and encouraging lecture format that overcomes social inequalities in physics education.

Discussion AKC 1.2 Mon 15:45 H1

Diversity in Physics? — •Andrea B. Bossmann[1], Franziska Kaiser[1], and Helene Götschel[2] — [1]Technische Universität Berlin — [2]Technische Universität Darmstadt

Still today, the environment in physics departments and research institutes in Germany appears to be quite homogeneous: the vast majority of physicists is cis-male, white and heterosexual. Why is it like this and what are its implications?

In this session, we aim to open a space for discussion and empowerment. The session will start with a brief overview and talk. Then a moderated discussion will follow in which everyone in the audience is invited to participate. We are looking forward to discussing with you!

AKC 2: The time after: How COVID-19 crisis redefined the R&I leadership

Time: Tuesday 12:00–13:00 Location: H5

Discussion AKC 2.1 Tue 12:00 H5

The time after: How COVID-19 crisis redefined the R&I leadership — •Jeanne Rubner[1], Burghilde Wieneke-Toutaoui[2], Kees Van der Beek[3], Sara Pirrone[4], and Sunny Xin Wang[5] — [1]Bayerische Rundfunk — [2]VDI-Association of German Engineers — [3]EPS-European Physical Society — [4]SIF-Italian Physical Society — [5]PSHK-Physical Society of Hong Kong

In these challenging times, R&I leaders and their commitment to science, education, leadership and their best practices for value-creation are being put the test. The Working Group for Equal Opportunities (AKC) of the German Physical Society invited international R&I leaders to share their experiences, best leadership practices and lessons-learned through this panel discussion. Speakers of the discussion have been selected among the leaders who supported and participated in the AKC's "Managing Work-Life Balance during the COVID-19 Crisis" study. The AKC implores those leaders to continue the charge, and asks others to join the mission.

Working Group on Energy
Arbeitskreis Energie (AKE)

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Overview of Invited Talks and Sessions

(Lecture hall H8)

Invited Talks

AKE 1.1	Mon	13:30–14:00	H8	**Elektrische Energiespeicherung mit Flüssigmetallen und Salzschmelzen** — •Tom Weier, Gerrit M. Horstmann, Steffen Landgraf, Michael Nimtz, Paolo Personnettaz, Frank Stefani, Norbert Weber
AKE 1.2	Mon	14:00–14:30	H8	**Hydrogen and e-fuels – energy systems, technology, and projects** — •Alexander Tremel
AKE 2.1	Mon	14:30–15:00	H8	**NOx und andere luftverunreinigende Stoffe in der Außenluft und in Innenräumen: Ursachen und Wirkung** — •Tunga Salthammer
AKE 2.2	Mon	15:15–15:45	H8	**Highly Efficient Monolithic Tandem Devices with Perovskite Top Cells** — •Steve Albrecht
AKE 2.3	Mon	15:45–16:15	H8	**Limits to wind energy: From the physical basis to practical implications** — •Axel Kleidon
AKE 3.1	Tue	10:00–10:30	H8	**Zur Energiewende: Zweispeicher-Modell und Pumpspeicherkraftwerke im aufgelassenen Tagebauloch** — •Gerhard Luther, Horst Schmidt-Böcking
AKE 3.2	Tue	10:30–11:00	H8	**Bioenergy: Chances and Pitfalls** — •Katja Bühler
AKE 3.3	Tue	11:15–11:45	H8	**Import options for chemical energy carriers from renewable sources to Germany** — •Johannes Hampp, Michael Düren, Tom Brown
AKE 3.4	Tue	11:45–12:15	H8	**Geothermal Energy: Risks and benefits of utilizing hot fluids from the deep underground** — •Hannes Hofmann, Simona Regenspurg, Ernst Huenges
AKE 3.5	Tue	12:15–12:45	H8	**Einsatz bildgebender Messverfahren und numerischer Modellierungswerkzeuge für die Verbesserung der Energieeffizienz industrieller Mehrphasenprozesse** — •Uwe Hampel
AKE 4.1	Tue	13:30–14:00	H8	**Nukleare Entsorgung im Kontext der internationalen Nutzung der Kernenergie** — •Thorsten Stumpf
AKE 4.2	Tue	14:00–14:30	H8	**Nuclear fusion on the way to ITER and beyond** — •Thomas Pütterich, the ASDEX Upgrade Team
AKE 4.3	Tue	14:30–15:00	H8	**Hochbelastbare Materialien für die Kernfusion: Entwicklungen und Perspektiven** — •Christian Linsmeier

Invited talks of the joint symposium Climate and energy: Challenges and options from a physics perspectiv (SYCE)

See SYCE for the full program of the symposium.

SYCE 1.1	Thu	13:30–14:00	Audimax 1	**The challenge of anthropogenic climate change - Earth system analysis can guide climate mitigation policy** — •Matthias Hofmann
SYCE 1.2	Thu	14:00–14:30	Audimax 1	**Towards a carbon-free energy system: Expectations from R&D in renewable energy technologies** — •Bernd Rech, Rutger Schlatmann
SYCE 1.3	Thu	14:30–15:00	Audimax 1	**Decarbonizing the Heating Sector - Challenges and Solutions** — •Florian Weiser
SYCE 1.4	Thu	15:15–15:45	Audimax 1	**A carbon-free Energy System in 2050: Modelling the Energy Transition** — •Christoph Kost, Philip Sterchele, Hans-Martin Henning
SYCE 1.5	Thu	15:45–16:15	Audimax 1	**The transition of the electricity system to 100% renewable energy: agent-based modeling of investment decisions under climate policies** — •Kristian Lindgren

Sessions

AKE 1.1–1.2	Mon	13:30–14:30	H8	**Thermische und chemische Energiespeicher**
AKE 2.1–2.3	Mon	14:30–16:15	H8	**Technologien für die Energiewende und ihre Implikationen I**
AKE 3.1–3.5	Tue	10:00–12:45	H8	**Technologien für die Energiewende und ihre Implikationen II**
AKE 4.1–4.3	Tue	13:30–15:00	H8	**Herausforderungen bei nuklearen Energietechnologien**

Sessions

– Invited Talks –

AKE 1: Thermische und chemische Energiespeicher

Time: Monday 13:30–14:30 Location: H8

Invited Talk AKE 1.1 Mon 13:30 H8

Elektrische Energiespeicherung mit Flüssigmetallen und Salzschmelzen — •Tom Weier, Gerrit M. Horstmann, Steffen Landgraf, Michael Nimtz, Paolo Personnettaz, Frank Stefani und Norbert Weber — Helmholtz-Zentrum Dresden - Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Deutschland

Stationäre Elektroenergiespeicher können helfen, momentane Differenzen von Elektrizitätsangebot und -nachfrage zu balancieren. Mit zunehmender Nutzung volatiler Stromquellen wird diese Aufgabe wichtiger. Dabei stehen verschiedene Speichertechnologien untereinander, aber auch mit Alternativen im Wettbewerb.

Flüssigmetallbatterien sind Hochtemperaturspeicher. Sie basieren auf der stabilen Dichteschichtung eines Alkalimetalls, einer Salzschmelze und eines Schwermetalls. Vermittelt durch die hohe Betriebstemperatur, die über den Schmelztemperaturen der einzelnen Phasen liegen muss, verlaufen Grenzflächenreaktionen und Transportvorgänge sehr rasch, was in hohen Strom- und Leistungsdichten resultiert. Der vollständig flüssige Zellinhalt ermöglicht einerseits eine konzeptionell einfache Skalierbarkeit auf Zellebene, die sehr günstige energiebezogene Investitionskosten verspricht. Andererseits gewinnen durch den flüssige Aggregatzustand strömungsmechanische Vorgänge, die eng an den Ladungstransport und -übergang gekoppelt sind, stark an Bedeutung.

Der Vortrag wird sowohl ausgewählte physikalische Phänomene in Flüssigmetallbatterien vorstellen, als auch ihre mögliche Rolle in einem zukünftigen Energiesystem diskutieren.

Invited Talk AKE 1.2 Mon 14:00 H8

Hydrogen and e-fuels – energy systems, technology, and projects — •Alexander Tremel — Siemens Energy, New Energy Business, Erlangen, Germany

Electricity is traditionally the most valuable form of energy – from a thermodynamic and economic perspective. This paradigm is likely to erode in the coming years since renewable power generation will be among the lowest cost energy options in many countries of the world. Power-to-X technologies are suited for the conversion of fluctuating renewable electricity and provide hydrogen and e-fuels. The presentation will outline recent developments in energy systems and will focus on technology and projects in the Power-to-X value chain.

AKE 2: Technologien für die Energiewende und ihre Implikationen I

Time: Monday 14:30–16:15 Location: H8

Invited Talk AKE 2.1 Mon 14:30 H8

NOx und andere luftverunreinigende Stoffe in der Außenluft und in Innenräumen: Ursachen und Wirkung — •Tunga Salthammer — Fraunhofer WKI, Bienroder Weg, 38108 Braunschweig

Regional gesehen wirken sich die derzeitigen klimatischen Veränderungen sehr unterschiedlich aus, da neben den Treibhausgasen auch die Freisetzung von Luftschadstoffen wie Partikel, Ozon und NOx eine wichtige Rolle spielt. Für die in Deutschland herrschenden Verhältnisse sind mögliche Auswirkungen des Klimawandels bereits recht gut untersucht. Umso mehr überrascht es, dass Aussagen zu den möglichen Konsequenzen für das im Innenraum herrschende Mikroklima bislang weitgehend fehlen. Aber auch im Innenraum selbst sind viele potentielle Quellen vorhanden, die zur Bildung von Partikeln und NOx führen. Dies sind in der Regel diverse Verbrennungsprozesse, insbesondere Kerzen, Ethanolöfen, holzbefeuerte Öfen und nach wie vor das Rauchen. Ozon wird heute im Wesentlichen von Luftreinigern und andere elektrischen Geräten in die Raumluft freigesetzt. Darüber hinaus tragen die durch Reaktionen von NOx und Ozon mit ungesättigten Kohlenwasserstoffen entstehenden Abbauprodukte und gebildeten Nanopartikel ebenfalls zur Innenraumluftbelastung bei. Unter Berücksichtigung der Bildungsmechanismen von Partikeln, NOx, Ozon und weiterer luftverunreinigender Stoffe in Innen- und Außenluft, sowie unter Einbeziehung klimatischer Parameter, lassen sich zeitliche Trends analysieren und Annahmen über zukünftige Entwicklungen treffen, was ggf. Konsequenzen für Neu- und Bestandsbauten sowie für zukünftiges Wohnverhalten bedingt.

15 min. break

Invited Talk AKE 2.2 Mon 15:15 H8

Highly Efficient Monolithic Tandem Devices with Perovskite Top Cells — •Steve Albrecht — Helmholtz-Center Berlin, Young Investigator Group Perovskite Tandem Solar Cells

Integrating metal halide perovskite top cells with crystalline silicon or CIGS bottom cells into monolithic tandem devices has recently attracted increased attention due to the high efficiency potential of these cell architectures. To further increase the tandem device performance to a level well above the best single junctions, optical and electrical optimizations as well as a detailed device understanding of this advanced tandem architecture need to be developed. In this talk, Prof. Albrecht will present the recent results on monolithic tandem combinations of perovskite with crystalline silicon and CIGS, as well as tandem relevant aspects of perovskite single junction solar cells. Finally, it will be shown how utilization of a self-assembled molecular monolayer (SAM) and fine tuning of the perovskite band gap in perovskite/silicon tandem solar cells further improved the efficiency to 27.5% and to 23.3% for perovskite/CIGS tandems, the latter being a certified world record efficiency.

Invited Talk AKE 2.3 Mon 15:45 H8

Limits to wind energy: From the physical basis to practical implications — •Axel Kleidon — Max-Planck-Institut für Biogeochemie, Jena

Wind energy plays an increasing role in the transition to a carbon-free sustainable energy system. In this talk, I first use thermodynamics to describe how and how much wind energy is generated by the atmosphere from differences in radiative heating. I then show that only a fraction of the kinetic energy can at best be used as renewable energy because the more wind turbines draw energy from the atmosphere at the regional scale, the lower the wind speeds, thus lowering power output and efficiencies of wind turbines. This results in much lower wind power potentials of about 0.5 Watt per square meter of surface area at the regional scale than estimates that are based on observed wind fields and that neglect the effects that wind turbines have on the atmosphere. I demonstrate the practical implications of this Earth system approach to wind energy by re-evaluating German energy scenarios for the year 2050, which rely on a substantial fraction of offshore wind energy.

AKE 3: Technologien für die Energiewende und ihre Implikationen II

Time: Tuesday 10:00–12:45 Location: H8

Invited Talk AKE 3.1 Tue 10:00 H8

Zur Energiewende: Zweispeicher-Modell und Pumpspeicherkraftwerke im aufgelassenen Tagebauloch — •Gerhard Luther[1] und Horst Schmidt-Böcking[2] — [1]Universität des Saarlandes, Saarbrücken, Experimentalphysik, F.St. Zukunftsenergie — [2]Universität Frankfurt/Main, Institut für Kernphysik

Die *Energiewende* umfasst die nahezu vollständige Abdeckung der elektrischen Stromversorgung durch regenerative Energien (RE) und hier vor allem durch Wind und Photovoltaik (PV). Wegen des durch Wetter und Astronomie bedingten ungleichmäßigen Dargebotes der RE lässt sie sich nur mit dem Einsatz von Speichern durchführen. Das Speicherproblem in Deutschland wurde durch eine Kombination von Kurz- und Langzeitspeichern mit dem *Zwei-Speichermodell* modelliert. Es ergab sich, dass eine Kapazität des Kurzzeitspeichers von nur 0,20 bis 0,30 Volllasttage für Deutschland ausreicht.

Es wird ein Vorschlag gemacht, wie man diese Speicherkapazität durch geeignete Nachnutzung aufgelassener Tagebaulöcher bereitstellen kann, indem man den Rekultivierungs- Restsee sowohl als Ober- als auch als Unterbecken einer großen Pumpspeicherkraftwerksanlage einsetzt.

Invited Talk AKE 3.2 Tue 10:30 H8

Bioenergy: Chances and Pitfalls — •Katja Bühler — Helmholtz Center for Environmental Research, Leipzig, Germany

In times of climate change and severe pressure on the natural resources of our planet bioenergy is a very controversial discussed topic. Bioenergy covers a broad field, reaching from the production of biofuels like ethanol and diesel from crop-based sugars, to the conversion of lignocellulose and microalgae. All mentioned approaches rely on the exploitation of biomass for energy production. Although significant progress was achieved in those technologies in recent years, biofuels still have problems to become established in the market. One reason certainly is the current low oil price which is a negative incentive for this technology. However, another major point in this discussion is the environmental footprint of bioenergy. Issues connected to land use, low efficiencies, tedious product isolation and the low energy return of invest make it questionable whether bioenergy in its current form is able to make a contribution to sustainable, CO2-neutral energy production. This presentation will lead through the different generations of bioenergy, discussing potentials and drawbacks. The focus will be on the so-called fourth-generation fuels, for which microorganisms are utilized as light-driven cell factories for fuel production directly from carbon dioxide, in my opinion the only concept with the chance to become a true bioenergy technology one day.

15 min. break

Invited Talk AKE 3.3 Tue 11:15 H8

Import options for chemical energy carriers from renewable sources to Germany — •Johannes Hampp[1], Michael Düren[1,2], and Tom Brown[3,4] — [1]Center for international Development and Environmental Research, Justus Liebig University Giessen — [2]II. Physikalisches Institut, Justus Liebig University Giessen — [3]Institute for Automation and Applied Informatics, Karlsruhe Institute of Technology — [4]Department of Digital Transformation in Energy Systems, Technische Universität Berlin

Ambitious climate targets and the need for a more sustainable energy system will require significant changes to the energy sectors of transport, heating and industry. Electrification will be the most sustainable option in many areas. Some applications however but certain applications will continue to require chemical energy carriers in future, especially long-distance aviation, shipping vessels and the chemical industry.

At present Germany is importing most of its primary energy (> 70%) in the form of fossil chemical energy carriers from foreign countries. Since Germany is lacking abundant potentials for renewable energy, it can be expected that Germany will continue imports of chemical energy carriers in the future.

We model potential energy supply chains for most prominent chemical energy carriers (hydrogen, methane, methanol, ammonia, Fischer-Tropsch fuels) and different transport options (electrical transmission lines, pipelines, shipping). Thereby we obtain the cost of energy and hydrogen for each energy supply chain allowing us to compare potential future export partners.

For example, Denmark makes for a good export partner with a combination of large offshore wind potentials and its close proximity to Germany. The Danish export volume however is limited. Thus, it is necessary to consider other potential exporters for larger import volumes within the EU (e.g. Spain), across the Mediterranean Sea (e.g. Morocco, Egypt, Saudi Arabia) or even worldwide (e.g. Argentina or Australia).

Depending on the individual chemical energy carrier and mode of transport, different export partners show different techno-economic potentials for exports to Germany.

Invited Talk AKE 3.4 Tue 11:45 H8

Geothermal Energy: Risks and benefits of utilizing hot fluids from the deep underground — •Hannes Hofmann, Simona Regenspurg, and Ernst Huenges — Helmholtz Centre Potsdam GFZ German Research Centre for Geosciences Section 4.8 Geoenergy Telegrafenberg, D-14473 Potsdam, Germany

In a geothermal fluid loop, formation water is pumped from a deep reservoir through a production well to the surface, where the heat is extracted and used for heating or electricity production. The cooled fluid is injected through another well back into the reservoir. The geological formations that are suitable for geothermal energy exploitation need to show two main characteristics: High temperature and high permeability. Typically, geothermal energy is exploited in areas with high geothermal gradient which are mainly located along tectonic plate boundaries. However, nowadays, the exploitable geothermal resources are found throughout the world and are utilized in 83 countries. Because of the lower temperatures in German geothermal plants, here most geothermal wells provide heat (about 1.49 GWh/a; source: www.Geotis.de). One of the main challenges when operating a geothermal plant is the correct handling of the geothermal fluids that carry the heat from the deep reservoirs to the surface. The high salinity and high amount of dissolved gasses of formation waters results in a variety of chemical reactions during fluid processing such as mineral precipitation and corrosion. However, these risks may be mitigated with different reservoir engineering methods and fluid chemistry might also represent a benefit if the dissolved components are of economic value.

Invited Talk AKE 3.5 Tue 12:15 H8

Einsatz bildgebender Messverfahren und numerischer Modellierungswerkzeuge für die Verbesserung der Energieeffizienz industrieller Mehrphasenprozesse — •Uwe Hampel — Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — Technische Universität Dresden, 01062 Dresden, Germany

Stoff- und Energieumwandlungsprozesse in technischen Apparaten sind oft an Mehrphasenströmungen gekoppelt. Beispiele dafür sind Chemiereaktoren, Stoffaustauschapparate, Kraftwerksanlagen oder Abwasserbehandlungsanlagen. Für die Modellierung der Strömungsvorgänge wurden in der jüngeren Vergangenheit numerische Berechnungsverfahren der Computational Fluid Dynamics entwickelt. Für diese besteht immer wieder die Aufgabe, sie mit realen Messdaten aus Strömungsexperimenten unter prozessähnlichen Bedingungen zu validieren bzw. aus solchen Messdaten Modelle und Korrelationen abzuleiten.

Der Vortrag gibt einen Einblick in die Nutzung innovativer schneller Bildgebungsverfahren für Mehrphasenströmungen für diesen Zweck. Vorgestellt werden die Gittersensortechnik sowie die ultraschnelle Röntgentomographie, welche am Helmholtz-Zentrum Dresden-Rossendorf entwickelt wurden. Mit beiden Bildgebungsverfahren ist die tomographische Analyse von Mehrphasenströmungen mit Bildraten von mehr als 1000 Bildern pro Sekunde sowie einer räumlichen Auflösung im Millimeterbereich möglich. Ihre Anwendung wird anhand verschiedener Beispiele für die Optimierung energieintensiver Prozesse, wie etwa Destillation und Abwasserbehandlung, exemplarisch diskutiert.

AKE 4: Herausforderungen bei nuklearen Energietechnologien

Time: Tuesday 13:30–15:00 Location: H8

Invited Talk AKE 4.1 Tue 13:30 H8

Nukleare Entsorgung im Kontext der internationalen Nutzung der Kernenergie — •Thorsten Stumpf — Helmholtz-Zentrum Dresden-Rossendorf e.V.

Im Jahr 2022 wird das letzte deutsche Kernkraftwerk abgeschaltet werden. Die bis dahin angefallenen hochradioaktiven Abfälle warten auf ihre Entsorgung. Zu diesem Thema hat im Juli 2016 die *Kommission zur Lagerung hoch radioaktiver Abfallstoffe gemäß * 3 Standortauswahlgesetz* ihren Abschlussbericht veröffentlicht. Auf Basis dieses Berichtes der Endlagerkommission wurde im März 2017 eine Novelle des Standortauswahlgesetzes durch Bundestag und Bundesrat beschlossen. Das Gesetz schreibt nun eine mehrphasige Suche nach einem Standort mit bestmöglicher Sicherheit vor. Die damit verbundene Diskussion um mögliche zukünftige Standorte zur Errichtung eines Endlagers für hochradioaktive Abfälle in Deutschland rückt auch die Endlagerforschung in den öffentlichen Fokus. Die wissenschaftlichen Grundlagen zur Unterstützung des Auswahlverfahrens werden in dem Vortrag vorgestellt und diskutiert. Zudem wird ein Blick auf den aktuellen Stand zur Forschung, zur Planung und zum Bau eines Endlagers im Ausland geworfen.

Invited Talk AKE 4.2 Tue 14:00 H8

Nuclear fusion on the way to ITER and beyond — •Thomas Pütterich and the ASDEX Upgrade Team — Max Planck Institute for Plasma Physics, Garching, Germany

One of the paths to achieving nuclear fusion on earth is the confinement of hot plasma in a magnetic device, called tokamak. In the largest one, ITER, which is currently being built in the south of France, a burning deuterium-tritium plasma will require core ion temperaturesabove 10 keV (100 Mio °C) at densities around 10^20 m^-3. In the core of a tokamak plasma turbulence is the dominant transport mechanism limiting the temperature gradient length. Therefore, the plasma edge acts as boundary condition to the core, and its temperature value is a crucial quantity which determines the performance of a tokamak plasma. In steady state conditions, all heat, that is deposited or produced in the centre, is transported across the plasma edge towards the wall. It is therefore crucial to taylor the plasma edge in a way to provide conditions for safe operation without damaging the plasma facing components. In this talk the most important ingredients of the physical properties of the tokamak plasma will be explained. The status of knowledge will be shown together with possible options for the operation in ITER, and the path to a demonstration power plant is illustrated.

Invited Talk AKE 4.3 Tue 14:30 H8

Hochbelastbare Materialien für die Kernfusion: Entwicklungen und Perspektiven — •Christian Linsmeier — Forschungszentrum Jülich, Institut für Energie- und Klimaforschung - Plasmaphysik, 52425 Jülich

Wolfram ist derzeit das bevorzugte Wandmaterial für zukünftige Fusionsreaktoren. Es verbindet eine geringe Tritiumrückhaltung für sicheren Betrieb mit sehr geringen Erosionsraten und einem hohen Schmelzpunkt für eine lange Lebensdauer der Wandkomponenten. Darüber hinaus erlaubt die hohe Wärmeleitfähigkeit eine gute Energieabfuhr und das relativ schnelle Abklingen der neutroneninduzierten Radioaktivität ein Recycling nach Stilllegung des Reaktors ohne geologische Lagerung. Sprödigkeit und die hohe Oxidationsrate bei hohen Temperaturen sind jedoch große Herausforderungen an die Fertigung und mechanische Belastbarkeit der Komponenten sowie den sicheren Umgang im Falle eines Kühlmittelverlusts.

Wir beschreiben in diesem Beitrag neue Konzepte zur Weiterentwicklung von Wolfram auf der Basis von faserverstärkten Verbundwerkstoffen und Legierungen, die den Einsatzbereich des Wandmaterials deutlich erweitern. Für die zügige Entwicklung dieser Konzepte zu fertigen Komponenten ist die Qualifizierung dieser neuen Materialkonzepte unter fusionsrelevanten Lastbedingungen notwendig. Bestehende und derzeit im Forschungszentrum Jülich neu gebaute Testanlagen werden vorgestellt, die auch den Einfluss von Neutronenschäden untersuchen lassen.

Working Group on Physics, Modern IT and Artificial Intelligence
Arbeitskreis Physik, moderne Informationstechnologie und Künstliche Intelligenz (AKPIK)

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Overview of Posters and Sessions

(Poster P)

Sessions

AKPIK 1.1–1.4	Tue	11:15–12:45	H1	**RDM I: NFDI consortia (joint session AGI/AKPIK)**
AKPIK 2.1–2.5	Tue	13:30–16:30	H1	**RDM II: Perspectives in Research Data Management (joint session AGI/AKPIK)**
AKPIK 3.1–3.7	Thu	13:30–15:30	P	**AKPIK Postersession**

Sessions

– Invited, Topical Talks, and Posters –

AKPIK 1: RDM I: NFDI consortia (joint session AGI/AKPIK)

Time: Tuesday 11:15–12:45 Location: H1

See AGI 1 for details of this session.

AKPIK 2: RDM II: Perspectives in Research Data Management (joint session AGI/AKPIK)

Time: Tuesday 13:30–16:30 Location: H1

See AGI 2 for details of this session.

AKPIK 3: AKPIK Postersession

Time: Thursday 13:30–15:30 Location: P

AKPIK 3.1 Thu 13:30 P

Towards optical neuromorphic hardware at Cesium wavelength — •Elizabeth Robertson[1,2], Mingwei Yang[1], Luisa Esguerra[1], Leon Messner[1], Lina Jaurigue[2], Guillermo Gallego[2,3], Kathy Lüdge[2], and Janik Wolters[1,2,3] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Institute for Optical Sensor Systems, Rutherfordstraße 2, 12489 Berlin, Germany — [2]Technische Universität Berlin, Str. des 17. Junis 135, 10623 Berlin, Germany — [3]Einstein Center Digital Future Robert-Koch-Forum, Wilhelmstraße 67, 10117 Berlin, Germany

With the exponential growth of research in Machine Learning, so too has the demand for fast, energy efficient neuromorphic hardware, to execute such algorithms. Optics provides an attractive tool for implementing neuromorphic hardware due to is speed, low crosstalk and high parallelism. In particular, convolutional- and recurrent neural networks benefit from an optics implementation; by using passive optics to carry out convolution [1], and time division multiplexing to demonstrate a reservoir computer [2]. We present our results towards realizing an optical convolutional neural network with an atomic nonlinearity [3] and an all-optical reservoir computer based on a delay loop with an additional optical random-access memory (RAM)[4].

[1] Miscuglio, M. et al. Optica 7, 1812-1819 (2020).
[2] Brunner, D., et al. Nat Commun 4, 1364 (2013).
[3] Yang, M. et al. CLEO/Europe-EQEC, poster JSIV-P.4 (2021).
[4] Wolters, J., et al. Phys. Rev. Lett. 119, 060502 (2017).

AKPIK 3.2 Thu 13:30 P

Optical Convolutional Neural Network with Atomic Non linearity — •Mingwei Yang[1,2], Elizabeth Robertson[2,3], Luisa Esguerra[2,3], and Janik Wolters[2,3] — [1]Humboldt Universität zu Berlin, Newtonstr.15, D 12489 Berlin, Germany — [2]Deutsches Zentrum für Luft und Raumfahrt e.V. (DLR), Rutherfordstraße 2, D 12489, Berlin, Germany — [3]Technische Universität Berlin, Straße des 17. Juni 135, D 10623, Berlin, Germany

An optical convolutional neural network is demonstrated in which linear operations are implemented by lenses and spatial light modulators (SLMs), while an optical nonlinearity is realized by a cesium vapor cell as a saturable absorber. We use this network to demonstrate non-linear image processing, as well as to improve the classification of the MNIST data by a single layer fully connected.

AKPIK 3.3 Thu 13:30 P

Convolutional Neural Network Framework for the Analysis of X-ray photoelectron spectra — •Lukas Pielsticker[1], Rachel L. Nicholls[1], Gudrun Klihm[1], Robert Schlögl[1,2], and Mark Greiner[1] — [1]Department Heterogeneous Reactions, Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr — [2]Department Inorganic Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin

X-ray photoelectron spectroscopy (XPS) enables studying the electronic structure and chemical state of solid materials and their surfaces. Quantitative analysis of the phases present in XP spectra is typically performed by manual peak fitting. However, such elemental quantification often suffers from, among other things, superposition of core-levels of different elements, incorrect instrument calibration, poor choice of backgrounds and lineshapes, as well as from noise in the data. Moreover, as XPS instruments are becoming increasingly automated and capable of producing large amounts of data, an equally automated approach to elemental quantification is desirable.

Here, a scalable automation framework for XPS analysis using Convolutional Neural Networks (CNNs) is presented. For model training, synthetic mixed metal-oxide spectra were generated based on known reference spectra. CNNs are shown to be capable of quantitatively determining the presence of metallic and oxide phases, as well as identifying morphological features such as over- and sublayers, exhibiting more reliable performance than standard XPS users. The use of Bayesian CNNs for the determination of quantification uncertainty is illustrated.

AKPIK 3.4 Thu 13:30 P

Conversion of Molecular Dynamics (MD) simulations to Neutronand X-Ray Scattering Data using High Performance Computing — •Arnab Majumdar[1], Sebastian Busch[1], and Martin Müller[2] — [1]Lichtenberg Strasße 1, 85747, Garching b. München — [2]Leibnitz Straße 19, 24098, Kiel

Sassena is one of the software solutions to convert molecular dynamics (MD) simulations into elastic and quasi-/inelastic neutron and X-ray scattering curves. Current work makes an effort to introduce different strategies of parallel computing into sassena. Parallel computing can be a huge leap in the journey of reducing the computing time within sassena. It consists of different strategies like distributed memory parallelization(MPI), shared memory parallelization (OpenMP) and vectorization. Sassena inherits distributed memory parallelization from its previous version. This work further augments vectorization and shared memory parallelization into it. Through vectorization, this work bolsters the computing speed of sassena to a new height of up to an order of magnitude faster than its previous version. On the other hand, shared memory parallelization introduces a possibility of doing hybrid parallelization within sassena. Furthermore, this work plans to benefit from the achieved performance gain by validating simulations of hydrogen storage materials with neutron scattering data.

AKPIK 3.5 Thu 13:30 P

Making computation material science data FAIR — •Jens Bröder[1,2], Volker Hofmann[1,2], Daniel Wortmann[3], Stefan Blügel[3], and Stefan Sandfeld[1,2] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Helmholtz Metadata Collaboration, Hub Information — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

For research data to be reusable by scientists or machines, the gathered research data and metadata should comply with the so-called "FAIR principles", i.e. it should be findable, accessible, interoperable, and reusable [1], a task which is not straightforward. In computational materials science, workflows often encompass many different simulation steps. The enrichment of data with detailed metadata is often only feasible close to the data creation process. Therefore, designated software, workflows, tools and standards will be needed throughout the community. Using an exemplary research project, we show in detail how to reconcile data from simulations with FAIR principles. The project contains data from a high-throughput simulation performed with the program FLEUR (www.flapw.de) using the AiiDA framework (https://aiida.net) on over 5000 different materials. All data and software is openly available and FAIR through the materialscloud archive [2]. We also discuss challenges for the domain of material science and how the Helmholtz Metadata Collaboration (HMC) tries to address these issues. [1] Wilkinson, M.D.et al. Sci Data 3, 160018 (2016) [2] L. Talirz et al., Sci Data 7, 299 (2020)

AKPIK 3.6 Thu 13:30 P

Design and validation of a Digital Twin for prostate cancer from a physics point of view — •Carlos Andres Brandl[1], Anna Nitschke[1], and Matthias Weidemüller[1,2] — [1]Physikalisches Institut, Ruprecht-Karls Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany — [2]National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, and CAS Center for Excellence and Synergetic Innovation Center in Quantum Information and Quantum Physics, Shanghai Branch, University of Science and Technology of China, Shanghai 201315, China

Digital Twins (DT) are virtual representations of physical assets and e.g. promise improved decision making. DT can help to personalize healthcare for complex diseases like prostate cancer by combining large amount of clinical parameters and answering the questions of tumor risk, tumor stage and optimal treatment. In medical applications interpretability and uncertainty quantification are crucial.

Combining data-driven approaches with interpretable machine-learning models and evidence based clinical guidelines will lead to more reliable and confidential outcomes. Correlation analysis gives an insight to the data and enables to unravel the dependencies of important clinical parameters like prostate specific antigen (PSA) with others and determine their distributions in the Heidelberg patient cohort. The backpropagation of outcome errors to the found distributions of the input parameters with Bayesian methods allows to determine the impact of the input parameter uncertainties on the twin predictions and helps clinicians to interpret the results accordingly.

AKPIK 3.7 Thu 13:30 P

Comparison of structural representations for machine learning-accelerated *ab initio* calculations — •Johannes Wasmer, Philipp Rüssmann, and Stefan Blügel — Forschungszentrum Jülich, Germany

Quantum mechanical calculations based on density functional theory (DFT) are the workhorse in today's computational materials design. Here we explore the possibility to accelerate the DFT calculations with potentials generated from a surrogate machine learning model. Finding a better starting potential could drastically reduce the number of required self-consistency steps during the convergence of DFT calculations. The juKKR code (jukkr.fz-juelich.de) allows high-throughput *ab initio* impurity embedding calculations which we use to generate a training dataset of 10'000 impurities from most elements of the periodic table embedded into elemental crystals with the help of the workflow engine AiiDA. The choice of a structural representation of the atomic environment which a machine learning model can understand has been identified as a crucial step. We compare a variety of such representations as training input for our surrogate model. Finally, we benchmark results for the converged impurity potential from DFT calculations against the output of the trained surrogate model.

We acknowledge support by the Joint Lab Virtual Materials Design, by the DFG under Germany's Excellence Strategy Cluster of Excellence ML4Q, by the AIDAS2 virtual lab, and thank for computing time provided on the JARA Partition part of the supercomputer CLAIX at RWTH Aachen University.

Working Group on Physics and Disarmament
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Zur Abrüstung, der Verhinderung der Verbreitung von Massenvernichtungsmitteln und der Beurteilung neuer Waffentechnologien sind naturwissenschaftliche Untersuchungen unverzichtbar. Auch bei der Verifikation von Rüstungskontrollabkommen werden neue Techniken und Verfahren benötigt und eingesetzt. Schwerpunkte in diesem Jahr bilden Themen wie die nukleare Abrüstung, Verifikation bzw. die Detektion von Nuklearanlagen und Materialien, Raketenabwehr und Zerstörung von Nuklearsprengköpfen, neue militärrelevante Technologien wie Drohnen. Die Fachsitzung wird von der DPG gemeinsam mit dem Forschungsverbund Naturwissenschaft, Abrüstung und internationale Sicherheit FONAS durchgeführt. Die 1998 gegründete Arbeitsgruppe Physik und Abrüstung ist für die Organisation verantwortlich. Die Sitzung soll international vorrangige Themen behandeln, Hintergrundwissen vermitteln und Ergebnisse neuerer Forschung darstellen.

Overview of Invited Talks and Sessions

(Lecture hall H8)

Max von Laue Lecture

PV XVI	Thu	18:30–19:30	MVL	**Max von Laue Lecture: What physicists can do to improve international security?** — •Steve Fetter

Invited Talks

AGA 2.1	Thu	11:15–12:00	H8	**TPNW Verification: Domains, Boundary Conditions, Priorities & Problems** — •Thomas E. Shea
AGA 2.2	Thu	12:00–12:45	H8	**International Partnership for Nuclear Disarmament Verification: Current Status and Future Prospects** — •Irmgard Niemeyer, Gerald Kirchner, Götz Neuneck
AGA 3.1	Thu	13:30–14:15	H8	**Denuclearization of the Korean Peninsula** — •Tariq Rauf
AGA 3.2	Thu	14:15–15:00	H8	**The DPRK's SLBMs and SRBMs - A Brief Update on North Korea's Missile Activities** — •Markus Schiller
AGA 3.3	Thu	15:15–16:00	H8	**One Size does not Fit All: Greatly Different Mandates for Denuclearizing Nuclear States** — •Robert Kelley
AGA 4.1	Thu	16:00–16:45	H8	**The Space Debris Challenge and ESA's Space Safety Programme** — •Holger Krag

Sessions

AGA 1.1–1.2	Thu	10:00–11:15	H8	**Disarmament Verification I**
AGA 2.1–2.2	Thu	11:15–13:30	H8	**Disarmament Verification II**
AGA 3.1–3.3	Thu	13:30–16:00	H8	**North Korea: Denuclearization**
AGA 4.1–4.1	Thu	16:00–16:45	H8	**Space Security**
AGA 5	Thu	17:00–18:00	MVAGA	**Annual General Meeting**
AGA 6.1–6.2	Fri	10:00–11:15	H8	**Non-Proliferation and Nuclear Verification**
AGA 7.1–7.2	Fri	11:15–12:30	H8	**Nuclear Archeology**
AGA 8.1–8.2	Fri	12:30–13:30	H8	**Preventive Arms Control**

Annual General Meeting of the Working Group on Physics and Disarmament

Thursday 17:00–18:00 MVAGA

1. Report of the activities 2020/2021
2. Election of the speakers
3. Future Activities

Sessions

– Invited and Contributed Talks –

AGA 1: Disarmament Verification I

Time: Thursday 10:00–11:15 Location: H8

AGA 1.1 Thu 10:00 H8

Zur Validierung von Monte-Carlo-Simulationen mit GEANT4 im Rahmen nuklearer Abrüstungsverifikation — •Manuel Kreutle[1], Alessandro Borella[2], Riccardo Rossa[2], Celine Scholten[1], Gerald Kirchner[1] und Claas van der Meer[2] — [1]Carl-Friedrich von Weizsäcker-Zentrum für Naturwissenschaften und Friedensforschung, Universität Hamburg — [2]Belgian Nuclear Research Centre SCK CEN, Mol, Belgien

Im Rahmen der Arbeit der Internationalen Partnerschaft zur Verifikation nuklearer Abrüstung (IPNDV) wurde eine internationale Übung im Kernforschungszentrum SCK CEN in Mol, Belgien, durchgeführt. Zusätzlich zu den Messungen wurden Monte-Carlo-Simulationen durchgeführt, um die Neutronensignaturen der verschiedenen vorhandenen Aufbauten zu rekonstruieren. In diesem Beitrag werden Simulationsergebnisse zum effektiven Neutronenmultiplikationsfaktor k_{eff}, zu Neutronenflussdichten und zur räumliche Verteilungen von Neutronenwechselwirkungsprozessen vorgestellt, welche mit Hilfe von GEANT4 berechnet wurden. Im Vergleich von k_{eff}-Ergebnissen mit MCNP- und KENO-Simulationen konnte die gute Leistung von GEANT4 nachgewiesen werden. Auch die Flussdichten für epithermische und schnelle Neutronen, welche mit GEANT4 und KENO berechnet wurden, stimmen in zufriedenstellendem Maß überein. Die vorliegenden Daten tagen somit zur Validierung der GEANT4-Neutronenphysik in Systemen mit spaltbarem Material, so wie z.B. im Rahmen von nuklearer Abrüstungsverifikation, bei.

AGA 1.2 Thu 10:30 H8

Einfluss von Betonwänden auf Neutronenstrahlung — •Svenja Sonder und Gerald Kirchner — Universität Hamburg, Carl Friedrich von Weizsäcker-Zentrum für Naturwissenschaft und Friedensforschung (ZNF), Beim Schlump 83, 20144 Hamburg

Neutronenmessungen spielen sowohl bei der Abrüstungsverifikation von nuklearen Waffen als auch bei zivilen Safeguards eine wichtige Rolle. Dabei haben die Größe des Raumes und die Beschaffenheit der Wände einen deutlichen Einfluss auf die Neutronenflussdichten, sodass begleitende Simulationen ohne Berücksichtigung der Wände die Realität nicht adäquat abbilden. Daher wurden am ZNF Simulationen durchgeführt, um den Einfluss von Betonwänden auf die Neutronenmessungen zu untersuchen.

Zur Simulation wurde das am CERN entwickelte Programm GEANT4 verwendet, welches aufgrund seiner Vielseitigkeit in verschiedensten Bereichen der Physik – von Hochenergiephysik bis zur medizinischen Bildgebung – eingesetzt wird. Dabei wird mithilfe von Monte-Carlo-Simulationen der Teilchentransport simuliert.

In diesem Vortrag soll der Einfluss von Betonwänden auf die Messungen innerhalb eines Raumes quantifiziert werden. Dabei wird ein besonderer Fokus auf die Änderung der Neutronenflussdichten und deren Energieverteilungen in räumlicher Nähe zu den Wänden gelegt. Darüber hinaus werden die verschiedenen Wechselwirkungsprozesse zwischen Neutronen und Beton beleuchtet.

15 min. break

AGA 2: Disarmament Verification II

Time: Thursday 11:15–13:30 Location: H8

Invited Talk AGA 2.1 Thu 11:15 H8

TPNW Verification: Domains, Boundary Conditions, Priorities & Problems — •Thomas E. Shea — Vienna

The TPNW provides a potential framework for eliminating existing arsenals in all nine nuclear-armed states, eliminating critical nuclear weapons infrastructure, and detecting any attempts to rearm in the future. The TPNW will require a verification system tailored to each nuclear-armed state reflecting its nuclear programs and respecting its laws governing nuclear safety and security. Each verification system should address eleven pursuits. Full verification will be costly, sometimes controversial, and will likely require prolonged periods before a state can be declared to be disarmed. Finding hidden weapons and clandestine manufacturing and support facilities will require the use of information obtained by the verification authorities together with information provided by states and other parties. Cybersecurity considerations will govern which verification technologies will be approved by each nuclear-armed state to prevent espionage and approved by the verification authorities to assure scientific authenticity

Invited Talk AGA 2.2 Thu 12:00 H8

International Partnership for Nuclear Disarmament Verification: Current Status and Future Prospects — •Irmgard Niemeyer[1], Gerald Kirchner[2], and Götz Neuneck[3] — [1]Forschungszentrum Jülich — [2]ZNF Universität Hamburg — [3]IFSH Universität Hamburg

The International Partnership for Disarmament Verification (IPNDV) includes technical experts and government representatives from Nuclear Weapon States and Non-Nuclear Weapon States to work jointly on procedures and technologies that would allow for effective verification of nuclear disarmament. In Phase I (2016-2017), IPNDV identified 14 key steps in the nuclear weapons dismantlement lifecycle. In Phase II (2018-2019), IPNDV broadened its work to consider wider aspects of nuclear disarmament verification while at the same time deepen the work on specific elements of verification. In moving from paper to practice, five practical exercises and technology demonstrations were conducted, including the Nuclear Disarmament Verification (NuDiVe) Exercise, co-hosted by Germany and France. Phase III (2020-2025) builds on current working methods and engages in further hands-on activities, including scenario-based discussions, practical exercise, such as NuDiVe 2021, and technology demonstrations. The talk will discuss the Partnerships' achievements so far and give an outlook to the next steps.

45 min. lunch break

AGA 3: North Korea: Denuclearization

Time: Thursday 13:30–16:00 Location: H8

Invited Talk AGA 3.1 Thu 13:30 H8

Denuclearization of the Korean Peninsula — •Tariq Rauf — Vienna

Tariq Rauf (former Head of Verification and Security Policy, International Atomic Energy Agency, responsible for the Director General's report on Application of Safeguards in the Democratic People's Republic of Korea). Nuclear weapons were first introduced into the Korean Peninsula in January 1958 by the US through its defence alliance with South Korea. During the inter-Korean war, the US threatened three times to use nuclear weapons against DPRK. There was no DPRK nuclear weapon programme until decades later.

South Korea's nuclear weapons research programme was wound up in 1975 with its ratification of the Non-Proliferation Treaty (NPT). In August 2004, the IAEA cited South Korea for previously undeclared nuclear activities involving the reprocessing of nuclear material. Between 9 October 2006 and 3 September 2017, the DPRK carried out six nuclear weapon tests and more than 100 missile tests. Until very recently, annual US-South Korea military exercises had been expanding both in their scope and numbers of troops, including decapitation strikes, and invasion and occupation of major military and other strategic locations in North Korea.

After early mutual threats and insults, DPRK leader Kim Jong Un and US President Donald Trump have held three bilateral summits but as yet no agreement has been possible on denuclearization of the Korean peninsula.

This presentation will cover developments regarding the DPRK's nuclear and missile programmes, and assess the prospects and possible measures for achieving the denuclearization of the Korean Peninsula.

Invited Talk AGA 3.2 Thu 14:15 H8

The DPRK's SLBMs and SRBMs - A Brief Update on North Korea's Missile Activities — •Markus Schiller — ST Analytics GmbH, München, Germany

After having successfully launched the Hwasong-15 road-mobile ICBM in November 2017, the Democratic People*s Republic of Korea (DPRK) apparently adhered to a self-imposed missile launch moratorium for almost 18 months. In May 2019, though, North Korea started to launch missiles again; about two dozen were fired over the summer months of 2019. However, contrary to 2017, these launches were limited to Short Range Ballistic Missiles (SRBMs) and a Submarine-Launched Ballistic Missile (SLBM), and relied on technologies that had nothing in common with the previous ICBM activities.

This presentation will give an update on the observed North Korean missile activities since 2018, including an attempt to distill some possible strategic motives for these activities.

15 min. break

Invited Talk AGA 3.3 Thu 15:15 H8

One Size does not Fit All: Greatly Different Mandates for Denuclearizing Nuclear States — •Robert Kelley — Vienna

The International Atomic Energy Agency (IAEA) has dealt with nuclear materials verification inspections in many states. In only a few cases has the IAEA actually had to deal with extensive programs, nuclear weapons components, and very sensitive nuclear weapon design information. In three significant cases, Iraq (1991-2003), Libya (2004) and South Africa (1993) there were very sensitive nuclear investigations required. All three had widely varying mandates, discoveries and constraints. Future investigations of actual weaponization activities can learn many lessons from these cases. A third, denuclearization active, Project Sapphire in Kazakhstan provided yet another model for extracting dangerous weaponization materials. Hopefully these cases will be studied in preparations for another denuclearization campaign, possibly in the DPRK.

AGA 4: Space Security

Time: Thursday 16:00–16:45 Location: H8

Invited Talk AGA 4.1 Thu 16:00 H8

The Space Debris Challenge and ESA's Space Safety Programme — •Holger Krag — ESA/ESOC Darmstadt

In line with EU and ESA's 'Shared vision and goals for the future of Europe in space', ESA has prepared a new programme that aims for Europe to ensure European autonomy in accessing and using space in a safe and secure environment. The primary goal of this programme is the protection of our planet, humanity and assets in space and on Earth from hazards originating in Space. The major hazards from space to be tackled by the programme have been identified as the Space Weather originating from our Sun, Planetary Defence from Asteroids and Space Debris. The talk will concentrate on the space debris-related aspects of the programme and provide details on ESA*s plans to develop sensor technology for debris monitoring in the area of laser, ground- and space-based optical telescopes and radar. One of the flagships of the programme will be an element entitled CREAM (Collision Risk Estimation and Automated Mitigation), which is a series of activities for the development of automated collision avoidance capabilities and alternate fast commanding option for public and private entities coping with enhanced space traffic, including a demonstration of such capabilities by 2023. The most prominent cornerstone will be the first ever active debris removal mission as an enabler of European industrial capability to conduct in-orbit servicing. The goal is to remove an ESA-owned space debris target object >100kg before the end of 2025 on orbit in a service approach, building on the industrial interest in gaining access to the rising in-orbit servicing market.

AGA 5: Annual General Meeting

Time: Thursday 17:00–18:00 Location: MVAGA

Annual General Meeting

AGA 6: Non-Proliferation and Nuclear Verification

Time: Friday 10:00–11:15 Location: H8

AGA 6.1 Fri 10:00 H8

Nuclear Weapon or Hoax Object? Imitating Gamma Spectra in Verification Measurements — •Christopher Fichtlscherer[1,2] and Moritz Kütt[2] — [1]Nuclear Verification and Disarmament Group, RWTH Aachen, Aachen, Germany — [2]Arms Control and Emerging Technologies, IFSH, Hamburg, Germany

Nuclear weapon authentication often relies on the passive gamma spectrum of a warhead. Measurement systems for such authentication need to provide sufficient information to judge whether the measured object is a warhead. At the same time, they need to protect information considered sensitive. Authentication is only possible if the measured spectrum is unique to a specific warhead type for a given measurement system. If it were possible to produce hoax objects whose emissions create the same measured signal, states could present those in verification processes, effectively undermining disarmament efforts. To determine the uniqueness of warhead spectra, we attempted to replicate detector responses of a notional warhead model with mixtures of radioactive isotopes. In the talk, we present simulation results for existing warhead authentication prototypes.

AGA 6.2 Fri 10:30 H8

Simulation Calculations for the Conversion of FRM-II — •Matthias Englert and Christoph Pistner — Institute for Applied Ecology, Rheinstr. 95, 64295 Darmstadt

Minimization of the civil use of highly enriched uranium (HEU) is one of the cornerstones of international nonproliferation efforts to prevent access to fissile material suitable to build nuclear weapons. The only reactor in Germany still using HEU is the FRM-II at the Technical University in Munich (TUM). Since almost 20 years there is a push to convert the reactor to lower enrichment. The extremely compact design of the fuel element, made possible by new uranium silicide fuel, has made the conversion of the reactor into a demanding task ever since. In a series of papers, new promising conversion options were published in recent years by TUM scientists. Especially conversion with the current uranium silicide fuel - an option that was almost neglected in the first 15 years - has seen new interest. We present complementing results from our simulation calculations regarding uranium silicide conversion with the burnup routine VESTA, the latest version of the neutron transport code MCNPX 6.2 and updated evaluation and core design tools implemented in Mathematica 12. For the new simulation environment, a benchmark was performed against older results on the HEU reference model. A new reactor geometry was modeled according to a design choice published by TUM with uranium silicide fuel with a density of 6 gU/cm3 at an enrichment of 35% and burn calculations will be presented. Since the results were promising we investigated whether the uranium silicide fuel qualified for LEU enrichment at 4.8 gU/cm3 would be suitable for use with up to 50% enrichment. Uranium silicide fuel has been used for 16 years at a density of 3.0 gU/cm3 with a high enrichment of 93% in FRM-II. Two strategies were identified to explore the possibilities of a uranium silicide fuel with higher density than 3.0 gU/cm3 (1.5 gU/cm3) with lower enrichment: First, to operate with fuel >4.8 gU/cm3 with as few changes in fuel assembly geometry as possible; second, to operate with the current fuel at a density of 3.0 gU/cm3. Further analysis focused on an investigation of the purely geometrical changes with the current fuel of a density of 3.0 gU/cm3. The dependence on enrichment was investigated and an enrichment of 50-60% was found to be promising. However, the burnup calculations showed that an enrichment of 50% leads to a reduction of the cycle length. Subsequently, the same model was used to investigate the effect of varying the length of the fuel element. We finally present an outlook for further optimizations such as a change in the density jump (or cancellation by using neutron absorbers) or other geometrical changes, such as a reduction in the number of plates and an increase in the cooling channel width.

15 min. break

AGA 7: Nuclear Archeology

Time: Friday 11:15–12:30 Location: H8

AGA 7.1 Fri 11:15 H8

Forensic measurements for nuclear archaeology - A new approach — •Lukas Rademacher and Malte Göttsche — Nuclear Verification and Disarmament, RWTH Aachen

The availability of effective and widely accepted verification tools is an essential prerequisite for any lasting and successful effort towards nuclear disarmament. One such verification toolbox is nuclear archaeology - it aims to reconstruct the production and removal history of weapons-usable fissile materials. A central method of nuclear archaeology is the deduction of a shut-down reactor's lifetime plutonium production using samples taken from within its core. Specific isotopic ratios are measured to assess neutron fluence and thus estimate plutonium production.

We will present a new approach aiming to strengthen the potential of the method by analyzing a larger set of measured isotopic ratios. This allows for the reconstruction of operational histories of the considered reactor in more detail , therefore providing more information to cross-check declarations. However, this requires a considerably more complex analysis. A feasibility study for this new approach using state-of-the-art mathematical and computational methods has been conducted and will be presented, showing that it is indeed possible to reconstruct additional information.

AGA 7.2 Fri 11:45 H8

Uncertainty Quantification of Plutonium Production Estimates Using the Isotope Ratio Method — •Benjamin Jung and Malte Göttsche — RWTH Aachen University, Aachen, Germany

An understanding of fissile material production histories is essential to enable nuclear disarmament. The Isotope Ratio Method is a technique to estimate the lifetime plutonium production of shut-down reactors. Robust uncertainty assessments are crucial to determine whether these plutonium estimates are consistent with a state's declaration. With Monte Carlo methods and sensitivity analysis techniques, we examine which impact different magnitudes of various uncertainty sources have, using a CANDU 6 and the graphite-moderated Yongbyon reactors as models. The results show that, in particular, uncertain burnup values and, to a lesser degree, nuclear data uncertainties impact the overall uncertainty. To appropriately consider this, we propose a new sequence of applying the Isotope Ratio Method, which calculates tolerance intervals (as opposed to mean values with a standard deviation). The scenarios considered here result in intervals of approximately +/- 10% around the plutonium estimate, suggesting possibly larger uncertainties of the Isotope Ratio Method than previously assumed.

15 min. break

AGA 8: Preventive Arms Control

Time: Friday 12:30–13:30 Location: H8

AGA 8.1 Fri 12:30 H8

Small Armed Aircraft and Missiles - Technology Assessment and Preventive Arms Control — •Jürgen Altmann, Mathias Pilch, and Dieter Suter — Exp. Physik III, TU Dortmund University, Dortmund, Germany

Numerous countries are deploying armed uninhabited aerial vehicles (UAVs), with wingspans of many metres and payloads of hundreds of kg. But work for and deployment of smaller systems have intensified. We have created a database of technical information on small (size <= 2 m) and very small (<= 0.2 m) UAVs (https://url.tu-dortmund.de/pacsam-db). In May 2021 the UAV database contains 152 types from 27 countries, among them 24 armed types from 10 countries. The database of small and very small missiles (diameter <= 70 m and 40 mm, respectively) counts 12 entries in July 2021 (4 of which date back several decades, 4 newer ones are <= 40 mm).

Because of limited payloads, small UAVs and missiles would bring limited weapon effects, but due to low cost they could be produced in high numbers, and attacks against soft spots or in swarms could be militarily relevant. Vertical and horizontal proliferation could endanger military stability and international security; preventive arms control is needed.

AGA 8.2 Fri 13:00 H8

Renaissance of Directed Energy Weapons? — •Götz Neuneck — IFSH University of Hamburg

The call to introduce Directed Energy Weapons on the battlefield goes back to Ronald Reagan's Strategic Defense Initiative, but is renewed from time to time. Russia's President Putin introduced a new ground-based combat laser (Peresvet)and U.S. President Trump's Missile Defense Review calls for new laser weapons for defense purposes. The development of high-power lasers for research and industrial purposes has been improved significantly. The talk analyses the current state ofthe art for laser sources, their dual-use potential and possible solutions for arms control. Esp. in the era of emerging power rivalry it is utmost important to organize dialogues with conflicting states.

Working Group on Information
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Overview of Invited Talks and Sessions

(Lecture hall H1)

Invited Talks

AGI 1.1	Tue	11:15–11:45	H1	**Challenges in data preservation in high energy physics** — •Ulrich Schwickerath
AGI 1.2	Tue	11:45–12:05	H1	**The PUNCH4NFDI Consortium in the NFDI** — •Thomas Schörner
AGI 1.3	Tue	12:05–12:25	H1	**DAPHNE4NFDI - Daten aus Photonen und Neutronenexperimenten** — Anton Barty, Bridget Murphy, Astrid Schneidewind, Wiebe Lohstroh, •Christian Gutt
AGI 1.4	Tue	12:25–12:45	H1	**FAIRmat – Making Materials Data Findable and AI Ready** — Claudia Draxl, •FAIRmat team
AGI 2.1	Tue	13:30–14:00	H1	**NFDI4Phys research data management for the next decades** — •Hans-Günther Döbereiner
AGI 2.2	Tue	14:00–14:30	H1	**Semantic Research Data Management in the National Research Data Initiative (NFDI)** — •Sören Auer
AGI 2.3	Tue	14:30–15:00	H1	**NFDI, EOSC, Gaia-X: Three Data Clouds - One Goal?** — •Klaus Tochtermann
AGI 2.4	Tue	15:30–16:00	H1	**Research Data Management and Higher Education in Physics** — •Janice Bode, Philipp Jaeger

Sessions

AGI 1.1–1.4	Tue	11:15–12:45	H1	**RDM I: NFDI consortia (joint session AGI/AKPIK)**
AGI 2.1–2.5	Tue	13:30–16:30	H1	**RDM II: Perspectives in Research Data Management (joint session AGI/AKPIK)**
AGI 3	Wed	16:30–18:00	MVAGI	**Mitgliederverdammlung der AGI**

Annual General Meeting of the Working Group on Information

Mittwoch 16:30–18:00 MVAGI

- Begrüßung
  Genehmigung des Protokolls der letzten Mitgliederversammlung
  Wahl der Protokollführerin oder des Protokollführers
- Bericht des Sprechers und der stellvertretenden Sprecherin
- Wahl des/der Sprecher/in
  Wahl des/der stellvertretenden Sprecher/in
- Aktuelle Projekte und Schwerpunkte
- Verschiedenes

Sessions

– Invited and Topical Talks –

AGI 1: RDM I: NFDI consortia (joint session AGI/AKPIK)

Time: Tuesday 11:15–12:45 Location: H1

Invited Talk AGI 1.1 Tue 11:15 H1

Challenges in data preservation in high energy physics — •Ulrich Schwickerath — CERN, CH-1211 Genf 23

We preserve our data to extend the scientific reach of our experiments. In high energy physics it is cost-efficient to warehouse data from completed experiments on the tape archives of our national and international laboratories. To use data archived in such a way we must also preserve our ability of use the data, specifically the documentation, computing environment and software of the experiments and analyses. Successful data preservation thus requires careful planning and ongoing effort. The contribution illustrates the challenges of long-term data preservation with experience especially from LEP, and will give a brief overview over the ongoing efforts in the LHC experiments at CERN.

Invited Talk AGI 1.2 Tue 11:45 H1

The PUNCH4NFDI Consortium in the NFDI — •Thomas Schörner — Deutsches Elektronen-Synchroton (DESY), Hamburg, Germany

With the "Nationale Forschungsdateninfrastruktur" (NFDI, national research data infrastructure), a massive effort is undertaken in Germany to provide a coherent research data management, to make research data sustainably utilisable and to implement the FAIR data principles.

PUNCH4NFDI is the consortium of particle, astro- and astroparticle, as well as hadron and nuclear physics within the NFDI. It aims for a FAIR future of the data management of its community and at harnessing its massive experience not least in "big data" and "open data" for the benefit of "PUNCH" sciences (Particles, Universe, NuClei and Hadrons) as well as for physics in general and the entire NFDI.

In this presentation, we will introduce the work programme of PUNCH4NFDI, its connection to everyday work in the physical sciences and beyond, and in particular the idea of digital research products and the PUNCH science data platform.

Invited Talk AGI 1.3 Tue 12:05 H1

DAPHNE4NFDI - Daten aus Photonen und Neutronenexperimenten — Anton Barty[1], Bridget Murphy[2], Astrid Schneidewind[3], Wiebe Lohstroh[4] und •Christian Gutt[5] — [1]DESY, Hamburg — [2]CAU Kiel — [3]FZ Jülich — [4]TU München — [5]Universität Siegen

Die Methoden der Synchrotron- und Neutronenstreuung werden in einer großen, interdisziplinären Bandbreite von Wissenschaftsfeldern angewendet. Die Nutzer repräsentieren dabei verschiedene Fachbereiche in den Naturwissenschaften, die sich dem gemeinsamen Bedarf an anspruchsvoller, schneller und tiefer Datenanalyse sowie den Herausforderungen der Implementierung eines qualifizierten Forschungsdatenmanagements gegenübersehen.

Ziel von DAPHNE4NFDI ist es, eine übergreifende Infrastruktur zu schaffen, welche die Forschungsdaten entsprechend den FAIR-Prinzipien verarbeitet. DAPHNE4NFDI bringt dazu Großforschungseinrichtungen und Nutzer/innen aus den wichtigsten Anwendungsbereichen zusammen, um das Datenmanagement im Sinne der FAIR-Kriterien voranzutreiben.

Invited Talk AGI 1.4 Tue 12:25 H1

FAIRmat – Making Materials Data Findable and AI Ready — Claudia Draxl[1] and •FAIRmat team[2] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]https://www.fair-di.eu/fairmat/fairmatteam

The enormous amounts of research data produced every day in the field of condensed matter physics and the chemical physics of solids represent a gold mine of the 21st century. This gold mine is, however, of little value, if these data are not comprehensively characterized and made available. How can we refine this feedstock, i.e., turn data into knowledge and value? Here, a FAIR (Findable, Accessible, Interoperable, and Re-usable) data infrastructure plays a decisive role. Only then, data can be readily shared and explored by data analytics and artificial-intelligence (AI) methods. Making data Findable and AI Ready (a forward-looking interpretation of the acronym) will change the way how science is done today.

In this talk, we discuss how the NFDI consortium FAIRmat (https://fair-di.eu/fairmat) is approaching these goals, and how researchers can profit from our first steps already now.

AGI 2: RDM II: Perspectives in Research Data Management (joint session AGI/AKPIK)

Time: Tuesday 13:30–16:30 Location: H1

Invited Talk AGI 2.1 Tue 13:30 H1

NFDI4Phys research data management for the next decades — •Hans-Günther Döbereiner — Institut für Biophysik, Universität Bremen

NFDI4Phys.de is applying to become part of the NFDI.de process. We are working towards digital transformation of academia from the viewpoint of physics with an emphasis on disciplinary and transdisciplinary research. For a list of our domains, see https://nfdi4phys.de/domains/. Data need to become FAIR (Findable, Accessible, Interoperable, Reusable). We promote FAIR Digital Objects (FDOs). These are, e.g., digital twins of objects in real life with a unique identifier. For a detailed list of our task areas and strategy, see https://nfdi4phys.de/task-areas/. We strive to categorise data according to their structure based on the hierarchical emerge of levels in nature, see https://nfdi4phys.de/emergence/. This implies building a bridge between natural and social sciences, engineering, and the humanities. Key to these efforts is to develop physics of complex systems further. We need to structure the qualitative by quantifying it with semantic metrics. Generally, the techniques to do so are mainly available, scattered across various disciplines, waiting to be picked up. We need to overcome the complexity barrier in our minds to make progress. Quantum supremacy provided by quantum computing will eventually provide another level of computing power. Finally, faced with tremendous opportunities, we urgently need to develop ethics of information in order to guide us in judging the impact of technology on our society.

Invited Talk AGI 2.2 Tue 14:00 H1

Semantic Research Data Management in the National Research Data Initiative (NFDI) — •Sören Auer — TIB, Welfengarten 1b, 30167 Hannover, Germany

In this talk, we will give an overview of the concepts and implementation of semantic Research Data Management for the National Research Data Initiative (NFDI). We will introduce vocabularies and ontologies for establishing a common understanding of research data and showcase their use in the context of the NFDI initiatives NFDI4Ing, NFDI4Chem, and NFDI4DataScience. We give an overview of three open technology components, ready to be used: - Terminology service for the collaborative creation of terminologies, vocabularies, and ontologies: https://service.tib.eu/ts4tib/index - Open Research Knowledge Graph (ORKG) for organizing scientific contributions in a knowledge graph: https://www.orkg.org - Leibniz Data Manager as a meta-data repository for research data: https://labs.tib.eu/info/projekt/leibniz-data-manager/

Invited Talk AGI 2.3 Tue 14:30 H1

NFDI, EOSC, Gaia-X: Three Data Clouds - One Goal? — •Klaus Tochtermann — Düsternbrooker Weg 120, 24105 Kiel

Currently, there are three data clouds having an influence on how data management will be shaped in Europe in the future: NFDI, Gaia-X and EOSC. This talk will focus on the synergies of and difference between these three major projects.

The talk will explore how the alignment of these Open Science infrastructures will significantly shape (open) science system of the future. It will shed light on the following questions: Which cooperations are necessary to successfully organise the exchange of scientific resources? How do they complement each other to advance the implementation of the FAIR principles as a whole? Which aspects are crucial for future engagement?

break

Invited Talk AGI 2.4 Tue 15:30 H1

Research Data Management and Higher Education in Physics — •Janice Bode[1] and Philipp Jaeger[2] — [1]Westfälische Wilhelms-Universität Münster, Germany — [2]University of Manitoba, Canada and Bergische Universität Wuppertal, Germany

This year, funding has been awarded to three NFDI consortia from the physics community. DPG is involved in all of them, aiming to provide a platform for collaboration and exchange of ideas. As its students organization, jDPG also got involved as well as representatives of the Federal Conference of Physics Student Councils (ZaPF - Zusammenkunft aller deutschsprachigen Physikfachschaften).

If research data management (RDM) is to be promoted throughout the physics community, there is no way around reaching out to physicists in their early stages of education. This should be achieved in close alignment between the consortia and the stakeholders in higher education in physics to avoid redundant work and incompatible developments. To this end, we discuss possible routes towards implementing RDM in the physics curricula at low expenses in terms of both effort and funds.

Topical Talk AGI 2.5 Tue 16:00 H1

Discussion — •Philipp Jäger[1], Uwe Kahlert[2], and Tim Ruhe[3] — [1]University of Manitoba, Canada and Bergische Universität Wuppertal, Germany — [2]RWTH Aachen University — [3]Technische Universität Dortmund

In order to provide data obtained in physics experiments to the respective communtities and to society as a whole, these data need not only to be stored in a sustainable way, but also be prepared and maintained. Such an effective research data management (RDM) does not only require unified solutions with respect to the anticipated resources, but also common standards across various scientific disciplines. We will discuss current and future intiative of RDM with the speakers of the session.

AGI 3: Mitgliederverdammlung der AGI

Time: Wednesday 16:30–18:00 Location: MVAGI

Mitgliederversammlung der AGI

Science meets Industry (SMI)

Martin Wolf
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Scientific work relies on sophosticated instrumentation and measurements techniques provided by specialized industries. Such techniques are often developed in close interaction between companies and research groups. This session with provide some insights to state of the art products presented by representatives from several companies.

Overview of Talks and Sessions

(Lecture hall H1)

Talks

SMI 1.1	Wed	13:30–13:45	H1	**Collaboration of Science and Industry: Developments towards Novel and Revolutionary Analytical Approaches** — •Andreas Thissen
SMI 1.2	Wed	13:50–14:05	H1	**Hamamatsu Photonics – ein „Hidden Champion" der Optoelektronik** — •Christoph Seibel
SMI 1.3	Wed	14:10–14:25	H1	**Basics and concepts of optical parametric chirped-pulse amplification (OPCPA)** — •Robert Riedel
SMI 1.4	Wed	14:30–14:45	H1	**Boost your signal detection – while keeping the setup simple** — •Claudius Riek, Heidi Potts
SMI 1.5	Wed	14:50–15:05	H1	**Next steps in Cryogenics** — •David Gunnarsson
SMI 1.6	Wed	15:10–15:25	H1	**Novel approaches for future challenges in nanofabrication** — •Jörg Stodolka

Sessions

SMI 1.1–1.6	Wed	13:30–15:30	H1	**Science meets industry**

Sessions

– Talks –

SMI 1: Science meets industry

Scientific work relies on sophosticated instrumentation and measurements techniques provided by specialized industries. Such techniques are often developed in close interaction between companies and research groups. This session with provide some insights to state of the art products presented by representatives from several companies.

Time: Wednesday 13:30–15:30 Location: H1

SMI 1.1 Wed 13:30 H1

Collaboration of Science and Industry: Developments towards Novel and Revolutionary Analytical Approaches — •Andreas Thissen — SPECS Surface Nano Analysis GmbH, Voltastraße 5, 13355 Berlin, Germany

Nowadays modern materials and device developments in industry require a deep analytical insight into relevant materials' properties and their correlation to technical device parameters. The determination of this property-to-device parameter correlation is one of the biggest tasks of modern science. This leads to novel analytical approaches allowing to access the relevant data under relevant conditions. This presentation summarizes new approaches to surface chemical analysis from the perspective of a leading instrument manufacturing company.

5 min. break

SMI 1.2 Wed 13:50 H1

Hamamatsu Photonics – ein „Hidden Champion“ der Optoelektronik — •Christoph Seibel — Group Leader Academic Solutions, Hamamatsu Photonics Deutschland GmbH, Arzbergerstr. 10, 82211 Herrsching

Hamamatsu Photonics ist einer der weltweit führenden Hersteller von optoelektronischen Detektoren, Lichtquellen und Systemen. Unsere innovativen Lösungen decken ein breites Spektrum ab – von Röntgenstrahlen, über UV- und sichtbares Licht bis hin zu Infrarot- und Terahertz-Wellenlängen.

Unsere Mission ist es, das Leben durch photonische Technologien zu verbessern. Basierend auf dieser Unternehmensphilosophie entwickeln wir kontinuierlich neue Produkte für wissenschaftliche, industrielle und kommerzielle Anwendungen.

Entdecken Sie im Vortrag unseres Experten für High Energy Physics, Dr. Christoph Seibel, die Welt von Hamamatsu Photonics und welche Möglichkeiten sie für junge Talente bereithält.

5 min. break

SMI 1.3 Wed 14:10 H1

Basics and concepts of optical parametric chirped-pulse amplification (OPCPA) — •Robert Riedel — Class 5 Photonics GmbH, Notkestr. 85, 22607 Hamburg

Class 5 Photonics delivers ultrafast, high-power laser technology at outstanding performance to advance demanding applications from bio-imaging to ultrafast material science and attosecond science. The basis of Class 5 Photonics' high-power femtosecond laser technology is the nonlinear amplifier concept called optical parametric chirped pulse amplification (OPCPA). The concept of OPCPA combines the laser chirped-pulse amplification (CPA) scheme with optical parametric amplification (OPA). With this powerful combination, the advantages of both methods are merged. Ultrashort femtosecond pulses can be amplified at different wavelengths to high pulse energies at high repetition rates.

5 min. break

SMI 1.4 Wed 14:30 H1

Boost your signal detection – while keeping the setup simple — •Claudius Riek and Heidi Potts — Zurich Instruments AG, Technoparkstrasse 1, 8005 Zürich

Controlling measurements with high precision and capturing the signals with a good signal-to-noise ratio is vital for outstanding research. At Zurich Instruments, we are passionate about providing cutting-edge instrumentation for advanced laboratories, e.g. lock-in amplifiers, impedance analyzers, and arbitrary waveform generators, and quantum computing control systems.

In this talk, we will provide an overview of the working principles of lock-in amplifiers. We will elaborate on how this can help measure tiny signals buried in noise while reducing the setup complexity for fields from impedance analysis to quantum computing.

5 min. break

SMI 1.5 Wed 14:50 H1

Next steps in Cryogenics — •David Gunnarsson — Bluefors Oy, Arinatie 10, 003700 Helsinke, Finland

Cryogenics is an integral part of today's quantum technology and as such it need to keep the same high pace of development. In this presentation David Gunnarsson will look ahead and present how Bluefors prepare for the next steps in Cryogenics.

5 min. break

SMI 1.6 Wed 15:10 H1

Novel approaches for future challenges in nanofabrication — •Jörg Stodolka — Raith GmbH, Konrad-Adenauer-Allee 8, 44263 Dortmund

Requirements in Electron Beam Lithography (EBL) are becoming increasingly demanding, often exceeding what is possible when using standard patterning technologies. Improving and combining well known technologies enables new approaches for future developments.

We present two examples where cooperation with research groups gave room to a full new range of applications: Stitch-free writing of gratings with sub-nanometer periodicity control for high precision DFB lasers, and EBL at positions preselected by local generation of light detected by Cathodoluminescence spectroscopy for high yield fabrication of quantum devices.

5 min. break

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