Crystalline Solids and their Microstructure Division
Fachverband Kristalline Festkörper und deren Mikrostruktur (KFM)

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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

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 $T_{JT} = 45\,\mathrm{K}$. 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 $\sim$ 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* Molekülardynamik 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 bio-medical 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 $1.5\,\mathrm{x}\,1.5\,\mathrm{mm}^2$ 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

Invited Talk KFM 6.1 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).

KFM 6.2 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]

KFM 6.3 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

KFM 6.4 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).

KFM 6.5 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)

KFM 6.6 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).

KFM 6.7 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.

KFM 6.8 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).

KFM 6.9 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)

KFM 6.10 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).

KFM 6.11 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).

KFM 6.12 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.

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

Invited Talk KFM 11.1 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.

KFM 11.2 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.

KFM 11.3 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.

KFM 11.4 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.

KFM 11.5 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

KFM 11.6 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)

KFM 11.7 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 submicrometer 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.

KFM 11.8 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.

KFM 11.9 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.

KFM 12: Skyrmions II (joint session MA/KFM)

Time: Friday 10:00–13:15 Location: H5

Invited Talk KFM 12.1 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.

KFM 12.2 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).

KFM 12.3 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.

KFM 12.4 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

KFM 12.5 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

KFM 12.6 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.

KFM 12.7 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)

KFM 12.8 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)

KFM 12.9 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.

KFM 12.10 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).

This work was supported by DFG through SPP 2137 "Skyrmionics" (Project BL444/16-1), SFB 1238 (project C01) and SFB/TRR 173 (project MO 1731/5-1), DARPA TEE program, through grant MIPR# HR0011831554 from DOI, and ERC- consolidator grant 681405-DYNASORE.

KFM 12.11 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).

KFM 12.12 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)

KFM 13: Topological Insulators and Semimetals (joint session TT/KFM)

Time: Friday 10:00–12:45 Location: H7

KFM 13.1 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)

KFM 13.2 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.

KFM 13.3 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)

KFM 13.4 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 measure-

ments 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.

KFM 13.5 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)

KFM 13.6 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)

KFM 13.7 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)

KFM 13.8 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

KFM 13.9 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)

KFM 13.10 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 an-

gle 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.