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

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Overview of Invited Talks and Sessions

(Lecture halls H5 and H7; Poster P2)

Invited Talks

KFM 2.1	Mon	9:30–10:00	H5	**Domain-wall engineering in multiferroic materials** — •Guillaume Nataf
KFM 2.5	Mon	11:15–11:45	H5	**Charged Higher Order Topologies in Room Temperature Magnetoelectric Multiferroic Thin Films** — •Shelly Conroy, Kalani Moore, Sinead Griffin, Lynette Keeney, Eoghan O'Connell
KFM 7.1	Mon	15:00–15:30	H5	**Multiferroic coupling on the level of domain walls** — •Mads C. Weber, Yannik Zemp, Marcela Giraldo, Ehsan Hassanpour, Quintin Meier, Yusuke Tokunaga, Yoshinori Tokura, Sang-Wook Cheong, Nicola N. Spaldin, Thomas Lottermoser, Manfred Fiebig
KFM 10.2	Tue	10:00–10:30	H5	**Negative capacitance and voltage amplification in ferroelectric heterostructures** — •Jorge Iniguez
KFM 10.4	Tue	11:15–11:45	H5	**Magnetization processes in $SmFeO_3$** — •Thomas Schrefl, Alexander Kovacs, Roman Beigelbeck, Hubert Brückl, Shixun Cao, Wei Ren
KFM 18.1	Wed	15:00–15:30	H5	**Deep understanding of advanced optical and dielectric materials for fusion diagnostic applications** — •Anatoli I. Popov, E Kotomin, V Kuzovkov, A Lushchik, Theo A Scherer

Invited Talks of the joint Symposium Frontiers of Orbital Physics: Statics, Dynamics, and Transport of Orbital Angular Momentum (SYOP)

See SYOP for the full program of the symposium.

SYOP 1.1	Mon	9:30–10:00	H1	**Orbital degeneracy in transition metal compounds: Jahn-Teller effect, spin-orbit coupling and quantum effects** — •Daniel Khomskii
SYOP 1.2	Mon	10:00–10:30	H1	**Orbital magnetism out of equilibrium: driving orbital motion with fluctuations, fields and currents** — •Yuriy Mokrousov
SYOP 1.3	Mon	10:30–11:00	H1	**Orbitronics: new torques and magnetoresistance effects** — •Mathias Kläui
SYOP 1.4	Mon	11:15–11:45	H1	**Orbital and total angular momenta dichroism of the THz vortex beams at the antiferromagnetic resonances** — •Andrei Sirenko
SYOP 1.5	Mon	11:45–12:15	H1	**Observation of the orbital Hall effect in a light metal Ti** — •Gyung-Min Choi

Invited Talks of the joint Symposium SKM Dissertation Prize 2022 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:15–10:45	H2	**Charge localisation in halide perovskites from bulk to nano for efficient optoelectronic applications** — •Sascha Feldmann
SYSD 1.2	Mon	10:45–11:15	H2	**Nonequilibrium Transport and Dynamics in Conventional and Topological Superconducting Junctions** — •Raffael L. Klees
SYSD 1.3	Mon	11:15–11:45	H2	**Probing magnetostatic and magnetotransport properties of the antiferromagnetic iron oxide hematite** — •Andrew Ross

SYSD 1.4	Mon	11:45–12:15	H2	**Quantum dot optomechanics with surface acoustic waves** — •Matthias Weiss

Invited Talks of the joint Symposium United Kingdom as Guest of Honor (SYUK)

See SYUK for the full program of the symposium.

SYUK 1.1	Wed	9:30–10:00	H2	**Structure and Dynamics of Interfacial Water** — •Angelos Michaelides
SYUK 1.2	Wed	10:00–10:30	H2	**A molecular view of the water interface** — •Mischa Bonn
SYUK 1.3	Wed	10:30–11:00	H2	**Motile cilia waves: creating and responding to flow** — •Pietro Cicuta
SYUK 1.4	Wed	11:00–11:30	H2	**Cilia and flagella: Building blocks of life and a physicist's playground** — •Oliver Bäumchen
SYUK 1.5	Wed	11:45–12:15	H2	**Computational modelling of the physics of rare earth - transition metal permanent magnets from $SmCo_5$ to $Nd_2Fe_{14}B$** — •Julie Staunton
SYUK 2.1	Wed	15:00–15:30	H2	**Hysteresis Design of Magnetic Materials for Efficient Energy Conversion** — •Oliver Gutfleisch
SYUK 2.2	Wed	15:30–16:00	H2	**Non-equilibrium dynamics of many-body quantum systems versus quantum technologies** — •Irene D'Amico
SYUK 2.3	Wed	16:00–16:30	H2	**Quantum computing with trapped ions** — •Ferdinand Schmidt-Kaler
SYUK 2.4	Wed	16:45–17:15	H2	**Breaking the millikelvin barrier in cooling nanoelectronic devices** — •Richard Haley
SYUK 2.5	Wed	17:15–17:45	H2	**Superconducting Quantum Interference Devices for applications at mK temperatures** — •Sebastian Kempf

Sessions

KFM 1.1–1.3	Sun	16:00–18:15	H3	**Tutorial: Functional Ferroics (joint session KFM/TUT)**
KFM 2.1–2.7	Mon	9:30–12:25	H5	**Focus Session: Defects and Interfaces in Multiferroics 1**
KFM 3.1–3.4	Mon	9:30–10:50	H7	**Microscopy and Tomography with X-ray, Photons, Electrons, Ions and Positrons**
KFM 4.1–4.11	Mon	9:30–12:45	H34	**Perovskite and Photovoltaics 1 (joint session HL/CPP/KFM)**
KFM 5.1–5.9	Mon	10:30–13:00	S053	**New Methods and Developments: Scanning Probe Techniques 1 (joint session O/KFM)**
KFM 6.1–6.4	Mon	11:05–12:25	H7	**Instrumentation and Methods for Micro- and Nanoanalysis**
KFM 7.1–7.6	Mon	15:00–17:25	H5	**Focus Session: Defects and Interfaces in Multiferroics 2**
KFM 8.1–8.6	Mon	15:00–17:15	H7	**Crystallography in Materials Science, Microstructure and Dielectric Properties**
KFM 9.1–9.5	Mon	15:00–16:15	S053	**New Methods and Developments: Scanning Probe Techniques 2 (joint session O/KFM)**
KFM 10.1–10.6	Tue	9:30–12:25	H5	**Focus session: Polar Materials Meet Energy demands**
KFM 11.1–11.5	Tue	9:30–11:10	H7	**Crystal Structure Defects / Real Structure / Microstructure**
KFM 12.1–12.12	Tue	9:30–12:45	H37	**Skyrmions 1 (joint session MA/KFM)**
KFM 13.1–13.5	Tue	10:15–11:30	H46	**Materials for Storage and Conversion of Energy (joint session MM/KFM)**
KFM 14.1–14.7	Wed	9:30–12:05	H5	**Ferroics – Domains and Domain Walls 1**
KFM 15.1–15.7	Wed	9:30–12:05	H7	**Materials for Energy Storage (joint session KFM/CPP)**
KFM 16.1–16.11	Wed	9:30–12:30	H33	**Oxide Semiconductors (joint session HL/KFM)**
KFM 17.1–17.10	Wed	15:00–18:30	H3	**Focus Session: Surfaces and Interfaces of (Incipient) Ferroelectrics (joint session O/KFM)**
KFM 18.1–18.5	Wed	15:00–16:50	H5	**Focus Session: Diamond and related dielectric materials**
KFM 19.1–19.3	Wed	15:00–16:00	H7	**Ferroics – Domains and Domain Walls 2**
KFM 20.1–20.11	Wed	15:00–18:15	H34	**Perovskite and Photovoltaics 2 (joint session HL/CPP/KFM)**
KFM 21.1–21.12	Wed	15:00–18:30	H36	**Functional semiconductors for renewable energy solutions (joint session HL/KFM)**
KFM 22	Wed	17:00–18:00	H5	**Members' Assembly**
KFM 23.1–23.13	Thu	9:30–12:45	H37	**Skyrmions 2 (joint session MA/KFM)**
KFM 24.1–24.7	Thu	10:30–12:30	H6	**New Methods and Developments: Spectroscopies, Diffraction and Others (joint session O/KFM)**
KFM 25.1–25.21	Thu	15:00–18:00	P2	**Poster**
KFM 26.1–26.8	Thu	15:00–18:30	H10	**Focus Session: Topological Devices (joint session TT/KFM)**

KFM 27.1–27.6	Thu	15:00–16:30	H31	**Perovskite and Photovoltaics 3 (joint session HL/CPP/KFM)**
KFM 28.1–28.10	Thu	15:00–17:45	H37	**Topological Insulators (joint session MA/KFM)**
KFM 29.1–29.7	Thu	15:00–16:45	H47	**Multiferroics and Magnetoelectric Coupling (joint session MA/KFM)**
KFM 30.1–30.13	Fri	9:30–12:45	H37	**Skyrmions 3 (joint session MA/KFM)**
KFM 31.1–31.4	Fri	11:30–12:30	H38	**Electrical, Dielectrical and Optical Properties of Thin Films (joint session CPP/KFM)**

Members' Assembly of the Crystalline Solids and their Microstructure Division

Wednesday 17:00–18:00 H5

KFM 1: Tutorial: Functional Ferroics (joint session KFM/TUT)

Chair: Dr. Jan Schultheiß (Augsburg University / NTNU Trondheim)

Time: Sunday 16:00–18:15 Location: H3

Tutorial KFM 1.1 Sun 16:00 H3

Domains and domain walls in functional ferroics — •Dennis Meier — Department of Materials Science and Engineering, Norwegian University of Science and Technology — Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway

Ferroic materials with spontaneous magnetic or electric long-range order are a rich source for functional phenomena. Ferromagnets, for example, are used in hard discs and read heads, whereas ferroelectrics find application as capacitors, energy harvesters, and in tunnel junctions. The rich functionality of ferroic materials is closely linked to their domain structures and the responses of the domains to external stimuli.

In this tutorial, I will give an introduction to the fundamentals that underpin the domain formation in ferroics and discuss different microscopy techniques that allow for imaging electric and magnetic domains. Furthermore, we will talk about more exotic systems, such as improper ferroelectrics and multiferroics, where the interplay of coexisting order parameters gives rise to completely new domain and domain wall properties at the nanoscale. Open experimental challenges will be addressed, as well as future application and research opportunities.

Tutorial KFM 1.2 Sun 16:45 H3

Theory and simulations of ferroelectrics and related materials — •Jorge Iniguez — Luxembourg Institute of Science and Technology — University of Luxembourg

In this tutorial I will introduce the theoretical and simulation methods most frequently employed to investigate ferroelectrics and related materials (antiferroelectrics, multiferroics). I will start from the general electronic-structure methods that permit predictive calculations at the atomic scale, and introduce successive simplifications to eventually reach continuum field schemes that give us access to the mesoscale. I will illustrate the specificity and usefulness of the different approaches by presenting, for each of them, one or two classic examples of application. In passing, this will allow me to emphasize the key role that simulation has played in our field, and to touch upon interesting possibilities for application in energy-related problems.

Jorge Íñiguez's work on ferroelectrics and related materials is mainly funded by the Luxembourg National Research Fund, currently through projects FNR/C18/MS/12705883/REFOX/Gonzalez, INTER/NWO/20/15079143, and C21/MS/15799044.

Tutorial KFM 1.3 Sun 17:30 H3

Atomic scale analysis of ferroic domain walls — •Shelly Conroy — Department of Materials, London Centre of Nanotechnology, Imperial College London, United Kingdom

The dynamic interfaces of ferroic materials known as domain walls bypass the static limitations of traditional nano-device designs. In contrast to hetero-interfaces between different materials, domain walls can be created, moved and removed via an applied stimulus. By combining multiple ferroic properties such as electricity and magnetism, new multi-functional interactive device applications are possible. As these mobile walls can be atomically sharp, it is essential to have physical characterisation at this scale spatially and time-resolved. In this tutorial, I will give an introduction to electron microscopy techniques starting with how to identify domain patterns in the bulk samples, and the most appropriate electron microscopy techniques to use with increasing magnification, leading to pico-meter characterisation. We will discuss some of the most recent advances in electron microscopy characterisation methods for ferroelectrics such as visualising electric charge density at sub-angstrom resolution, and the benefits of coupling polarisation characterisation with electron energy loss spectroscopy band structure analysis. We will then talk about how one can probe multiferroic properties such as magnetic field, strain and phonon modes. As one of the most exciting aspects of ferroic domain walls is their mobility, the various in situ options to investigate their dynamics will be detailed.

KFM 2: Focus Session: Defects and Interfaces in Multiferroics 1

The focus session is dedicated to advanced nano scale-characterization, property-engineering, and modelling methods of multiferroic materials focusing on defects and interfaces. Typical examples may include ferroic domain walls, microstructural levers, or strain effects. Further, applications in novel nanoelectronic devices and nano-related engineering concepts of macroscopic properties of multiferroics are of interest.

Organizers: Dr. Jan Schultheiß (Augsburg University, NTNU Trondheim) and Dr. Marion Höfling (DTU Copenhagen)

Chair: Dr. Marion Höfling (DTU Copenhagen)

Time: Monday 9:30–12:25 Location: H5

Invited Talk KFM 2.1 Mon 9:30 H5

Domain-wall engineering in multiferroic materials — •Guillaume Nataf — GREMAN UMR7347, CNRS, University of Tours, INSA Centre Val de Loire, 37000 Tours, France

Ferroelectric and ferroelastic domain walls are two-dimensional topological defects with thicknesses approaching the unit cell level that can move in response to an electric-field or an applied stress. They exhibit emergent functional properties, such as polarity in non-polar systems or electrical conductivity in otherwise insulating materials, and due their complex strain profiles they interact with phonons as 'defects' would.

In this talk I will: (1) Show how to characterize domain walls with optical techniques (polarized light optical microscopy, liquid crystal decoration, Raman spectroscopy); (2) Discuss how domain walls move in response to an electric field or an applied stress, through discrete impulsive jumps, indicators of avalanches on a broad range of scales; (3) Show that domain walls can be used to induce large thermal conductivity variations in materials.

KFM 2.2 Mon 10:00 H5

Engineering of improper ferroelectric vortex- and stripe-like domains in polycrystalline $ErMnO_3$ — •Max Haas, Jan Schultheiss, and Dennis Meier — Norwegian University of Science and Technology (NTNU), 7034 Trondheim, Norway

The functionality and physical properties of ferroelectric materials are intimately coupled to their domain structure. An exciting recent discovery are topologically protected vortex domains in hexagonal manganites, which are of interest for different fields ranging from nanoelectronics to cosmology-related questions. A key characteristic of the domain structure is the vortex density, that can readily be tuned via the cooling rate across the ferroelectric phase transition.

Here, we explore the effect of cooling rate variations in combination with three-dimensional spatial confinement in high-quality $ErMnO_3$ polycrystals. Utilizing piezoresponse force microscopy, we demonstrate a propensity for the formation of stripe-like domains. Analogous to the vortex-like domains observed in $ErMnO_3$ single crystals, we find that the periodicity of the stripe-like domains depends on the cooling

rate through the Curie temperature. For cooling rates in the range of 10^{-2} to 10^{1} K/min, the periodicity of the stripe-domains increases logarithmically. This scaling behavior is explained based on the interplay between cooling rate and long-ranging strain fields, offering new possibilities for the engineering of domains and domain walls in polycrystalline improper ferroelectrics.

KFM 2.3 Mon 10:20 H5

Tuning multiferroic properties in hexagonal $YMnO_3$ by manipulation of the structural order — •M. Giraldo[1], H. Sim[2], A. Simonov[1], M. Lilienblum[1], A. Samir[1], E. Gradauskaite[1], Y. Heo[1], M. Rossell[3], M. Trassin[1], J.-G. Park[2], Th. Lottermoser[1], and M. Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Department of Physics and Astronomy, Seoul National University — [3]Electron Microscopy Center, EMPA

We investigate the enhancement and suppression of the structural distortion (Q) in hexagonal $YMnO_3$ upon substituting Mn by Al and Ga. We demonstrate its consequences on the electric and magnetic long-range order. We deploy various techniques for a systematic investigation. We observe a progressive decrease in the structural order. This behaviour is caused by the chemical pressure induced by the ionic size of Al and Mn. On the level of the ferroelectric domains, the suppression of the structural order manifests in a progressive size decrease upon increased Al concentration. We do not observe a domain size variation upon Ga substitution. Our experiments suggest that, surprisingly, the progressive reduction on the structural distortion is not directly proportional to a decrease in ferroelectric polarization. On the magnetic level, we find a progressive decrease of the ordering temperatures. This is due to the direct perturbation of the magnetic sublattices formed by the Mn^{3+} moments and the progressive dilution of the magnetic long-range order. By tracing changes in the inherent properties of these systems, we aim to broaden the understanding for new routes in the manipulation of ferroic properties in these compounds.

KFM 2.4 Mon 10:40 H5

Strain-induced multiferroic ribbons in non-multiferroic phase of $MnWO_4$ — •Lea Forster[1], Shingo Toyoda[2], Manfred Fiebig[1,2], Taka-hisa Arima[2,3], Yoshinori Tokura[2,4,5], and Naoki Ogawa[2,5,6] — [1]Deptartment of Materials, ETH Zurich, Switzerland — [2]RIKEN CEMS, Saitama, Japan — [3]Department of Advanced Materials Science, University of Tokyo, Kashiwa, Japan — [4]Tokyo College, University of Tokyo, Tokyo, Japan — [5]Department of Applied Physics, University of Tokyo, Tokyo, Japan — [6]PRESTO, JST, Kawaguchi, Japan

Local structures, such as structural defects, interfaces, and domain walls have the potential to exhibit different physical properties than the bulk. The occurrence of magnetic and electric orders in a confined area may be of particular interest for technological applications, for example, to electrically control the magnetization in memory devices. However, probing local multiferroic structures is challenging caused by a lack of experimental techniques. In this study, we demonstrate a ribbon-shaped, spatially confined multiferroic phase in a non-multiferroic environment in $MnWO_4$. We use optical second harmonic generation imaging to show that a multiferroic phase can be generated by local strain within a non-multiferroic bulk structure. Furthermore, we reveal within the confined multiferroic regions domains with different electric polarization directions and demonstrate deterministic writing of a multiferroic state by the application of strain.

15 min. break

Invited Talk KFM 2.5 Mon 11:15 H5

Charged Higher Order Topologies in Room Temperature Magnetoelectric Multiferroic Thin Films — •Shelly Conroy[1,2], Kalani Moore[2], Sinead Griffin[3], Lynette Keeney[4], and Eoghan O'Connell[2] — [1]Imperial College London, London, United Kingdom — [2]University of Limerick, Limerick, Ireland — [3]Lawrence Berkeley National Laboratory, Berkeley, USA — [4]Tyndall National Institute, Cork, Ireland

Multiferroic topologies are an emerging solution for future low-power magnetic nanoelectronics due to their combined tuneable functionality and mobility. Here, we show that in addition to being magnetoelectric multiferroic at room temperature, thin film Aurivillius phase Bi6TixFeyMnzO18 is an ideal material platform for both domain wall and vortex topology based nanoelectronic devices. Utilising atomic resolution electron microscopy and atom probe tomography, we reveal the presence and structure of 180 type charged head-to-head and tail-to-tail domain walls passing throughout the thin film. Theoretical calculations confirm the sub-unit cell cation site preference and charged domain wall energetics for Bi6TixFeyMnzO18. Finally, we show that polar vortex type topologies also form at out-of-phase boundaries of stacking faults when internal strain and electrostatic energy gradients are altered. This study could pave the way for controlled polar vortex topology formation via strain engineering in other multiferroic thin films. Moreover, these results confirm the sub-unit-cell topological features play an important role in controlling the charge and spin state of Aurivillius phase films and other multiferroic heterostructures.

KFM 2.6 Mon 11:45 H5

X-ray investigation of a multiferroic $YBaCuFeO_5$ single crystal — •Arkadiy Simonov[1], Marisa Medarde[2], and Ruggero Frison[3] — [1]ETH Zürich, Zürich, Switzerland — [2]Paul Scherrer Institut (PSI), Willigen, Switzerland — [3]University of Zürich, Zürich, Switzerland

Recent reports have shown that type-II multiferroic materials can be created using chemical disorder. Disorder frustrates magnetic interaction and induces a magnetic spiral state which breaks the inversion symmetry of the crystal [1]. Such a mechanism is robust since it involves only nearest-neighbor magnetic exchanges and can stabilize the spiral state almost up to room temperature in materials like $YBaCuFeO_5$. However, due to the complexity of characterizing and controlling chemical disorder, this mechanism is rarely used in practice to design novel multiferroic materials.

In this work we propose single-crystal x-ray diffuse scattering as a method for characterizing disorder. Using YBaCuFeO5 as our model system, we show that diffuse scattering can efficiently probe the local structure induced by chemical disorder. Moreover, when measured at sufficiently high resolution, diffuse scattering is also sensitive to the magnetic phase transition from antiferromagnetic to spiral state of the $YBaCuFeO_5$. This is unusual, and likely indicates that atomic relaxations induced by this transition are larger than the values observed in typical type-II multiferroics.

[1] M. Morin et al. Nat. Comms. 7, (2016): 133758.

KFM 2.7 Mon 12:05 H5

A phase-field model for ferroelectrics with local chemical defects — •Dilshod Durdiev[1], Frank Wendler[1], Takahiro Tsuzuki[2], Shuji Ogata[2], Ryo Kobayashi[2], Masayuki Uranagase[2], and Hikaru Azuma[2] — [1]Friedrich-Alexander University Nuremberg-Erlangen, Fürth, Germany — [2]Nagoya Institute of Technology, Nagoya, Japan

In this work, an electromechanical fully coupled phase-field model (PFM) is developed, based upon the approach [1], to study domain evolution and polarization switching under the combined influence of the mechanical and electrical loads and local chemical defects in a $BaTiO_3$ single crystal. The free energy density of the system includes the Landau potential, gradient, mechanical, piezoelectric and electrical energy, respectively. We apply a Fourier spectral method to solve the coupled constitutive equations. Molecular dynamics simulations with core-shell potentials are conducted to capture the domain wall dynamics including vacancies and cation-anion vacancy dipoles [2]. We develop procedures to obtain kinetic and energetic parameters of the PFM from these simulations. Scaling relations are applied to transfer local fields (of vacancies and aliovalent dopants) as well as local bond effects (from vacancies) from the micro- to the continuum scale.

[1] D. Schrade, et al., Arch. Appl. Mech., 83,1393–1413 (2013).
[2] T. Tsuzuki, et al., Appl. Phys. 131, 194101 (2022).

KFM 3: Microscopy and Tomography with X-ray, Photons, Electrons, Ions and Positrons

Time: Monday 9:30–10:50 Location: H7

KFM 3.1 Mon 9:30 H7

Small-Angle X-ray Scattering: Characterization of arbitrarily shaped nanoparticles using the Debye equation — •Jérôme Deumer[1], Brian Richard Pauw[2], Sylvie Marguet[3], Dieter Skroblin[1], Olivier Taché[3], Michael Krumrey[1] und Christian Gollwitzer[1] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [2]Federal Institute for Materials Research and Testing (BAM), Unter den Eichen 87, 12205 Berlin — [3]Université Paris-Saclay, CEA, CNRS, NIMBE, 91191 Gif-sur-Yvette, France

We propose a versatile software package in the form of a Python extension, named CDEF (Computing Debye's scattering formula for Extraordinary Formfactors), to approximately calculate scattering profiles of arbitrarily shaped nanoparticles for small-angle X-ray scattering (SAXS). CDEF generates a quasi-randomly distributed point cloud in the desired particle shape and then applies the open source software DEBYER for efficient evaluation of Debye's scattering formula to calculate the SAXS pattern. The usage of the software is demonstrated for the evaluation of scattering data of Au nanocubes with rounded edges, which were measured at the four-crystal monochromator beamline of PTB at the synchrotron radiation facility BESSY II in Berlin. Our implementation is fast enough to run on a single desktop computer and perform model fits within minutes. The accuracy of the method was analyzed by comparison with analytically known form factors.

KFM 3.2 Mon 9:50 H7

Flat-field correction of highly-dynamic processes — •Thea Engler[1], Johannes Hagemann[1], Christian Schroer[1], and Mathias Trabs[2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Karlsruhe Institue of Technology KIT, Germany

Using hard coherent x-rays, as produced in PETRA III at DESY and in the European XFEL, objects with a size of μm to nm can be imaged with full-field phase-contrast imaging. With single-pulse imaging, specifically dynamic processes on the nanosecond-timescales can be investigated. A recorded single-pulse hologram of the object under investigation in a lens-less imaging setup is disturbed by illumination artifacts. The origin of these artifacts are aberrations in the optics, such as figure errors and surface roughness. For further analysis, the illumination artifacts have to be removed, which is achieved by a flat-field correction. Therefore, the x-ray image of the object of interest is divided by an empty-beam image. This approach assumes temporal stability of both illumination and object. In the case of XFEL experiments, the pulse-to-pulse fluctuations stemming from the SASE process violate this assumption. For the imaging conducted at PETRA III, in addition to vibrations in the beamline's optical components, the object itself incorporates dynamic movements. The common case of the flat-field correction can be improved by recording an empty-beam image-series. With principal component analysis (PCA) of the image series and a careful selection of the principal components, a synthetic flat-field can be reconstructed for each object-image.

KFM 3.3 Mon 10:10 H7

Formation and time dynamics of hydrogen-induced vacancies in nickel — •Maik Butterling[1], Luca Chiari[2], Masanori Fujinami[2], Maciej Oskar Liedke[1], Eric Hirschmann[1], Ahmed Gamal Attallah[1], and Andreas Wagner[1] — [1]Institute for Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Department of Applied Chemistry and Biotechnology, Chiba University, 1-33 Yayoi, Inage, Chiba 263-8522, Japan

The formation of hydrogen-induced defects in nickel was investigated by positron annihilation lifetime spectroscopy and the time dynamics of those defects during room temperature aging was tracked with an unprecedented time resolution of the order of minutes using an ultrahigh-flux slow positron beam. Those measurements showed the formation of a large number of atomic vacancies simply by hydrogen addition at room temperature. It could be proved that they were monovacancy-level defects and that hydrogen was trapped and bound to those vacancies during the hydrogen charge. Room temperature aging, i.e. below the stage III temperature in Ni, and the concomitant hydrogen desorption induced the agglomeration of those monovacancies into large vacancy clusters which remained even after all the hydrogen had desorbed and hydrides had disappeared. These results constitute the first empirical evidence that vacancy-hydrogen complexes are induced in Ni only by hydrogen charging and demonstrate that hydrogen has a primary role in the formation and stabilization of vacancies even at room temperature.

KFM 3.4 Mon 10:30 H7

Stereo X-Ray Microscopy: Seeing the nanocosm in 3D — •Sina Röper[1,2], Karolina Stachnik[2], Lukas Grote[2], Mattias Åstrand[3], Hanna Ohlin[3], Martin Seyrich[1], Sarah-Alexandra Hussak[2], Thomas Frisk[3], Andreas Schropp[1], Ulrich Vogt[3], Dorota Koziej[2], and Christian Schroer[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]University of Hamburg, Hamburg, Germany — [3]KTH Royal Institute of Technology, Stockholm, Sweden

Understanding the nucleation and growth mechanisms involved in the synthesis of nanomaterials is a key factor in determining their performance and functionality. In many cases, these processes are still not well understood in particular, due to the difficulty of observing them *in situ* or *operando*. Scanning hard X-ray microscopy offers the potential for *in situ* nanoimaging of complex chemical systems under relevant environmental conditions. However, standard X-ray tomography relies on the rotation of the sample with respect to the X-ray beam. This is typically not possible for the synthesis of nanoparticles in solution, which requires an extended reaction cell.

We have developed a new stereoscopic X-ray imaging technique with improved depth resolution to overcome these challenges. By simultaneously illuminating the sample with two nanofocused X-rays at different angles, we increased the effective numerical aperture and improved the spatial resolution along the X-ray beam path. This provides a significant gain in depth-sensitivity in ptychography with multi-slicing and allows us to obtain 3D structural information from 2D scans.

KFM 4: Perovskite and Photovoltaics 1 (joint session HL/CPP/KFM)

Time: Monday 9:30–12:45 Location: H34

KFM 4.1 Mon 9:30 H34

The Electronic Structure of $Cs_2AgBiBr_6$ at Room Temperature — •Julian Gebhardt[1,2] and Christian Elsässer[1,2,3] — [1]Fraunhofer Institute for Mechanics of Materials IWM, 79108 Freiburg — [2]Cluster of Excellence livMatS at FIT - Freiburg Center for Interactive Materials and Bioinspired Technologies, Albert-Ludwigs-University Freiburg, 79104 Freiburg — [3]Freiburg Materials Research Center (FMF), Albert-Ludwigs-University Freiburg, 79104 Freiburg

$Cs_2AgBiBr_6$ is a stable halide double perovskite with a band gap of about 2.2 eV. Therefore, it is intensively studied as possible lead free alternative to hybrid perovskite solar cell absorber materials such as methylammonium-lead iodide. However, power conversion efficiencies of solar cells with this material have not yet exceeded 3%. A detailed understanding of the electronic structure of this material is difficult, due to the variance of reported data and experimental as well as theoretical difficulties that occur in going beyond a qualitative understanding of such an indirect semi-conductor at device operation temperature. Here we combine self-energy corrected electronic-structure theory including spin-orbit coupling and structural dynamics at room temperature to model and understand this compound in a quantitative manner, and we compare our theoretical findings with experimental ones. Based on an achieved good agreement, we propose that the observed low power conversion efficiencies can be attributed to the density of states in the conduction band region. From the relation between dimensionality and electron conductivity, we suggest a general design principle for absorber material search.

KFM 4.2 Mon 9:45 H34

Photon-echo spectroscopy of a $CH_3NH_3PbI_3$ perovskite single crystal — •Stefan Grisard[1], Artur V. Trifonov[1,2], Aleksandr N. Kosarev[1,3], Ilya A. Akimov[1,3], Dmitrii R. Yakovlev[1,3], Julian Höcker[4], Vladimir Dyakonov[4], and Manfred Bayer[1,3] — [1]Experimentelle Physik 2, Technische Universität Dortmund — [2]Spin Optics Laboratory, St. Petersburg State University, Russia — [3]St. Petersburg, Russia — [4]Experimental Physics 6, Julius-Maximilian University of Würzburg

Lead halide perovskites such as $CH_3NH_3PbI_3$ ($MAPbI_3$) show outstanding characteristics important for photovoltaic and optoelectronic applications. However, the peculiarities of light-matter interactions in these materials are far from being fully explored. Here, we applied time-resolved photon echo spectroscopy to a high quality $MAPbI_3$ single crystal highlighting the importance of inhomogeneous broadening of excitonic transitions even at cryogenic temperatures. Furthermore, we developed an experimental photon-echo polarimetry method that unambiguously identifies contributions from exciton and biexciton to the coherent optical response. Most importantly, our method allows to accurately extract the biexciton binding energy of 2.4meV, even though the period of the observed quantum beats exceeds the coherence times of exciton and biexciton.

KFM 4.3 Mon 10:00 H34

Structural properties of (hot-)pressed $MAPbI_3$ films revealed by detailed temperature-dependent optical analyses — •Christina Witt[1], Konstantin Schötz[1], Nico Leupold[2], Simon Biberger[1], Philipp Ramming[1], Ralf Moos[2], and Fabian Panzer[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, Bayreuth 95440, Germany — [2]Department of Functional Materials, University of Bayreuth, Bayreuth 95440, Germany

Halide perovskites attracted much attention in recent years, due to the remarkable increase in corresponding solar cell efficiencies. More recently, hot-pressing has emerged as attractive method for manufacturing and post-treatment of perovskite films [1, 2]. However, a detailed understanding regarding the role of temperature during hot-pressing on resulting film properties is still missing. Thus, we use temperature-dependent PL and absorption measurements of $MAPbI_3$ thin films pressed with different temperatures and in detail analyze their optical properties. This allows us to draw conclusions about structural and optoelectronic properties, revealing that an increased temperature improves film morphology, structural and optoelectronic film properties.

[1] Witt, C. et al. Impact of Pressure and Temperature on the Compaction Dynamics and Layer Properties of Powder-Pressed Methylammonium Lead Halide Thick Films. ACS Appl. Electron. Mater. 2020, 2 (8), 2619-2628.

[2] Pourdavoud, N. et al. Room-Temperature Stimulated Emission and Lasing in Recrystallized Cesium Lead Bromide Perovskite Thin Films. Adv. Mater. 2019, 31, 1903717.

KFM 4.4 Mon 10:15 H34

Application of atomic layer deposition and x-ray photoelectron spectroscopy in perovskite solar cells — •Małgorzata Kot[1], Chittaranjan Das[2], Lukas Kegelmann[3], Hans Koebler[3], Mikhailo Vorokhta[4], Carlos Escudero[5], Steve Albrecht[3], Antonio Abate[3], and Jan Ingo Flege[1] — [1]BTU Cottbus-Senftenberg, Cottbus, Germany — [2]KIT, Eggenstein-Leopoldshafen, Germany — [3]HZB, Berlin, Germany — [4]Charles University, Prague, Czech Republic — [5]ALBA Synchrotron, Cerdanyola del Vallès, Spain

In this work we have utilized near-ambient pressure and ultra-high vacuum X-ray photoelectron spectroscopy as well as atomic layer deposition to investigate perovskite solar cells (PSCs). We have demonstrated that ultrathin room temperature atomic layer-deposited aluminium oxide on the perovskite surface very effectively suppresses iodine migration[1] and improves the long term stability and efficiency of PSCs [2,3]. Furthermore, exposure to light proves more detrimental to the perovskite film than exposure to water vapor.[2] Absorbed photons create Frenkel defects in the perovskite crystal and their number strongly depends on the used illumination. The higher the photon flux, the higher the concentration of Frenkel defects, and thus the stronger the degradation of power conversion efficiency and the stronger the hysteresis in the J-V characteristics. [1] C. Das, M. Kot et al., Cell Reports Physical Science 2020, 1, 100112. [2] M. Kot et al., ChemSusChem 2020, 13, 5722. [3] M. Kot et al., ChemSusChem 2018, 11, 3640.

KFM 4.5 Mon 10:30 H34

Chemical Engineering of Ferroelastic Twin Domains in $MAPbI3$ Thin Films — •Yenal Yalcinkaya[1], Ilka Hermes[1], Tobias Seewald[2], Katrin Amann-Winkel[1], Lothar Veith[1], Lukas Schmidt-Mende[2], and Stefan A.L. Weber[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Physics, University of Konstanz, Universitätsstr. 10, 78464, Germany

In this study, we introduce a new chemical method for controlling the strain in methylammonium lead iodide (MAPbI3) perovskite crystals by varying the ratio of Pb(Ac)2 and PbCl2 in the precursor solution. We used a combination of piezoresponse force microscopy (PFM) and X-ray diffraction (XRD) to observe the effect on crystal strain. We observed larger ferroelastic twin domains upon increasing the PbCl2 content, indicating increased crystal strain via PFM images. We confirmed the increased crystal strain via the XRD patterns with strong crystal twinning features. We suggest that this behaviour is caused by different evaporation rates of methylammonium acetate and methylammonium chloride which led to a strain gradient during the crystallization as revealed by time-of-flight secondary ion mass spectroscopy (ToF-SIMS) and grazing incidence x-ray diffraction (GIXRD) measurements. We observed films with larger twin domain structures show an increased carrier via time-resolved photoluminescence (TRPL). The results demonstrate the potential of chemical strain engineering as an easy method for controlling strain-related e*ects in lead halide perovskites.

KFM 4.6 Mon 10:45 H34

Inspecting the local structure of cubic phase halide perovskites from first-principles — •Xiangzhou Zhu, Sebastián Caicedo-Dávila, Christian Gehrmann, and David A. Egger — Department of Physics, Technical University of Munich, Garching, Germany

Halide perovskites (HaPs) have been identified as one of the most promising optoelectronic materials in recent years. Different from the conventional inorganic semiconductors, HaPs exhibit profound deviations from their average atomic structure at finite temperature, which have important consequences for their optoelectronic properties. However, a detailed understanding of these local structural fluctuations, the underlying physical mechanisms as well as their consequences is far from complete. Here, we perform molecular dynamics (MD) calculations based on density functional theory (DFT) to investigate the local structure and anharmonic dynamics of $CsPbBr_3$ in the cubic phase at T=425 K and 525K. We find that motions of neighboring Cs-Br atoms interlock within a nominal cubic unit cell. This manifests in the most likely Cs-Br distance being significantly shorter than what is inferred from an ideal cubic structure. Furthermore, we use the statistical information on the dynamic atomic distributions to quantify the effective potential associated with certain atomic motions at two temperatures. We find that Br motions occur in a dynamically disordered potential energy landscape and relate the Cs motion as well the Cs-Br coupling to $PbBr_6$ octahedral rotations.

30 min. break

KFM 4.7 Mon 11:30 H34

Distinct Resonances in Absorption Spectra of Lead Halide-based Quantum Dots — •Anja Barfüsser, Quinten A. Akkerman, Sebastian Rieger, Amrita Dey, Ahmet Tosun, Tushar Debnath, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

In recent years, perovskite nanocrystals have attracted much attention for their unique optical properties. Here, we discuss sphere-like lead halide-based quantum dots with diameters in the range of 4.5-12 nm featuring a multitude of distinct resonances in their absorption spectra. We have investigated the nature of these resonances by comparing experimental data with model calculations based on weak and strong confinement. In transient absorption experiments, bleaching and induced absorption signals are observed, which we discuss in terms of confined excitons and biexcitonic contributions.

KFM 4.8 Mon 11:45 H34

Revealing the doping density in perovskite solar cells and its impact on device performance — •Francisco Peña-Camargo and Martin Stolterfoht — Physik weicher Materie, Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str.

24-25, 14776 Potsdam, Germany

Inorganic semiconductors can be electronically doped with high precision. Conversely, there is still conjecture regarding the assessment of the electronic doping density in metal-halide perovskites, not to mention of a control thereof. This study presents a multifaceted approach to determine the electronic doping density for a range of different lead-halide perovskite systems. Optical and electrical characterisation techniques comprising intensity-dependent and transient photoluminescence, AC Hall effect, transfer-length-methods, and charge extraction measurements were instrumental in quantifying an upper limit for the doping density. The obtained values are subsequently compared to the electrode charge per cell volume at short-circuit conditions (CU_{bi}/eV), which amounts to roughly 10^{16} cm^{-3}. This figure of merit represents the critical limit below which doping-induced charges do not influence the device performance. The experimental results demonstrate consistently that the doping density is below this critical threshold ($< 10^{12}$ cm^{-3} which means $\ll CU_{\mathrm{bi}}/eV$) for all common lead-based metal-halide perovskites. Nevertheless, although the density of doping-induced charges is too low to redistribute the built-in voltage in the perovskite active layer, mobile ions are present in sufficient quantities to create space-charge-regions in the active layer.

KFM 4.9 Mon 12:00 H34

Ground-state structures, electronic structure, transport properties and optical properties of anion-ordered anti-Ruddlesden-Popper phase oxide perovskites — •Dan Han, Shizhe Wang, Thomas Bein, and Hubert Ebert — Department Chemie, Ludwig-Maximilians-Universität München, Germany

Anti-Ruddlesden-Popper (ARP) phase oxide perovskites Ca4OA2 (A = P, As, Sb, Bi) have recently attracted great interest in the field of ferroelectrics and thermoelectrics, while their optoelectronic application is dominantly limited by their indirect band gaps. In this work, we consider A-site anion ordering in Ca4OA2 (A = P, As, Sb, Bi), and find that it induces an indirect-to-direct band gap transition. Using first-principles calculations, we study the ground-state structures, electronic structure, transport properties and optical properties of anion-ordered ARP phase oxide perovskites Ca4OAA'. Based on an analysis of the lattice dynamics, the ground-state structures of Ca4OAsSb, Ca4OAsBi, Ca4OPSb and Ca4OPBi are identified. In contrast to the Ruddlesden-Popper (RP) phase oxide and halide counterparts, Ca4OAA' show larger band dispersion along the out-of-plane direction, smaller band gaps and highly enhanced out-of-plane mobilities, which is ascribed to the short interlayer distances and enhanced covalency of the pnictides. Although the out-of-plane mobilities of these n = 1 ARP phase perovskites highly increase, comparatively strong polar optical phonon (POP) scattering limits the further enhancement of their mobilities. This work shows that these anion-ordered Ca4OAA' exhibit the potential for optoelectronic applications.

KFM 4.10 Mon 12:15 H34

Including light management concepts in performance prediction modelling of perovskite-silicon tandem solar cells by implementing transfer matrix method — Aminreza Mohandes[1,2], Peymaneh Rafieipour[1,2], Mohammad Moaddeli[1], and •Mansour Kanani[1] — [1]Department of Materials Science and Engineering, School of Engineering, Shiraz University, Shiraz, Iran — [2]Department of Physics, Shiraz University, Shiraz, Iran

The 2-T monolithic perovskite-silicon tandem design holds a record efficiency of 29.80%, recently. To perform more accurate, complete and experimentally reliable modelling of tandem solar cell, we adopt the transfer matrix method (TMM) which incorporates the interfacial reflections, light scattering and parasitic absorption losses in the calculation of the light transmitted from the top perovskite solar cell. The results reveal that the light scattering and interfacial reflection losses cannot be ignored and the previously used Beer-Lambert exponential relation is insufficient for studying tandem configuration. Including TMM method in the performance optimization of the tandem solar cells lets to consider light management concepts more extensively. Therefore, identifying and reducing optical losses in each layer/interface and designing appropriate anti-reflection coatings in a multilayer tandem simulation can be achieved. In this study, standalone and tandem devices have been analyzed and the effect of absorber layer thickness variation, J-V curves, external quantum efficiency (EQE), filtered spectra, current matching, and tandem performance parameters on the cell efficiency is considered.

KFM 4.11 Mon 12:30 H34

Highly Efficient Perovskite-on-Silicon Tandem Solar Cells on Planar and Textured Silicon — •Christian M. Wolff[1], Xin Yu Chin[2], Kerem Artuk[1], Deniz Türkay[1], Daniel Jacobs[1], Quentin Jeangros[2], and Christophe Ballif[1,2] — [1]École polytechnique fédérale de Lausanne, STI IEM PVLAB, Rue de la Maladière 71b, 2000 Neuchâtel — [2]Centre Suisse d'Electronique et de Microtechnique, Rue Jaquet-Droz 1, 2002 Neuchâtel

Multi-junction devices offer the possibility to harness the sun's light beyond the limitations of single-junction solar cells. Among the different combinations perovskite-on-silicon (Pk/Si) tandems hold the great promise of high efficiencies >30%, while maintaining low cost. I will report on our latest progress in the development of Pk/Si tandems comparing our efforts on single-side and double-side textured Pk/Si tandems, reaching a V_{OC} up to 1.95V, summed short-circuit currents above 41mA/cm^2, and certified efficiencies >29%, on an active area of 1cm^2. We achieved these results by dedicated electrical and optical optimizations of all layers within the stack. Specifically, we reduced recombination and transport losses in the Pk absorbers through process and additive engineering for both solution-processed one-step and hybrid two-step deposited Pks, and improved the transparency of the front stack electrodes and contacts through simulation-guided optimizations of the front grid and layer thicknesses. Furthermore, we investigated the stability of single-junction Pk and tandem devices under reverse-bias and standardized accelerated aging conditions.

KFM 5: New Methods and Developments: Scanning Probe Techniques 1 (joint session O/KFM)

Time: Monday 10:30–13:00 Location: S053

Topical Talk KFM 5.1 Mon 10:30 S053

Identification of active electrocatalytic centers using EC-STM under reaction conditions — •Aliaksandr Bandarenka — Technical University of Munich, Department of Physics, James-Franck-Str 1, 85748 Garching bei München, Germany

Identification of so-called active electrocatalytic centres can be very complicated under reaction conditions. In many cases, electrochemical scanning tunnelling microscopy can be efficiently used to do so by comparing the tunnelling noise in the presence and the absence of the electrocatalytic reactions. I the presentation, I will discuss examples, which deal with finding the active sites at the surface of various electrodes for hydrogen evolution, oxygen reduction, and oxygen evolution reactions. Pt, HOPG, Pt-alloys, and transition metal oxides are used as the model systems.

KFM 5.2 Mon 11:00 S053

Coherent Noise Removal for Scanning Probe Microscopy — Jens Oppliger, Danyang Liu, and •Fabian Donat Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

Despite the best efforts to isolate the weak signals in scanning probe microscopes from sources of noise, white and coherent noise remain major nuisances. While the presence of Gaussian white noise can be handled with temporal averaging, the influence of high-Q coherent noise, such as coming from ground-loops or mechanical resonances, is less straightforward to delete when rastering along the surface. Such noise leads to characteristic streaks and spurious Bragg peaks in the Fourier transform of two-dimensional data. Here we demonstrate a straightforward method to remove coherent noise using data-labelling and exemplify its working for quasiparticle interference and topographic imaging.

KFM 5.3 Mon 11:15 S053

General, Strong Impurity-Strength Dependence of Quasipar-

ticle Interference — •Seung-Ju Hong[1], Jae-Mo Lihm[1,2,3], and Cheol-Hwan Park[1,2,3] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, South Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, South Korea

Quasiparticle interference patterns induced by impurities contain information about electronic structures in momentum space. In this presentation, we show that the interpretation of quasiparticle interference patterns is not trivial and needs special care. Even in the simple case of a single-site impurity on the square lattice, the pattern is strongly dependent on the strength of impurity potential. For example, the wave vector with the strongest scattering differs by about 16% in spin-dependent JDOS and exact QPI computations. We also showed that this dependence can be analyzed by decomposing the pattern into the impurity-dependent T-matrix part and momentum-dependent Green function part. We applied our formalism to TaAs, an archetype Weyl semimetal with first-principles calculations. We find that the strong dependence on impurities is also present in TaAs. Thus, our work demonstrates that these quasiparticle interference patterns must be analyzed with care and needs more attention.

Reference [1] S.-J. Hong, J.-M. Lihm, and C.-H. Park, J. Phys. Chem. C 2021, 125, 13, 7488-7494

KFM 5.4 Mon 11:30 S053

Real-space sub-femtosecond imaging of quantum electronic coherences in molecules — Manish Garg[1], •Alberto Martin-Jimenez[1], Michele Pisarra[2], Yang Luo[1], Fernando Martin[2,3,4], and Klaus Kern[1,5] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA Nano), Madrid, Spain — [3]Universidad Autonoma de Madrid (UAM), Madrid, Spain — [4]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain — [5]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Tracking electron motion in molecules is the key to understand and control chemical transformations. Contemporary techniques in attosecond science have the capability to generate and trace the consequences of this motion in real time, but not in real space. Scanning tunnelling microscopy (STM), on the other hand, can locally probe the valence electron density in molecules, but cannot provide by itself dynamical information at this ultrafast time-scale. Here we show that, by combining STM and attosecond technologies, quantum electronic coherences induced in molecules by $<$ 6 femtosecond long carrier-envelope-phase (CEP) stable near-infrared laser pulses can be directly visualized with angstrom-scale spatial and sub-femtosecond temporal resolutions. We demonstrate concurrent real-space and real-time imaging of coherences involving the valence orbitals of perylenetetracarboxylic dianhydride (PTCDA) molecules, and full control over the population of the involved orbitals.

KFM 5.5 Mon 11:45 S053

Femtosecond Tip-Enhanced Coherent Anti-Stokes Raman Spectroscopy of a Single Graphene Nanoribbon — •Yang Luo[1], Alberto Martin-Jimenez[1], Manish Garg[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

By integration of ultrashort laser pulses with a scanning tunneling microscope (STM) one can study the electronic and carrier dynamics with very high spatial and temporal resolution. Nevertheless, molecular vibrational modes at the single-molecule level are difficult to track, owing to the lack of energy resolution. To overcome this barrier, we have now integrated a local spectroscopic tool, combining ultrafast laser pulses with an STM-based tip-enhanced Raman spectroscopy (TERS). By performing TERS with femtosecond laser pulses, we have tracked vibrational coherences and phonon dephasing dynamics in a single graphene nanoribbon (7-GNR). The decoherence time (T2/2 ~ 440 fs) of the phonons in a GNR has been obtained from the time-resolved coherent anti-Stokes Raman spectra. Temporal evolution of vibrational coherences (beatings) between different phonon modes in the GNR has been measured, which evolve on time scales as short as ~ 100 fs. This work lays the foundation for investigating intramolecular vibrational coherences and vibronic dynamics with utmost spatial, temporal and energy resolutions, simultaneously.

KFM 5.6 Mon 12:00 S053

Coherent phonon spectroscopy on the nanoscale — Shuyi Liu[1], Adnan Hammud[1], Ikutaro Hamada[2], Martin Wolf[1], •Melanie Müller[1], and Takashi Kumagai[3] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]College of Materials Science and Engineering, Hunan, China — [3]Institute for Molecular Science, Okazaki, Japan

Coherent phonon (CP) spectroscopy is a powerful tool to monitor ultrafast lattice dynamics under nonequilibrium conditions, providing insight into microscopic interactions that dictate macroscopic material properties. In imperfect crystals, the excitation and relaxation of CPs will be susceptible to the nanoscale environment, calling for real-space observation of ultrafast lattice dynamics. We demonstrate nanoscale coherent phonon spectroscopy by means of ultrafast laser-induced scanning tunneling microscopy (STM) in a plasmonic junction. Comparison of the CP spectra with tip-enhanced Raman spectroscopy allows us to identify the involved phonon modes. In contrast to the Raman spectra, the relative CP intensities exhibit strong nanoscale spatial variations, which correlate with changes in the local density of states recorded via scanning tunneling spectroscopy. Our work introduces a new approach to study the ultrafast structural response at solid surfaces using optical STM.

KFM 5.7 Mon 12:15 S053

Construction of a dry low temperature STM — •Simon Gerber[1] and Wulf Wulfhekel[2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology — [2]Physikalisches Institut, Karlsruhe Institute of Technology

Driven by rising helium prices, we design a dry, low temperature Scanning Tunneling Microscope with a closed helium cycle. We designed a compact dry four stage cryostat with an integrated dilution refrigerator which is cooled using helium from a 400 mW cold head. The STM is connected to the dilution refrigerator and allows measurements down to millikelvin temperatures. The system is mechanically decoupled at several points to minimize vibrations from the cold head reaching the STM. The microscope is positioned inside a split-coil magnet with magnetic fields up to 4T. Optical Access to the STM is possible in the parked position and allows fast tip and sample exchange. The tips and samples can then be prepared under UHV conditions. The complete cryostat and and the STM are home-built.

KFM 5.8 Mon 12:30 S053

Probing tunneling processes into YSR states with microwaves — •Janis Siebrecht[1], Haonan Huang[1], Piotr Kot[1], Sujoy Karan[1], Ciprian Padurariu[2], Björn Kubala[2], Joachim Ankerhold[2], Alfredo Levy Yeyati[3], Juan Carlos Cuevas[3], and Christian R. Ast[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Institut für Komplexe Quantensysteme and IQST, Universität Ulm, Ulm, Germany — [3]Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain

Microwaves are an important tool in the manipulation of multi-level systems such as single spins on a surface, nitrogen vacancies in diamond or double quantum dots. Here we use a scanning tunneling microscope (STM) at a base temperature of 0.56 K to probe the intrinsic YSR states in a Vanadium tip in contact with a V(100) surface. The addition of an E-Band (60-90 GHz) microwave antenna at the junction opens the possibility to study the behavior of YSR states with AC driving- a scenario which has been subject to many theoretical but very few experimental studies. Using microwave-assisted tunneling, we gain insight into how the excited state participates in the tunneling process and how this is related to Andreev processes and parity conservation. Our results point at a new path, namely microwave manipulation of YSR states, which could be an important step towards using YSR states as qubits.

KFM 5.9 Mon 12:45 S053

Compressed fingerprint spectroscopy based on scanning microscopy — •Bernd Kästner[1], Manuel Marschall[1], Arne Hoehl[1], Andrea Hornemann[1], Gerd Wübbeler[1], Selma Metzner[1], Piotr Patoka[2], Eckart Rühl[2], and Clemens Elster[1] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Freie Universität Berlin, Germany

The infrared spectral region between 400 and 4000 cm^{-1} is called the fingerprint region, because the absorption features are unique to individual organic substances. Such a spectrum usually contains many peaks, making it difficult to link individual peaks to the substance. Consequently, the spatial mapping of substances requires spectral

imaging, where at each point in space a complete spectrum needs to be recorded. Usually this can be achieved by spectrometers equipped with array detectors. Recently, scanning methods based on the optical nearfield and local thermal expansion with nanoscale spatial resolution have been developed allowing sub-diffraction spectral imaging. However, the inherently serial recording severely limits their imaging application due to long acquisition times involved and the resulting stability issues. In this work we demonstrate different strategies to significantly reduce the measurement time in spectral imaging measurement by compressing the measurement combined with a low-rank matrix reconstruction. Several examples from different fields of application will be discussed.

KFM 6: Instrumentation and Methods for Micro- and Nanoanalysis

Time: Monday 11:05–12:25 Location: H7

KFM 6.1 Mon 11:05 H7

Sub-nm Control of Radioactive Isotope Incorporation at Surfaces and Interfaces using Ultra-Low Energy Ion Implantation: The ASPIC and ASCII Vacuum Chambers — •Koen van Stiphout, Leonard-Alexander Lieske, Manuel Auge, and Hans Hofsäss — Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The use of radioactive tracer isotopes has a long history of providing unique insights into magnetic interactions, electric environments and crystal structures of materials at the atomic scale. Experimental techniques such as perturbed γ - γ angular correlations or emission Mössbauer spectroscopy require the incorporation of radioactive isotopes into the crystal lattice. However, as more research focuses on ever-smaller nano-scaled systems such as atomically thin 2D materials, precise and reproducible incorporation becomes challenging. One way of overcoming these difficulties is the introduction of ultra-low energy (ULE) ion implantation (10 - 100 eV), which enables sub-nm control of the implanted probe's location at the first few monolayers of the sample.

We present the refurbishment, design and application of two vacuum chambers that will soon be installed in the ISOLDE experimental hall of CERN: the *apparatus for surface physics and interfaces at CERN* (ASPIC), an experienced ultra-high vacuum chamber dedicated to surface characterization and modification, and the new *ASPIC's ion implantation* (ASCII) chamber, designed for ULE ion implantation of radioactive probes.

KFM 6.2 Mon 11:25 H7

Combined X-ray Raman Scattering Spectroscopy and X-Ray Diffraction on Shock-Compressed Vitreous SiO_2 — •Lena Bussmann[1], Mirko Elbers[3], Christian Albers[2], Johannes Kaa[2], Martin Sundermann[4], Hlynur Gretarsson[4], Nicola Thiering[2], Christian Sternemann[2], Sindy Fuhrmann[1], Thomas Schlothauer[1], and Gerhard Heide[1] — [1]TU Bergakademie Freiberg, Institut für Glas und Glastechnologie/Institut für Mineralogie, D-09599 Freiberg — [2]TU Dortmund, Fakultät Physik/DELTA, D-44221 Dortmund — [3]Universität Potsdam, Institut für Geowissenschaften, D-14467 Potsdam-Golm — [4]DESY, D-22609 Hamburg

Vitreous SiO_2 is a suitable model material for dynamic compression experiments: Many of its pressure-related properties are fairly well known, yet, several questions remain unsolved. Vitreous silica has been shock-compressed in the "Reiche Zeche" mine in Freiberg and investigated at the P01 beamline of PETRA III at DESY via X-ray Raman spectroscopy (XRS) and X-ray diffraction (XRD). XRS allows to classify the shock effects on a short scale, while XRD reflects the intermediate-range structure. Results are compared to crystalline SiO_2 modifications. The combination of both methods hence allows to analyse the samples in terms of the effective shock pressure achieved. Furthermore, time-resolved XRD acquisition revealed a structural 'relaxation' process in the shock-compressed samples induced by the X-ray irradiation. This process is studied for different heat-treated glass samples as a function of time and temperature, and characterized by collating the XRD and XRS results.

KFM 6.3 Mon 11:45 H7

X-ray diffraction with micrometer spatial resolution for highly absorbing samples — Prerana Chakrabarti[1,2], Anna Wildeis[1], Markus Hartmann[1], Robert Brandt[1], Giovanni Fevola[2], Christina Ossig[2,3], Michael Stuckelberger[2], Jan Garrevoet[4], Ken Vidar Falch[4], Vanessa Galbierz[4], Gerald Falkenberg[4], and •Peter Modregger[1,2] — [1]Universität Siegen — [2]CXNS, DESY, Hamburg — [3]Universität Hamburg — [4]DESY, Hamburg

We report on a novel goniometer-based setup for X-ray diffraction at high photon energies with micrometer spatial resolution, which was implemented at the P06 beamline of PETRA III. The 6-axes goniometer features 3 translations with 1 nm accuracy and 3 rotations with 0.1 μrad accuracy and allows for 5D scans: 2 in direct and 3 in reciprocal space. Utilizing X-ray focus sizes of 1 μm at a photon energy of 35 keV provided by P06, enables us to characterize the strain field of a 1 mm thick, poly-crystalline martensitic steel sample with micrometer spatial resolution. Further, we experimentally demonstrate the assessment of elemental distribution by fluorescence simultaneous with diffraction for high-Z materials in a ACIGS thin film solar cell. Future plans include the extension of multimodal experiment including ptychography or XBIC and improving spatial resolutions to 200 nm.

KFM 6.4 Mon 12:05 H7

How Silicon Crystals are Used to Disseminate the SI Base Units Mole and Kilogram — •Axel Pramann and Olaf Rienitz — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

It is explained how the SI base units mol and kilogram are disseminated in practice using the X-ray-crystal-density (XRCD) method *counting* silicon atoms in single-crystalline silicon spheres [1-3]. Few practical examples and the status are given how the revision of the SI base units impacts the application of such quantities in chemistry and physics. In case of the XRCD method, the availability of macroscopic single crystalline silicon spheres highly enriched in 28Si is emphasized and the method of the dissemination is shown in detail with regard to the experimental mass spectrometric procedures. [1] K. Fujii et al., Metrologia, 53, A19 (2016). [2] B. Guettler, O. Rienitz, A. Pramann, Annalen der Physik, 1800292 (2018). [3] R. J. C. Brown, P. J. Brewer, A. Pramann, O. Rienitz, and B. Guettler, Anal. Chem. 93, 12147 (2021).

KFM 7: Focus Session: Defects and Interfaces in Multiferroics 2

The focus session is dedicated to advanced nano scale-characterization, property-engineering, and modelling methods of multiferroic materials focusing on defects and interfaces. Typical examples may include ferroic domain walls, microstructural levers, or strain effects. Further, applications in novel nanoelectronic devices and nano-related engineering concepts of macroscopic properties of multiferroics are of interest.

Organizers: Dr. Jan Schultheiß (Augsburg University, NTNU Trondheim) and Dr. Marion Höfling (DTU Copenhagen)

Chair: Dr. Jan Schultheiß (Augsburg University, NTNU Trondheim)

Time: Monday 15:00–17:25 Location: H5

Invited Talk KFM 7.1 Mon 15:00 H5

Multiferroic coupling on the level of domain walls — •Mads C. Weber[1,2], Yannik Zemp[1], Marcela Giraldo[1], Ehsan Hassanpour[1,3], Quintin Meier[1], Yusuke Tokunaga[4], Yoshinori Tokura[4,5], Sang-Wook Cheong[6], Nicola N. Spaldin[1], Thomas Lottermoser[1], and Manfred Fiebig[1] — [1]ETH Zurich — [2]Le Mans University — [3]University of Bern — [4]University of Tokyo — [5]RIKEN — [6]Rutgers University

Multiferroic materials are of interest for the coupling of different ferroic properties on the level of the domains. However, this coupling is not only limited to the bulk but concerns the domain walls too. Here, we show on the example of three different multiferroic systems, that the multi order-parameter coupling on the domain wall level leads to a wide variety of intrinsic domain wall phenomena. In (Dy,Tb)FeO_3, we demonstrate that the interaction of two independent magnetic sublattices gives rise to a polar, multiferroic domain wall in a non-multiferroic environment. The crosstalk of ferroelectricity, structural distortions and magnetic order in hex-$ReMnO_3$ leads to spin rotations of 60°, 120° or 180° about the magnetic domain walls. Depending on the position of the magnetic domain walls with respect of the ferroelectric domain walls, these walls can exchange their rotational character. In the last example, we show that the interplay of two structural distortions in hybrid improper ferroelectrics induces head-to-head and tail-to-tail orientations of the polarization of adjacent ferroelectric domains. These examples illustrate the wide variety of domain wall phenomena thanks to (multi)ferroic coupling effects on the nanoscale.

KFM 7.2 Mon 15:30 H5

3D imaging of multiferroic $(LuFeO_3)_9/(LuFe_2O_4)_1$ superlattices by atom probe tomography — •Kasper Hunnestad[1], Hena Das[2], Constantinos Hatzoglou[1], Megan Holtz[3], Charles Brooks[3], Antonius T. J. Helvoort[1], Darrell Schlom[3,4], Julia Mundy[5], and Dennis Meier[1] — [1]Norwegian University of Science and Technology, Norway — [2]Tokyo Institute of Technology, Japan — [3]Cornell University, USA — [4]Kavli Institute at Cornell for Nanoscale Science, USA — [5]Harvard University, USA

Oxide interfaces are a rich source for novel physical phenomena, ranging from interfacial superconductivity to unusual (multi-)ferroic effects. Over the last decade, significant progress has been made in both the understanding and engineering of oxide interfaces, propelled by the ongoing progress in the development of atomic-scale characterization techniques.

Here, we introduce atom probe tomography (APT) as versatile tool for studying oxide interfaces, investigating the 3D atomic-scale structure and chemical composition of multiferroic $(LuFeO_3)_9/(LuFe_2O_4)_1$ superlattices. Our APT measurements reveal a substantial accumulation of oxygen vacancies at the $LuFe_2O_4$ layers. Based on the data, we quantify the vacancy concentration and discuss their accumulation in relation to calculated defect formation energies and the multiferroic domain structure. In general, this research establishes a new pathway for studying the interaction of interfaces and point defects in oxides, expanding related atomic-scale investigations into 3D.

KFM 7.3 Mon 15:50 H5

Electric-field control of oxygen defects and local transport properties in $ErMnO_3$ — •Jiali He[1], Ursula Ludacka[1], Donald M. Evans[1], Theodor S. Holstad[1], Erik D. Roede[1], Kasper A. Hunnestad[1], Konstantin Shapovalov[2], Zewu Yan[3,4], Edith Bourret[4], Antonius T. J. van Helvoort[1], Sverre M. Selbach[1], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Norway — [2]Institute of Materials Science of Barcelona, Spain — [3]ETH Zurich, Switzerland — [4]Lawrence Berkeley National Laboratory, USA

The electronic properties of complex oxides can be tuned via oxygen defects, offering intriguing opportunities for controlling conductivity. Recently, anti-Frenkel defects moved into focus for minimally invasive property engineering, and their creation makes it possible to adjust the electronic properties without long-range ionic migration or stoichiometry changes. Here, we present a detailed analysis of the electric-field-driven formation and time-voltage-dependent evolution of anti-Frenkel defects in hexagonal $ErMnO_3$. By combining atomic force microscopy and scanning electron microscopy, we investigate the local electronic transport properties associated with the written defects, complemented by numerical simulations. The study reveals that oxygen interstitial - vacancy pairs can be split under an applied electric field. This splitting leads to spatially separated and well-defined vacancy- and interstitial-rich regions, forming a bipolar nanoscale junction. The results provide new insight into the electric-field-driven ionic migration in $ErMnO_3$ and defects physics in functional oxides.

15 min. break

KFM 7.4 Mon 16:25 H5

Deep learning evaluation of conductive atomic force microscopy data — Lorenz Glück[1,2], •Manuel Zahn[1,3], Lukas Puntigam[1], Donald M. Evans[1], Somnath Ghara[1], Michael Heider[2], and Stephan Krohns[1] — [1]Experimental Physics V, University of Augsburg, 86159 Augsburg — [2]Organic Computing Group, University of Augsburg, 86159 Augsburg — [3]Institut für Angewandte Physik, Technische Universität Dresden, 01069 Dresden

Machine learning has gained an enormous interest in the past decade to boost data evaluation in many fields of applied physics. For example, feature recognition in high dimensional datasets in scanning probe microscopy (SPM) can be improved and hidden effects resolved. However, the physical relevance of resolved features is normally still determined by humans.

In this work, we investigate if the regularization of a deep learning (DL) neuronal network, composed of long-short term memory and temporal convolutional network based layers inside an autoencoder architecture, can be utilized to characterize physical significance. We do this on a conductive atomic force microscopy dataset, collected on ferroelectric GaV4S8, as the general properties have already been identified and there are emergent traits at the domain walls. The resolved features from the DL approach are compared to those derived from classical clustering algorithms and classically resolved local material properties. This set up is the first steps to automatic evaluation of physically significant properties in GaV4S8, and is expected to be applicable to other ferroelectric systems.

KFM 7.5 Mon 16:45 H5

Oxygen off-stoichiometry and domain wall conductance in $ErMnO_3$ — •Leonie Richarz[1], Jan Schultheiss[1], Edith Bourret[2,3], Zewu Yan[3], Antonius T.J. van Helvoort[1], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]ETH Zurich, Switzerland — [3]Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Ferroelectric domain walls are natural interfaces, separating volumes with different orientation of the spontaneous polarization. Due to their symmetry, electrostatics, and strain, the walls can develop completely different electronic properties than the surrounding domains. In ferroelectric oxides, oxygen off-stoichiometry is an additional versatile control parameter. This is reflected by the neutral ferroelectric domain

walls in hexagonal manganites: Depending on the oxygen content, their conduction behavior varies from insulating to highly conducting.

In this work, we monitor the electronic transport properties at the domain walls as a function of temperature and oxygen partial pressure with nanoscale spatial resolution. Conductive atomic force microscopy measurements on high-quality $ErMnO_3$ single crystals show anomalous conductance at the domain walls within the whole temperature range of 25 to 300°C. Furthermore, we find that by annealing the sample in nitrogen, the domain wall conductance can be enhanced. Our results provide new insight into the impact of environmental parameters on the electronic domain wall properties. This is of interest for the development of atmospheric sensors, adding a new direction to the field of domain wall nanotechnology.

KFM 7.6 Mon 17:05 H5

Manipulation of improper ferroelectric domains in $Gd_2(MoO_4)_3$ using temperature, electric fields, and mechanical stress — •Ivan Ushakov[1], Theodor Holstad[1], Didier Perrodin[2], Edith Bourret[2], Thomas Tybell[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology (NTNU), Norway — [2]Lawrence Berkeley National Laboratory, USA

In improper ferroelectrics, the spontaneous polarization arises as a biproduct of magnetic or structural order, promoting the formation of domains and domain walls with unusual electronic transport phenomena and scaling behavior. $Gd_2(MoO_4)_3$ is a classical example of an improper ferroelectric material where a structural instability leads to the formation of a polar axis.

Here, we expand previous mesoscale microscopy studies of the domain structure to the nanoscale. By using piezoresponse force microscopy, we image the patterns of ferroelectric and structural antiphase domains in $Gd_2(MoO_4)_3$. In addition to the established domain patterns, we resolve so far unexplored stripe-like nanodomains with a periodicity of about 60 nm. Temperature-dependent measurements show that the nanodomains are stable up to 70°C. Furthermore, we demonstrate reversible switching of these nanodomains by local electric fields and their control via mechanical stress. Our findings provide new insight into the nanoscale domain-physics of $Gd_2(MoO_4)_3$ and introduce novel opportunities for domain engineering in improper ferroelectrics.

KFM 8: Crystallography in Materials Science, Microstructure and Dielectric Properties

Time: Monday 15:00–17:15 Location: H7

KFM 8.1 Mon 15:00 H7

In Situ Structural and Optical Characterization of Laser Recrystallization in an Ultrafast TEM — •Jakob Hagen, Murat Sivis, and Claus Ropers — Max-Planck-Institute for Multidisciplinary Sciences, Göttingen, Germany

Surface-plasmon resonances (SPR) have gained increasing attention due to their widespread use in various scientific fields [1]. These resonantly excited collective free-electron oscillations are able to localize and enhance electromagnetic fields beyond the diffraction limit [2]. To this date, the fabrication of such structures with high optical quality remains challenging, since in general, bottom-up-approaches suffer from the poly-crystallinity of the metal which counteracts the plasmon propagation by damping at grain boundaries [3]. In this study, we created plasmonic nanodiscs by electron beam lithography (EBL) and subsequently performed in situ annealing with a pulsed laser source in an ultrafast transmission electron microscope (TEM). This method allows for live-tracking of the boundary migration and also for characterization of SPRs by photon-induced near-field electron microscopy (PINEM) [4]. Upon illumination, the number of grains reduces drastically leading to almost perfect mono-crystals while preserving the shape. Our approach combines the benefits of mono-crystalline plasmonics [5] with nanometrically precise positioning from EBL.

[1] S. Lal et al., Nat. Photonics 1, 641-648 (2007), [2] K. B. Crozier et al., J. Appl. Phys., 94, 4632 (2003), [3] M. Bosman et al., Sci. Rep. 4, 5537 (2014), [4] L. Piazza et al., Nat. Commun. 6, 6407 (2015), [5] J.-S. Huang, Nat. Commun., 1:150 (2010)

KFM 8.2 Mon 15:20 H7

Impact of the stacking sequence on the stability of transition-metal diborides — •Thomas Leiner[1], Nikola Koutná[2], Paul H. Mayrhofer[2], and David Holec[1] — [1]Department of Materials Science, Montanuniversität Leoben, Austria — [2]Institute of Materials Science and Technology, TU Wien, Austria

Transition-metal diborides are a very hard and brittle type of materials, which, among others, find their use as protective coatings, because of their excellent heat conductivity, oxidation stability and wear resistance.

The investigated diborides XB_2 X=(Cr, Hf, Mn, Mo, Nb, Re, Ta, Ti, V, Zr) occur in three different known stackings, the A-A-A-A stacking of e.g. TiB_2, the A-B-A-B stacking of ReB_2 and the A-B-B-A stacking of WB_2.

In this work, the impact of the stacking sequence on the stability of diborides is investigated via *ab initio* methods (VASP) and phonon analysis. The energy levels and the energy barriers for the different structures of the transition-metal diborides is calculated and evaluated. The stability of observed local and global energy minima are further investigated by assessing their phonon density of states and their phonon frequencies.

Predictions about a possible stability of certain stackings are made and the behaviour of different diborides was compared to each other.

KFM 8.3 Mon 15:40 H7

Pressure-driven insulator-to-metal transition and superconductivity in one-dimensional transition-metal-trichalcogenide microstructures — •Chin Shen Ong[1], L. F. Shi[2,3], Jin-Guang Cheng[2,3], Irina Gorlova[4], Sergey Zybtsev[4], Lingyi Ao[5], Junwei Huang[5], Hongtao Yuan[5], Raman Thiyagarajan[6], Vadim Pokrovskii[4], Olle Eriksson[1,7], and Mahmoud Abdel-Hafiez[1] — [1]Uppsala University, Uppsala, Sweden — [2]Chinese Academy of Sciences, Beijing, China — [3]University of Chinese Academy of Sciences, Beijing, China — [4]Moscow — [5]Nanjing University, Nanjing, China. — [6]Indian Institute of Technology Madras, Chennai, India — [7]Örebro University, Örebro, Sweden

Transition metal trichalcogenides exhibit large tunability of nontrivial electronic states by modifying chemical composition, temperature, and pressure. Despite great interest in TMTCs, very little information exists on how their electronic properties change with compression. Here, we systematically investigate the high-pressure behavior of n-type semiconducting TiS3 of one-dimensional microstructural form. High-pressure electrical resistance measurements up to 98 GPa identify an exotic sequence of transitions from being a semiconductor to insulator, then metal and finally, a hitherto undiscovered superconducting phase at pressures above 70 GPa. The experimental results are supported by first-principles theoretical calculations.

KFM 8.4 Mon 16:00 H7

Impact of point defects on the ferroelectric phase diagram: a molecular dynamics study on the defect arrangements — •Sheng-Han Teng and Anna Grünebohm — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany

Ferroelectric perovskites usually host imperfections and defects that affect their functional properties. Aging and fatigue are often related to the redistribution of these defects [1-3]. Microscopic insights are therefore needed to better apply these materials to different applications. In this study, we use the first-principle based effective Hamiltonian method [4] to screen the impact of distribution and agglomeration of point defects on the phase diagrams of $BaTiO_3$-based materials. With this approach, we can simulate up to 10^6 unit cells and efficiently investigate different defect arrangements. We find that the local fields induced by the defect dipoles play a key role in ferroelectric phase stability and the optimization of functional properties.

[1] Yuri A. Genenko, Julia Glaum, Michael J. Hoffmann, and Karsten Albe. *Mater. Sci. Eng. B*, **192**, 52-82 (2015)

[2] D. Lupascu and J. Rödel. *Adv. Eng. Mater.* **7**(10), 882-898 (2005)

[3] Xiaobing Ren. *Nat. Mater.* **3**(2), 91-94 (2004)

[4] T. Nishimatsu, A. Grünebohm, U. V. Waghmare, M. Kubo, *J. Phys. Soc. Jpn.* **85**, 114714 (2016)

15 min. break

KFM 8.5 Mon 16:35 H7

Strain-Induced Collapse of Landau Levels in TaAs — •Yang-Jun Lee[1,2,3], Cheol-Hwan Park[1,2,3], and Maria A.H Vozmediano[4] — [1]Center for Correlated Electron Systems, Institute for Basic Science, Seoul 08826, Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [3]Center for Theoretical Physics, Seoul National University, Seoul 08826, Korea — [4]Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, Madrid 28049, Spain

A Weyl semimetal, which has a topologically protected conic electronic structure, hosts interesting phenomena such as Fermi arc surface states and chiral anomaly. Recently, the deformation-driven pseudo gauge fields in strained Weyl semimetals have received attention. Among such examples is the collapse of strain-induced Landau levels in Weyl semimetal. In this study, we establish the theory for the effect of strain-induced gauge fields on realistic Weyl semimetals, and based on first-principles calculations, we investigate the conditions on the external strain for the collapse of Landau levels in TaAs.

KFM 8.6 Mon 16:55 H7

Hidden order in ferroelectric oxide thin films — •Joohee Bang[1], Nives Strkalj[2], Martin Sarott[1], Morgan Trassin[1], and Thomas Weber[1] — [1]Department of Materials Science, ETH Zurich, Zurich, Switzerland — [2]Department of Materials Science and Metallurgy, Cambridge University, Cambridge, United Kingdom

Nontrivial polar topologies such as flux-closure, vortex-antivortex pair, and skyrmions in ferroelectric thin films have recently garnered much interest as they have implications for the creation of new states of matter and hold promise for alternative device configurations for microelectronics [1]. These observations called for an in-depth structural investigation of the material as the polarization states such as orientation and domain architecture define the macroscopic ferroelectric properties in ferroelectric thin films. In fact, characterization of local order in such films using noninvasive probes is important as it not only allows access to the polarization states in the bulk, but also tracks structural local order. Here, we present a newly discovered local order state on ferroelectric lead titanate and dielectric strontium titanate superlattices from a comprehensive reciprocal space investigation analyzed with three-dimensional delta pair distribution function (3D-ΔPDF) method [2]. The structural analysis was performed by collecting a complete three-dimensional diffuse X-ray scattering data, which, to the best of our knowledge, was used for the first time to study local order in single-crystalline thin films.

[1]Yadav, A., et al. 2016
[2]Weber and Simonov 2012

KFM 9: New Methods and Developments: Scanning Probe Techniques 2 (joint session O/KFM)

Time: Monday 15:00–16:15 Location: S053

KFM 9.1 Mon 15:00 S053

The importance of the dipole at the metal tip apex when approaching closer with a CO tip — •Shinjae Nam, Oliver Gretz, Thomas Holzmann, Alfred John Weymouth, and Franz J. Giessible — University of Regensburg, Regensburg, Germany

By functionalizing the tip with a single CO molecule, the resolution of atomic force microscope (AFM) can be drastically increased. The contrast enhancement produced by a CO tip has been explained in terms of strong Pauli repulsion and the associated tilting of the probe molecule. Although these two interactions play a dominant role at very close distances, recent experiments show that other interactions, especially electrostatic forces, are also important to understand the observed contrast. Here, we used Lateral Force Microscope, a variant of frequency modulation atomic force microscopy, to quantify the interaction between a CO tip and a CO on the Cu (111) surface. Interestingly, one more feature appeared in the measurement when we measured closer to the surface at the side of the surface CO. Following the results of other investigations, we include the electrostatic force in our simulations. We modeled our tip as a quadrupole, including a dipole at both the metal tip and on the CO molecules. We found that the dipole of the metal apex of the tip becomes a much greater influence as we approach closer to the surface.

KFM 9.2 Mon 15:15 S053

Chemical bond imaging using torsional and flexural higher eigenmodes of qPlus sensors — •Daniel Martin-Jimenez[1], Michael G. Ruppert[2], Alexander Ihle[1], Sebastian Ahles[3], Hermann A. Wegner[3], André Schirmeisen[1], and Daniel Ebeling[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen (Germany). — [2]University of Newcastle, Callaghan, NSW, 2308 (Australia). — [3]Institute of Organic Chemistry, Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen (Germany).

Non-contact atomic force microscopy (AFM) with CO-functionalized tips allows to visualize the chemical structure of adsorbed molecules and identify individual inter- and intramolecular bonds. Herein, we analyze the suitability of qPlus sensors, which are commonly used for bond imaging, for the application of modern multifrequency AFM techniques. Two different qPlus sensors were tested for submolecular resolution imaging via actuating torsional and flexural higher eigenmodes and via bimodal AFM. The torsional eigenmode of the first sensor is perfectly suited for performing lateral force microscopy (LFM) with single bond resolution. The advantage of using a torsional eigenmode is that the same molecule can be imaged either with a vertically or laterally oscillating tip without replacing the sensor simply by actuating a different eigenmode. Submolecular resolution is also achieved by actuating the 2nd flexural eigenmode of our second sensor. With laser Doppler vibrometry measurements and AFM simulations we can rationalize the image contrast mechanism of the 2nd eigenmode.

KFM 9.3 Mon 15:30 S053

3D Force mapping of single organic molecules at room temperature — •Timothy Brown, Philip Blowey, Jack Henry, and Adam Sweetman — University of Leeds, Leeds, UK

Scanning probe microscopy has established itself as a highly effective technique in the study of surfaces and molecules. In particular, non-contact atomic force microscopy has yielded enormous progress in our ability to characterise materials at the atomic scale, including the ability to resolve the chemical structure of individual molecules, and to acquire 3D force-maps with intramolecular resolution.

Intramolecular imaging is almost exclusively performed using qPlus sensors at cryogenic temperatures, as the functionalisation of the tip via a CO molecule (required for intra-molecular imaging) is only stable at near liquid helium temperatures. Although it has been shown that intramolecular imaging may be performed at higher temperatures, via use of semi-conducting, rather than metallic substrates, acquisition of high density 3D data sets generally requires long acquisition times. Hence the lack of thermal equilibrium between the tip and sample at room temperature makes acquisition of these datasets at elevated temperatures extremely challenging.

In this talk we present the first demonstration of high resolution 3D force mapping of a single organic molecule at room temperature using conventional silicon cantilevers. We show how the challenges of operating in a room temperature experimental environment can be overcome to acquire reproducible 3D force maps of a resolution and quality previously only demonstrated at low temperature.

KFM 9.4 Mon 15:45 S053

Monitoring of molecular configurations during manipulation with a scanning probe microscope — •Joshua Scheidt[1,2], Alexander Diener[1,2], Michael Maiworm[3], Rolf Findeisen[3], Kurt Driessens[2], F. Stefan Tautz[1], and Christian Wagner[1] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany — [2]Maastricht University, Data Science and Knowledge Engineering, Maastricht, Netherlands — [3]Control and Cyber-Physical Systems Laboratory, Technische Universität Darmstadt, Darmstadt, Germany

A bold vision of nanofabrication is the assembly of functional molec-

ular structures with a scanning probe microscope (SPM). Such an approach allows the quick variation of conformation and composition of (supra)molecular systems and an assessment of these parameters on the envisioned functionality. However, monitoring the molecular conformations during manipulations remain elusive due to the dual role of the SPM tip as an actuator and an imaging probe. We present an approach which enables monitoring based on continuously gathered force gradient data using a particle filter approach, which solves the inverse problem of conformation monitoring by comparing current force gradient data to a structured set of simulations stored in the form of a finite state automaton. This allows using molecular simulations with wall-times for completion much longer than the time scale of the experiments. Our proof-of-principle investigations are based on the vertical SPM manipulation of a PTCDA (3,4,9,10-perylene-tetracarboxylic dianhydride) molecule on the Au(111) surface.

KFM 9.5 Mon 16:00 S053

Real-space imaging of σ-hole by means of Kelvin probe force microscopy. — •Aurelio Gallardo[1], Benjamín Mallada[2], Bruno de la Torre[2], and Pavel Jelínek[1] — [1]FZU of the CAS, Prague, Czech Republic — [2]RCPTM-CATRIN, Palacký University, Olomouc Czech Republic

Anisotropic charge distributions on individual atoms, such as σ-holes, are crucial for the structural properties of certain systems. Nevertheless, the existence of σ-holes has only been demonstrated indirectly, either observing the interaction between halogenated molecules or by theoretical calculations. However, there was no experimental technique that would allow the spatail resolution of anisotropic atomic charges.

To tackle this problem, we employed Kelvin probe force microscopy (KPFM) which imaging mechanism relays on the electrostatic tip-sample interaction. To achieve the requested resolution, we developed a theoretical description of the KPFM imaging mechanism on atomic scale, which enables optimize the experimental setup. Namely we demonstrated both theoretically and experimentally that probe tip functionalization by a single Xe atom enhances the spatial resolution to directly visualize the anisotropic charge of the σ-hole, as well as the quadrupolar character of the carbon monoxide molecule. [1]

We believe that this work large already outstanding imaging capabilities of scanning probe techniques. In particular, this KPFM technique will enable better description of charge distribution in molecular complexes as well as on surfaces.

References: [1] Mallada et al., Science 374, 863-867 (2021)

KFM 10: Focus session: Polar Materials Meet Energy demands

Polar materials, in particular in (anti-) ferroelectrics, play an important role in future energy storage and energy harvesting devices and have a high potential for ultra-low power memory and logic devices as well as energy efficient cooling technologies. The aim of this focus-session is to bring together scientists from theory and experiment to improve the fundamental understanding and optimization of the underlying material properties and microstructures in a multiphysics and multidisciplinary scenario.

Organizers: Prof. Dr. Anna Grünebohm (Bochum) and Prof. Dr. Bai-Xiang Xu (TU Darmstadt)

Chair: Prof. Dr. Anna Grünebohm (Bochum University)

Time: Tuesday 9:30–12:25 Location: H5

Prize Talk KFM 10.1 Tue 9:30 H5

Einfluss des Sauerstoffgehalts auf das Koerzitivfeld für die Polarisationsumschaltung in HfO_2 aus der Dichtefunktionaltheorie — •Luis Azevedo Antunes — Hochschule für angewandte Wissenschaften München — Laureate of the Georg-Simon-Ohm-Prize 2022

Die fortschreitende Miniaturisierung in der Mikroelektronik stößt beim Thema Energieeffizienz zunehmend an ihre Grenzen. Der Grund sind die Speicher- und Schaltkonzepte, welche auf dem Schalten von elektrischen Strömen basieren. Einen Ausweg könnte hier der ferroelektrische Feldeffekt-Transistor (FeFET) bieten, welcher stromsparend und ohne Kondensator viel besser skalierbar ist. Mit dem vor 15 Jahren in einem Industrielabor in Dresden gefundenen ferroelektrischen HfO_2 und ZrO_2 gibt es ein Material, welches die Anforderungen bei sehr kleinen Bauelementen zu erfüllen scheint. Die Fluorit-struktur basierte ferroelektrische Phase des HfO_2 weist im Vergleich zu den Perowskit basierten Ferroelektrika jedoch ein höheres Koerzitivfeld auf, welches die Zuverlässigkeit einschränkt. Derzeit wird der Einfluss von Dotierstoffen sowie von Sauerstoff auf die Eigenschaften des Koerzitivfeldes und weiterer Eigenschaften untersucht. In dem Vortrag wird über First-Principle-Berechnungen dieser Eigenschaften berichtet, welches Übergangszustände in den kristallinen Materialien betrachtet. Die Ergebnisse führen zu einem grundlegenden Verständnis von Sauerstoffdefekten auf die Bindungsstruktur und weiterführend auf das Koerzitivfeld. Die Ergebnisse werden mit experimentell gemessenen Koerzitivfeldern verglichen.

Invited Talk KFM 10.2 Tue 10:00 H5

Negative capacitance and voltage amplification in ferroelectric heterostructures — •Jorge Iniguez — Luxembourg Institute of Science and technology — University of Luxembourg

My group is interested in the behavior of ferroelectric materials that present non-trivial polar orders (vortexes, skyrmions) and properties (chirality, negative capacitance) in situations of reduced dimensionality (ultra-thin layers or films) and/or subject to suitable electrostatic boundary conditions. In this talk I will review our most recent theoretical results for one of the model systems in the field, the $PbTiO_3/SrTiO_3$ ferroelectric/dielectric superlattices where many of the above effects were first demonstrated. In particular, I will discuss the negative-capacitance response of such materials, with an emphasis on the attendant voltage amplification. I will show that this anomalous behavior is actually quite frequent, occurring in regular multi-domain structures as well as in novel topological states. Further, I will explain its atomistic underpinnings and show how it can be optimized (to obtain voltage amplifications beyond x10) if the polar layers are tuned to display an incipient ferroelectric state.

Most of the work done in collaboration with M. Graf and H. Aramberri (postdocs at the Luxembourg Institute of Science and Technolgoy) and funded by the Luxembourg National Research Fund through Grants INTER/RCUK/18/12601980 and C18/MS/12705883/REFOX. Other key contributors include P. Zubko (UC London), J. Junquera (U. Cantabria), R. Ramesh (UC Berkeley), etc.

Topical Talk KFM 10.3 Tue 10:30 H5

Advanced Phase-field Simulation of Ferroelectrics and Antiferroelectrics — •Bai-Xiang Xu — Division Mechanics of Functional Materials, Institute of Materials Science, TU Darmstadt

Featured by high power density and high cyclic stability, ferroelectric (FE) and antiferroelectric (AFE) perovskites are distinct type of materials for energy storage and conversion particularly in pulse power equipment, miniaturized electronic devices and electronic control system in electric vehicles. The key issue is to increase the energy storage density, which is strongly related to ferroelectric domain structure in the materials and its interaction with defects.

In this talk I will present advanced phase-field simulations on the domain scale of such energy materials. In the first part, by combining phase-field simulations with dislocation mechanics and driving force theory (Zhou et al. IJSS 2021; Höfling et al. Science, 2021), I will show simulation results and mechanistic understanding on domain wall-dislocation interaction in mechanically hardened ferroelectrics and its impact on properties. In the second part, a high order gradient phase-field model for antiferroelectrics will be presented (Liu and Xu, Script Mat. 2020). It enables simulations of the newly observed incommensurate modulations of (anti-)ferroelectric polarization configuration, which goes beyond the capability of the established models

like the Kittel sublattice model. Simulations on the domain structure, hysteresis, and temperature induced FE-AFE phase transition will be shown, along with the comparison to experimental results.

15 min. break

Invited Talk KFM 10.4 Tue 11:15 H5

Magnetization processes in $SmFeO_3$ — •Thomas Schrefl[1], Alexander Kovacs[1], Roman Beigelbeck[1], Hubert Brückl[1], Shixun Cao[2], and Wei Ren[2] — [1]Department for Integrated Sensor Systems, Danube University Krems, Viktor Kaplan Straße 2E, 2700 Wiener Neustadt, Austria — [2]Department of Physics, Shanghai University, China

$SmFeO_3$ is an antiferromagnet with a canted spin structure. We analyzed the basic magnetic properties of monocrystalline $SmFeO_3$ samples through magnetic measurements and micromagnetic simulations. The measurements of the temperature dependent magnetization confirm a spin reorientation at 181°C. Hysteresis properties were found to depend on the magnetic history. We observed exchange bias at room temperature whereby the bias field is sensitive on and increases with the field which is applied after field cooling. Using the double sublattice weak ferromagnetic model we derived effective intrinsic material properties for micromagnetic simulations. The simulations show the existence of metastable multidomain states. In $SmFeO_3$ ferroelectricity is believed to arise from antiferromagnetic domain walls. In a phenomenological model, in which the electric polarization arises from the noncollinear magnetization distribution in the domain walls, the average electric polarization is directly proportional to the total number of domain walls. We show how the number of antiferromagnetic domain walls and the electric polarization changes with the applied magnetic field.

Work supported by The Austrian Research Promotion Agency (FFG) project 20087207, MagnifiSense.

KFM 10.5 Tue 11:45 H5

A first-principles study of electronic properties of lead iron niobate — •Madhura Marathe[1], Anna Grunebohm[2], Doru Lupascu[3], and Vladimir Shvartsman[3] — [1]Department of Physics and Astronomy, Uppsala University, 75120 Uppsala, Sweden. — [2]Interdisciplinary Center for Advanced Materials Simulations (ICAMS), Ruhr-University Bochum, 44801 Bochum, Germany — [3]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141 Essen, Germany

Efficient and cost-effective photovoltaic devices require materials which have optimal band gaps for absorption in the visible spectrum. Several ferroelectric perovskite materials have been investigated for their photovoltaic performance, but have too large band gaps. One promising candidate is multiferroic lead iron niobate $Pb(Fe,Nb)O_3$ (PFN) which has a narrower band gap [1].

We study the electronic and magnetic properties of PFN using density functional theory calculations. We explore how magnetic ordering and structure (ground-state rhombohedral versus high temperature cubic phases) influence the electronic structure and can thus be used to improve material performance.

References 1. N. Bartek, *et al.*, Materials, **14**, 6841 (2021).

KFM 10.6 Tue 12:05 H5

Lead-free Barium Zirconium Titanate-Based Ceramics for Energy Storage — •Eva Kröll, Vladimir Shvartsman, and Doru Lupascu — Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstr. 15, 45141 Essen, Germany

The growing world population and new technical developments request advanced energy storage systems which offer long life time, high power and energy densities. Relaxor ferroelectrics promise to provide these requirements for new energy storage systems due to their high dielectric permittivity and low hysteresis losses. In this work we added bismuth compounds, $Bi(Zn_{2/3}Nb_{1/3})O_3$ and $Bi(Zn_{2/3}Ta_{1/3})O_3$, to the ferroelectric barium zirconium titanate to induce a relaxor state. The heterovalent substitution at the A- and B-sites interrupts the long-range ferroelectric order. Concurrently, Bi^{3+} and Nb^{5+} as ferro active ions improve the polarizability of the materials. The addition of Ta^{5+} should increase the breakdown strength of the ceramic which is crucial to withstand high electric fields and to increase the stored energy density. We used X-ray diffraction for the phase characterization and scanning electron microscopy for the microstructure analysis. The dielectric spectroscopy and polarization measurement show that small amounts of 1.5 mol% BZNb and BZTa induce relaxor behavior in $Ba(Ti_{0.85}Zr_{0.15})O_3$. With increasing content of dopants, the polarization loops become linear. The samples with 2 mol% BZNb and BZTa show the highest energy storage performance with 0.417 J/cm^3 and 0.423 J/cm^3 at 100 kV/cm, respectively.

KFM 11: Crystal Structure Defects / Real Structure / Microstructure

Time: Tuesday 9:30–11:10 Location: H7

KFM 11.1 Tue 9:30 H7

HRTEM study of nanoparticle precipitation in additively manufactured 1.2709 maraging steel — •Anna Benediktová[1], Dagmar Jandová[1], Jiří Benedikt[2], Rostislav Medlín[1], and Ján Minár[1] — [1]New Technologies - Research Center, University of West Bohemia, Pilsen, Czech Republic — [2]Faculty of Applied Sciences, University of West Bohemia, Pilsen, Czech Republic

Maraging steels are known for their excellent properties, such as high strength and toughness, which are mainly due to the precipitation of intermetallic compounds during heat treatment. Up to now, mainly precipitation hardening from a temperature of about 500 °C has been studied, however, the hardening effect begins to show clearly at lower temperatures, even from 250 °C.

The HRTEM study was performed on maraging steel samples without tempering as well as after tempering at 350 °C and 490 °C, and the results were compared with simulations. Besides other relatively coarse precipitates, a high density of globular coherent nanoparticles with a superlattice was found in samples tempered at 350 °C. While the sample tempered at 490 °C contained slightly larger globular and rod-shaped Ni3Mo particles.

KFM 11.2 Tue 9:50 H7

Tuning local structure in Prussian Blue Analogues — •Yevheniia Kholina and Arkadiy Simonov — ETH Zurich, Switzerland

Prussian Blue analogues, $M[M'(CN)_6]_{1-x}\cdot nH_2O$, which we abbreviate here as M[M'] (M and M'=transition metal ions), is a diverse family of cyanide materials, which is intensely investigated for its potential application for hydrogen storage, as catalysts and as electrode materials. Applications that require efficient mass transport utilize the ability of the structure to accommodate a large number of $M'(CN)_6$ vacancies, which create a highly connected porous network. It was theoretically shown that the connectivity and the accessible volume of such a network depend on the local structure[1]. Therefore, to optimize mass transport properties not only the number of vacancies but also their distribution must be precisely controlled. In this work we show how to tune the local structure of Mn[Co] Prussian Blue analogues grown in gel by varying the crystallization parameters: the type of gel, the crystallization temperature, the concentration of reactants, and the concentration of chelating agents. We probe the defect distribution by single-crystal x-ray diffuse scattering, which allows quantitative characterization of the local structure. All of the above-mentioned parameters allow smooth continuous control of diffuse scattering and thus of the local order in Mn[Co] crystals.

[1] Simonov, Arkadiy, et al. "Hidden diversity of vacancy networks in Prussian blue analogues." Nature 578.7794 (2020): 256-260.

KFM 11.3 Tue 10:10 H7

Electronically driven anharmonicities in low-energy lattice models: Affordable molecular dynamics of charge-density-wave systems — Arne Schobert[1], •Jan Berges[1], Michael Sentef[2], Mariana Rossi[2], Erik van Loon[3], Sergey Brener[4], and Tim Wehling[4] — [1]University of Bremen, Bremen, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [3]Lund University, Lund, Sweden — [4]University of Ham-

burg, 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 build an ab-initio low-energy lattice model, which reproduces Born-Oppenheimer potential surfaces from density-functional-theory (DFT). The ab-initio low-energy lattice model is used for molecular dynamics in the CDW phase of 1H-TaS2.

KFM 11.4 Tue 10:30 H7

Ab Initio Thermodynamics for Surface Motifs of the M1 Selective Oxidation Catalyst — •K. Nam[1], Y. Lee[1], L. Masliuk[2], T. Lunkenbein[2], A. Trunschke[2], C. Scheurer[1], and K. Reuter[1] — [1]Theory Dept., Fritz-Haber-Institut der MPG, Berlin — [2]Inorganic Chemistry Dept., Fritz-Haber-Institut der MPG, Berlin

The activity and selectivity of heterogeneous catalysts can be altered noticeably by small changes in different factors such as bulk composition, dopants, defects, reaction conditions, etc. The effects of these factors are furthermore interrelated in non-trivial ways. As an important first step to rationally disentangle them, we here aim to understand their influences on the local atomic-scale structural motifs offered by the catalyst. Specifically, we do this for the M1 structural modification of (Mo,V)O_x and (Mo,V,Te,Nb)O_x as an active catalyst for the oxidative dehydrogenation reaction of ethane to ethylene.

The large primitive cell of this M1 catalyst challenges a detailed study by means of predictive-quality first-principles calculations. To this end, we deconstruct the primitive cell into 'rod-like structures' of surface motifs with various oxygen content, faithfully modeling reported data from electron microscopy [1]. *Ab initio* thermodynamics then allows us to explore the effect of varying reaction conditions on the stability of these motifs and thus on M1 catalyst surfaces. Exploiting the data thus generated to train a machine-learn potential we can specifically rationalize the influence of vanadium and niobium doping on the active surface structure.

[1] L. Masliuk *et al.*, J. Phys. Chem. C **121**, 24093 (2017).

KFM 11.5 Tue 10:50 H7

Raman spectroscopic structure analysis of colloidal semiconductor core-shell quantum dots for the achievement of near-unity quantum efficiency — •Sandra Hinz[1,2], Sonja Krohn[2,3], Hannes Van Avermaet[4], Zeger Hens[4], Jan Steffen Niehaus[3], Janina Maultzsch[1], and Holger Lange[2] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Institute of Physical Chemistry, University of Hamburg, Hamburg, Germany — [3]Fraunhofer IPA - Center for Applied Nano-Technology CAN, Hamburg, Germany — [4]Physics and Chemistry of Nanostructures, Ghent University, Ghent, Belgium

State of the art applications of quantum dots (QDs) require near-unity photoluminescence quantum yield (PLQY). This demand is rarely achieved and therefore the synthesis process is under constant optimization and nanocrystals consisting of a core with one or more shells of different materials are paving the way to achieve high PLQY. As those components have diverse lattice parameters, the induction of strain within the QDs is inevitable. Recently, we applied Raman spectroscopy for in depth structure characterization and a strain minimization approach to optimize the synthesis of InP/ZnSe/ZnS QDs towards near-unity PLQY. A similar effect plays a role in CdSe/CdS QDs when aiming for high PLQY. In these QDs, the formation of an alloyed interface between the CdSe core and CdS shell is assumed. By Raman spectroscopy, we are able to monitor the formation of these alloyed domains for different QD parameters and correlate it with the PLQY.

KFM 12: Skyrmions 1 (joint session MA/KFM)

Time: Tuesday 9:30–12:45 Location: H37

Invited Talk KFM 12.1 Tue 9:30 H37

Topological spin structures at surfaces — •Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany

Magnetic skyrmions are of great interest for future applications ranging from data storage to neuromorphic computing [1]. Fundamental insight into the properties of skyrmions and the underlying microscopic interactions can be obtained by studying them at surfaces [2,3]. Here, I will discuss the stabilization, creation, and annihilation mechanisms of nanoscale topological spin structures based on density functional theory and atomistic spin simulations [4-8]. A novel skyrmion annihilation mechanism, the Chimera collapse [4], is presented which has been confirmed by direct comparison with scanning tunneling microscopy (STM) experiments [5]. It is further shown that skyrmion stability can be tuned via applied electric fields [6] allowing writing and deleting of skyrmions. Higher-order exchange interactions (HOI) beyond Heisenberg exchange also play a role since they can stabilize skyrmion lattices [2] as well as isolated skyrmions or antiskyrmions [7]. Unexpectedly, HOI can induce not only non-collinear but also collinear two-dimensional multi-Q states observed via spin-polarized STM [8].

[1] A. Fert *et al.*, Nat. Rev. Mater. **2**, 1 (2017), [2] S. Heinze *et al.*, Nat. Phys. **7**, 713 (2011), [3] N. Romming *et al.*, Science **341**, 639 (2013), [4] S. Meyer *et al.*, Nat. Commun. **10**, 3823 (2019), [5] F. Muckel *et al.*, Nat. Phys. **17**, 395 (2021), [6] S. Paul *et al.*, npj Comput. Mater. **8**, 105 (2022), [7] S. Paul *et al.*, Nat. Commun. **11**, 4756 (2020), [8] M. Gutzeit *et al.*, arxiv:2204.01358 (2022).

KFM 12.2 Tue 10:00 H37

Controlling Magnetic Skyrmion Nucleation and Motion — •Lisa-Marie Kern[1], Victor Deinhart[1,4], Kathinka Gerlinger[1], Michael Schneider[1], Dieter Engel[1], Christian Günther[2,3], Katja Höflich[4,5], Riccardo Batistelli[4], Daniel Metternich[4], Felix Büttner[4], Bastian Pfau[1], and Stefan Eisebitt[1,3] — [1]Max-Born-Institut, Berlin, Germany — [2]Zentraleinrichtung für Elektronenmikroskopie (ZELMI), Technische Universität, Berlin, Germany — [3]Institut für Optik und Atomare Physik, Technische Universität, Berlin, Germany — [4]Helmholtz Zentrum für Materialien und Energie, Berlin, Germany — [5]Ferdinand-Braun-Institut, Berlin, Germany

Magnetic skyrmions are topological quasiparticles, stabilized in out-of-plane magnetized multilayers. Great advances have been reported in generating, annihilating and shifting skyrmions via spin-orbit torque from spin-polarized currents. Optical nucleation with single laser pulses offers a possibly faster and more energy-efficient alternative. While the underlying mechanisms of the nucleation are different, both methods suffer from a certain stochasticity in the spatial distribution of the skyrmions nucleated. However, in view of scientific and practical applications, a controllable localization of the skyrmion's nucleation site is typically required. Nanopatterning of a tailored magnetic anisotropy landscape using He+-ions provides a promising platform for enhanced control of skyrmions in thin films. Based on this technique, we have recently demonstrated reproducible skyrmion nucleation and motion - a prerequisite for any fundamental or applied research on topological structures.

KFM 12.3 Tue 10:15 H37

Current-Induced H-Shaped Skyrmion Creation and Their Dynamics in the Helical Phase — •Ross Knapman[1,4], Davi R Rodrigues[2], Jan Masell[3], and Karin Everschor-Sitte[4,5] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany — [2]Department of Electrical and Information Engineering, Politecnico di Bari, 70126 Bari, Italy — [3]RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan — [4]Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany — [5]Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47057 Duisburg, Germany

A potential application of magnetic skyrmions is in racetrack memory devices. [1] While efforts have often been concentrated on the use of ferromagnetic and antiferromagnetic 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. Moreover, inspired by previous works which demonstrated electric-current-controlled skyrmion injection at magnetic impurities, [3] we propose a method of creating

skyrmions in a helical background. [4]

[1] Fert, A. et. al., Nat. Nanotechnol. **8**, 152-156 (2013)
[2] Müller, J. et. al., Phys. Rev. Lett. **119**, 137201 (2017)
[3] Everschor-Sitte, K. et. al., New J. Phys. **19**, 092001 (2017)
[4] **Knapman, R.** et. al. J. Phys. D: Appl. Phys. **54**, 404003 (2021)

KFM 12.4 Tue 10:30 H37

Skyrmion automotion in confined geometries for applications — •Kilian Leutner[1], Thomas Brian Winkler[1], Hans Fangohr[2,3], and Mathias Kläui[1] — [1]Johannes Gutenberg University, Institute for Physics, Staudinger Weg 7, 55128 Mainz, Germany — [2]Max-Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany. — [3]University of Southampton, SO17 1BJ, Southampton, United Kingdom

Magnetic skyrmions are promising candidates for energy-efficient applications due to their quasi-particle nature and their topological stabilization. We present here a new concept for a multi-turn sensor-counter based on skyrmions. The skyrmion-boundary force in confined geometries leads with the topology-dependent dynamics to the effect of automotion in certain cases. Automotion describes the movement of magnetic structures without the supply of external energy. For our case, we describe and investigate this effect with micromagnetic simulations and the coarse-grained Thiele equation. Automotion has already been demonstrated for domain walls [1], but is not well explored in skyrmionic systems yet.

[1] M.-A. Mawass et al, Phys. Rev. Applied 7, 044009, 2017

KFM 12.5 Tue 10:45 H37

Walking Skyrmions — •Alla Bezvershenko and Achim Rosch — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

We study the pinning - unpinning transition of the skyrmion lattice in bulk MnSi under applying a slowly oscillating transverse magnetic field. We model the system using an elastic model for skyrmion strings in the presence of pinning forces. With this effective model we show that the presence of a transverse magnetic field reduces the critical current density needed to depin the skyrmion lattice, reaching zero at the critical magnetic field value. Further, the complete phase diagram of this model will be discussed. Below the threshold amplitude, the skyrmion lines stay fully pinned. Upon increasing the amplitude, a so-called "walking" phase starts, where the skyrmion lines start to unpin. If in this phase a sufficiently large electric current is being applied, the skyrmion lattice starts to move. Obtained results are compared to the experimental data on the transverse susceptibility measurements for this system.

KFM 12.6 Tue 11:00 H37

Small-angle neutron scattering of kinetically driven skyrmion lattice motion — •Denis Mettus[1], Alfonso Chacon[1], Andreas Bauer[1], Sebastian Mühlbauer[2], 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

Skyrmions are topologically non-trivial spin textures that exhibit an exceptionally efficient coupling to spin currents, notably spin-polarized charge currents and magnon currents as observed in MnSi, FeGe, and Cu_2OSeO_3. This raises the question for the microscopic mechanisms that control the pinning of the skyrmion lattice, and how they depend on the topology, electronic structure, and disorder. We report neutron scattering measurements of kinetically driven skyrmion lattice unpinning and motion by means of Time-Involved Small Angle Neutron scattering Experiment (TISANE). In our study we examined the unpinning process under changing field orientation for different materials including the metallic systems $Mn_{1-x}Fe_xSi$ and the insulator Cu_2OSeO_3. We discuss our results in the light of methodological aspects of the TISANE technique and recent theoretical predictions of walking skyrmions.

KFM 12.7 Tue 11:15 H37

Spin Wave Driven Skyrmions in Antiferromagnets — •Michael Lau[1], Wolfgang Häusler[2], and Michael Thorwart[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Institute of Physics, University of Augsburg

In a two-dimensional lattice of antiferromagnetically coupled classical magnetic moments of unit length it is theoretically possible to stabilize Skyrmions when appropriately adjusting the Dzyaloshinskii-Moriya interaction (DMI) and a uniaxial anisotropy. We present simulations on a discrete lattice which reveal that these Skyrmions can be moved by spin waves injected at one edge of the lattice. It is known that in ferromagnets spin waves are scattered by Skyrmions, imposing a driving force on them. In antiferromagnets, we find similar scattering of spin waves by Skyrmions, exerting a net driving force. However, contrary to ferromagnets, the driving force acts in the direction of spin wave propagation and the Skyrmion accelerates like a classical particle with finite mass, as typically found for antiferromagnetic solitons. Additionally, we exploit the fact that antiferromagnetic spin waves can appear left- or right handed and study the impact of spin waves of different polarizations on the Skyrmion. It turns out that chirality, frequency and amplitude of the spin waves all significantly influence the Skyrmion motion.

KFM 12.8 Tue 11:30 H37

Skyrmion lattice dynamics — •Daniel Schick, Markus Weissenhofer, Levente Rózsa, and Ulrich Nowak — Universität Konstanz, Konstanz, Germany

We investigate the movement of skyrmions in lattices by performing molecular dynamics simulations based on the Thiele equation [1], using different effective skyrmion-skyrmion interactions. We compare mean-square displacement and the dynamical orientational correlation function $g_6(t)$ for different values of damping α and different topological charges and find the topological charge to change the effect of damping on the examined quantities. Furthermore, we find that for finite topological charge, the mean-square displacement in low-density skyrmion lattices increases compared to free diffusion. By comparing to trivial topology, we can demonstrate the increase in mean-square displacement to be the result of the gyrocoupling of skyrmions.

[1] A.A. Thiele, Phys. Rev. Lett. 30, 6 (1973)

KFM 12.9 Tue 11:45 H37

Skyrmion Pinning Energetics in Thin Film Systems — Raphael Gruber[1], Jakub Zázvorka[1], •Maarten A. Brems[1], Davi R. Rodrigues[1], Takaaki Dohi[1], Nico Kerber[1], Boris Seng[1], Mehran Vafaee-Khanjani[1], Karin Everschor-Sitte[2], Peter Virnau[1], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany

Magnetic skyrmions in thin films have been shown to exhibit thermal diffusion, making them a promising system for applications in probabilistic computing [1] as well as Brownian computing [2]. In such applications, pinning effects are of crucial importance as the pinning strength is often comparable to thermal excitations and thus impacts the operation of skyrmion-based devices. Using thermal skyrmion dynamics, we characterize the pinning in a sample and ascertain the spatially resolved energy landscape [3]. To understand the mechanism of pinning, we image the skyrmion pinning details and find a strong size-dependence. We observe that the skyrmion is pinned at its boundary (domain wall) and not as previously considered at its core. As a consequence, we find that the size-dependence follows from different favorable overlaps of the skyrmion boundary with the pinning regions, which is supported by micromagnetic simulations. This allows us to switch pinning sites on and off by small tuning of external fields. [1] J. Zázvorka et al., Nat. Nanotechnol. 14, 658 (2019). [2] M. A. Brems et al., Appl. Phys. Lett. 119, 132405 (2021). [3] R. Gruber et al., under review (2021).

KFM 12.10 Tue 12:00 H37

Coexistence of topologically distinct spin textures — •Börge Göbel[1], Jagannath Jena[2], Stuart Parkin[2], and Ingrid Mertig[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle

Over the last decade, the field of skyrmionics has attracted great research interest, as skyrmions (small, whirl-like spin textures) possess a topologically-induced stability that allows to consider them as the carriers of information in future data storage devices. However, due to their integer topological charge there are two major shortcomings of skyrmion-based racetrack storages: The skyrmions do not move parallel to a current and multiple skyrmions attract and repell each other.

A solution to these problems is the utilization of alternative magnetic nano-objects that go beyond conventional skyrmions; see review [1]. In this talk, we show via simulations, Lorentz transmission electron microscopy measurements [2,3] and Hall transport measurements [4] that skyrmions, antiskyrmion and topologically trivial bubbles [5] can coexist in Heusler materials. They can even appear fractionally

near the sample's edges [6]. We propose an advanced version of the racetrack storage device based on these results.

[1] BG et al. Physics Reports 895, 1-28 (2021), [2] Jena, BG et al. Nat. Com. 11, 1115 (2020), [3] Jena, BG et al. Science Advances 6, eabc0723 (2020), [4] Sivakumar, BG et al. ACS Nano 14, 13463 (2020), [5] BG et al. PRAppl. 15, 064052 (2021), [6] Jena, BG et al. Nat. Com. 13, 2348 (2022)

KFM 12.11 Tue 12:15 H37

Topological magnetism in multiferroic lacunar spinels — •Vladislav Borisov[1], Patrik Thunström[1], Anna Delin[2], and Olle Eriksson[1,3] — [1]Ångström Laboratory, Uppsala University, Uppsala, Sweden — [2]Department of Applied Physics, School of Engineering Sciences, KTH Royal Institute of Technology, Stockholm, Sweden — [3]Örebro University, Örebro, Sweden

Several skyrmionic magnetic systems have been discovered since the first observation of skyrmions in a B20 compound MnSi. Only a few of them host not just magnetism but also ferroelectricity and prominent examples are lacunar spinels GaV_4S_8 and GaV_4Se_8. These bulk systems are rather unique, because they host Neel skyrmions, which are otherwise only observed in metallic multilayers. Detailed description of magnetic phenomena in the multiferroic spinels is challenging for theory due to correlations within the V_4 clusters.

We study the role of the magnetic state of these clusters and electronic correlations for the Heisenberg and Dzyaloshinskii-Moriya interactions in V- and Mo-based lacunar spinels. The character of magnetic interactions is discussed in relation to the crystal symmetry and electronic properties derived from the V_4 molecular orbitals. Based on micromagnetic simulations, we determine the role of different interactions for the formation of magnetic textures.

This work was supported by the Knut and Alice Wallenberg Foundation, the Swedish Research Council and the Swedish National Infrastructure for Computing.

KFM 12.12 Tue 12:30 H37

Systematic identification and assessment of topological spin textures via saddle point searches — •Hendrik Schrautzer[1,2], Grzegorz Kwiatkowski[1], Hannes Jónsson[1], Pavel F. Bessarab[1,3], and Stefan Heinze[2] — [1]University of Iceland, Reykjavik, Iceland — [2]Christian-Albrechts-University, Kiel, Germany — [3]Linnaeus University, Kalmar, Sweden

Magnetic systems hosting topological textures such as skyrmions have been of great technological and fundamental interest in recent years. The growing zoo [1] of co-existing meta-stable states makes investigation of such systems challenging. Here, we present a methodology combining global optimization based on recursive traversing between energy minima via saddle points on the energy surface [2,3], and harmonic transition state theory. The methodology provides a systematic approach to predict previously unknown metastable states, identify their lifetime at a given temperature and compute kinetics of their mutual transformations. We apply the method to the widely studied Pd/Fe/Ir(111) skyrmionic system, parametrized using density functional theory, and predict a variety of new transition mechanisms and spin textures including skyrmions with chiral kinks [1], which have been unknown so far in this system.

1: V. M. Kuchkin, *et al.*, Phys. Rev. B **102**.14 (2020): 144422.
2: A. Pedersen, *et al.*, International Workshop on Applied Parallel Computing (pp. 34-44) (2010). Springer, Berlin, Heidelberg.
3: G. P. Müller *et al.*, Phys. Rev. Lett. **121**.19 (2018): 197202

KFM 13: Materials for Storage and Conversion of Energy (joint session MM/KFM)

Time: Tuesday 10:15–11:30 Location: H46

KFM 13.1 Tue 10:15 H46

How Important are Long-Range Electrostatics in Machine-Learning Potentials for Battery Materials? — •Carsten Staacke[1], Hendrik Heenen[1], Christoph Scheurer[1], Gabor Csanyi[2], Karsten Reuter[1], and Johannes Margraf[1] — [1]Fritz Haber Institut, Berlin, Germany — [2]Engineering Department, Cambridge University, UK

All-solid-state Li-ion batteries promise gains in safety and durability by combining high Li-ion conductivity and mechanical ductility. In this respect, solid-state electrolytes (SSE) such as the $Li_7P_3S_{11}$ glass-ceramic have gained much attention. Modern machine learning (ML) potentials are increasingly being adopted as a tool for modeling SSEs at the atomistic level. However, the local nature of these ML potentials typically means that long-range contributions arising, e.g., from electrostatic interactions are neglected. To this end, we have combined short-ranged machine-learning potentials based on the Gaussian Approximation Potential (GAP) approach with a classical electrostatic model in the long-range (ES-GAP). We will present a first-principles validation of both, the pure GAP potential and the new ES-GAP for the LPS SSE. In particular, the role of Coulomb interactions in isotropic vs. non-isotropic system simulations will be evaluated. In standard isotropic simulation tasks, such as determining ionic conductivities, both GAP and ES-GAP yield similar results. In contrast, simulations on non-isotropic systems show the importance of ES contributions and provide new insights into interface stability of $Li_7P_3S_{11}$.

KFM 13.2 Tue 10:30 H46

Oxygen Hole Formation Controls Stability in $LiNiO_2$ Cathodes: DFT Studies of Oxygen Loss and Singlet Oxygen Formation in Li-Ion Batteries — •Annalena Genreith-Schriever[1,3], Hrishit Banerjee[1,2,3], Clare P. Grey[1,3], and Andrew J. Morris[2,3] — [1]Yusuf Hamied Department of Chemistry, University of Cambridge, Cambridge, United Kingdom — [2]School of Metallurgy and Materials, University of Birmingham, Birmingham, United Kingdom — [3]The Faraday Institution, Harwell Science and Innovation Campus, Didcot, United Kingdom

Ni-rich cathode materials achieve both high voltages and capacities in Li-ion batteries but are prone to structural instabilities and oxygen loss via the formation of singlet oxygen. Using ab initio molecular dynamics simulations, we observe spontaneous O_2 loss from the (012) surface of delithiated $LiNiO_2$, singlet oxygen forming in the process. We find that the origin of the instability lies in the pronounced oxidation of O during delithiation, i.e., O plays a central role in Ni-O redox in $LiNiO_2$, as analysed with density-functional theory and dynamical mean-field theory calculations based on maximally localised Wannier functions. The O_2 loss route observed here consists of 2 surface $O^{\cdot -}$ radicals combining to form a peroxide ion, which is oxidised to O_2, leaving behind 2 O vacancies and 2 O^{2-} ions: effectively 4 $O^{\cdot -}$ radicals disproportionate to O_2 and 2 O^{2-} ions. Singlet oxygen formation is caused by the singlet ground state of the peroxide ion, with spin conservation dictating the preferential release of $^1O_2$.

KFM 13.3 Tue 10:45 H46

Defects and Phase Formation in Non-Stoichiometric $LaFeO_3$: A Combined Theoretical and Experimental Study — •Daniel Mutter[1], Roland Schierholz[2], Daniel Urban[1], Sabrina Heuer[2,3], Thorsten Ohlerth[2,3], Hans Kungl[2], Christian Elsässer[1,4], and Rüdiger-A. Eichel[2,3] — [1]Fraunhofer IWM, Freiburg — [2]Forschungszentrum Jülich, IEK-9 — [3]RWTH Aachen, Institute of Physical Chemistry — [4]FMF, Universität Freiburg

Defect engineering of perovskite compounds has become increasingly popular as it offers the possibility to influence their catalytic properties for applications in energy storage and conversion devices such as solid-oxide fuel- and electrolyser cells. We present results of a combined theoretical and experimental study exploring the feasibility for an active manipulation of the La stoichiometry, and thereby the valence state of Fe, in $LaFeO_3$, which can be regarded as a base compound of the family of catalytically active $La_{1-x}A_xFe_{1-y}B_yO_{3-\delta}$ compounds. Concentrations of point defects are presened, derived from formation energies which were calculated by first-principles DFT+U calculations as a function of experimental processing conditions, resulting in predictions of achievable stoichiometry ranges. In the experimental part, LFO was synthesized with a targeted La-site deficiency, and we analyzed the phases in detail by X-ray diffraction and various electron microscopy methods (STEM, EDS, EELS). Instead of a variation of the La/Fe ratio, a mixture of two phases, $Fe_2O_3/LaFeO_3$, was observed, resulting in an invariant charge state of Fe, which is in line with the theoretical results.

KFM 13.4 Tue 11:00 H46

Can we improve thermoelectric properties by microstructural manipulations? — •Leonie Gomell[1], Tobias Haeger[2], Moritz Roscher[1], Hanna Bishara[1], Ralf Heiderhoff[2], Thomas Riedl[2], Christina Scheu[1], and Baptiste Gault[1] — [1]Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf, Deutschland — [2]Institute of Electronic Devices, University of Wuppertal, Deutschland

Thermoelectric (TE) materials convert (waste) heat into electrical energy. Several material properties determine TE performance, with the influence of microstructure being the least understood. However, the microstructure plays a crucial role in the performance of TE materials.

We present microstructural investigations of Fe_2VAl, synthesized via laser surface remelting. Scanning electron microscopy and atom probe tomography were used to bridge the scale from nanometer to micrometer. The local electrical resistivity was analyzed by an in-situ four-probe technique and the thermal conductivity by scanning thermal microscopy.

We observed a high dislocation density in the order of 10^{13} m^{-2} and small grains separated by low-angle grain boundaries. Segregation of V and N was found at grain boundaries and dislocations, observed by atom probe tomography. These defects scatter electrons and phonons, influencing their transport within the material.

We conclude that by manipulating the microstructure, we were able to improve the properties of Fe_2VAl. The combination of detailed microstructural analysis and local measurement of properties offers the possibility of understanding the microstructure-property relationship.

KFM 13.5 Tue 11:15 H46

Enhanced efficiency of graphene-silicon Schottky junction solar cell through inverted pyramid arrays texturation — •Jiajia Qiu[1,2], Huaping Zhao[1], Wenhui Ma[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]State Key Laboratory of Complex Nonferrous Metal Resources Clean Utilization, Kunming University of Science and Technology, Kunming 650093, China

Recently, a growing interest of incorporating graphene (Gr) with silicon (Si) to develop Gr-Si Schottky junction solar cells is considered as a potential low-cost alternative to the conventional p-n junction silicon solar cells. In this work, silicon nanowries (SiNWs) and silicon inverted pyramid arrays (SiIPs) were introduced on surface of Gr-Si solar cell through silver and copper-catalyzed chemical etching, respectively. The effects of SiNWs and SiIPs on carrier lifetime, optical properties and efficiency of Gr-SiNWs/SiIPs solar cell were systematically analyzed. The results show that the inverted pyramid arrays have ability of balance of antireflectance and surface area simultaneously. Compared to the Gr-SiNWs solar cells, power conversion efficiency (PEC) and carrier lifetime of Gr-SiIPs devices increase by 62% and 34%, respectively. Finally, the Gr-SiIPs cell with efficiency of 5.63% was successfully achieved through doping nitric acid. This work proposes a new strategy to introduce the inverted pyramid arrays for improving the performance of Gr-Si solar cells.

KFM 14: Ferroics – Domains and Domain Walls 1

Chair: Dr. Donald Evans (Augsburg University)

Time: Wednesday 9:30–12:05 Location: H5

KFM 14.1 Wed 9:30 H5

Strain driven conducting domain walls in a Mott insulator — •Lukas Puntigam[1], Donald Evans[1], Markus Altthaler[1], Somnath Ghara[1], Lilian Prodan[1], Vladimir Tsurkan[1,2], Stephan Krohns[1], and Istvan Kezsmarki[1] — [1]Universität Augsburg, 86159, Augsburg, Deutschland — [2]Institute of Applied Physics, MD 2028 Chisinau, Moldova

Ferroelectric domain walls, which can be written, tuned or erased, are being considered as functional building blocks for nanoelectronics. Especially, conducting domain walls are of high interest to achieve this functionality. To date, the origin for increased conductivity in ferroelectrics domain walls has been typically attributed to the formation of screening charges driven by polar discontinuities.

Here, we establish that for the template system, the lacunar spinel GaV_4S_8 also strain can enhance the conductivity of specific domain walls. This system exhibits ferroelectric domain pattern below a Jahn-Teller transition at 42K. At this temperature a change in its crystal structure can result in mechanical stress at domain walls. Piezoresponse force microscopy revealed an interesting ferroelectric pattern. Each ferroelectric domain can be identified by structural considerations to be one of the four possible polar direction. In case of domain walls between structural incompatible domains measurements with conductive atomic force microscopy show strongly enhanced conductivity denoting an additional twist highly conductive domain walls. Further, spatially resolved IV spectroscopy enable the investigation of the underlying conductivity mechanism at the tip-sample interface.

KFM 14.2 Wed 9:50 H5

In-situ tracking of the evolution of polarization during the growth of layered-ferroelectric Aurivillius phases — •Ipek Efe, Elzbieta Gradauskaite, Manfred Fiebig, and Morgan Trassin — Department of Materials, ETH Zürich, Switzerland

The highly anisotropic nature of layered oxides is key to exotic functionalities such as superconductivity, magnetoresistance, and ferroelectricity, which are promising for applications. However, their integration in epitaxial design is challenging due to the complexity of the unit cell, which makes precise monitoring of the growth a necessity. Here, we directly access the polarization dynamics of the model system Aurivillius $Bi_5FeTi_3O_{15}$ films during the epitaxial growth using in-situ optical second harmonic generation (ISHG). We identify an oscillating intensity of the ISHG signal during two-dimensional layer-by-layer growth. We correlate these oscillations with the periodical evolution of the polarization of ferroelectric film dictated by the chemistry of the planes in the unit-cell, which consists of alternating positively charged fluorite-like $(Bi_2O_2)^{2+}$ layer and negatively charged $(Bi_3FeTi_3O_{13})^{2-}$ perovskite blocks. In combination with reflection high-energy electron diffraction, we show how polarization of the films consistently switches from an out-of-plane orientation during the perovskite blocks growth, to a fully-in-plane orientation with the completion of the unit-cell termination and the $(Bi_2O_2)^{2+}$ capping. Our findings reveal previously hidden polarization dynamics during the epitaxial design and bring new insights in the sub-unit cell control of layered oxide films properties for the development of energy efficient oxide electronics.

KFM 14.3 Wed 10:10 H5

Continuous polarization control at nanoscopic dimensions — •Martin F. Sarott[1], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Electron Microscopy Center, Empa Swiss Federal Laboratories for Materials Science and Technology, Switzerland

The switchable bistable polarization in ferroelectrics allows for the binary control of optical, electronic, and catalytic properties. Going beyond the limitation of a binary remanent polarization holds great promise for emerging neuromorphic concepts. Here, we demonstrate that we can arbitrarily set the magnitude of the remanent ferroelectric polarization at the nanoscale in epitaxial $PbZr_{0.52}Ti_{0.48}O_3$ thin films with a single DC bias. By approaching the PZT morphotropic phase boundary, we achieve a high degree of control over this unusually susceptible system via epitaxial strain. We employ this to accomplish the formation of decoupled nanometric 180° domains with a broad coercive field distribution. Using in-situ optical second harmonic generation and X-ray diffraction, we study the emergence of the nanoscopic domain configuration. We then use piezoresponse force microscopy to demonstrate the ability to locally and reversibly modulate the remanent polarization *continuously* between depolarized and saturated, while preserving the nanoscopic length scale of the domains. We highlight the technological relevance of nanoscale non-binary polarization switching, by showing (i) the voltage-controlled tunability of the nonlinear optical response and (ii) the quasi-continuous tunability of the tunnel electroresistance in ferroelectric tunnel junctions.

KFM 14.4 Wed 10:30 H5

Impact of strontium on domain wall mobility in barium ti-

tanate — •Aris Dimou[1], Pierre Hirel[2], and Anna Grünebohm[1] — [1]Ruhr-Uni. Bochum, Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Bochum, Germany — [2]Univ. Lille, Unité Matériaux et Transformations (UMET), Lille, France

Solid solutions of barium-strontium titanate are widely used, environmentally friendly ferroelectric materials that are important for a plethora of applications [1,2]. The presence of domain walls are known to change the properties of a material, and its mobility is of key interest in contemporary electronic devices [3]. Surprisingly little attention has so far been paid to the impact of Sr on the domain wall mobility in barium titanate.

Here we present a microscopic study on the case of Sr inclusions in barium titanate. Our simulations reveal an increase in the activation energy for domain wall movement at the Sr inclusion. Suggesting that a thin Sr plane is enough to pin the domain wall.

[1] Acosta et al., $BaTiO_3$-based piezoelectrics: Fundamentals, current status, and perspectives. *Applied Physics Review*, **4**, 2017.

[2] Grünebohm et al., Interplay of domain structure and phase transitions: theory, experiment and functionality. *J. Phys. L Condens. Matter*, **34**, 2022.

[3] Sharma et al., Functional ferroic domain walls for nanoelectronics. Currently. Open. *Solid State Mater. Sci.*, **9**, 2005.

15 min. break

KFM 14.5 Wed 11:05 H5

Stability of enhanced domain wall conductivity in single-crystalline lithium niobate — •Ahmed Samir Lotfy[1,2], Manuel Zahn[1], Michael Rüsing[1], and Lukas Eng[1] — [1]Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany — [2]Department of materials, ETH Zürich, Zürich, Switzerland

Domain-wall conductivity (DWC) in ferroelectrics has emerged as a key functionality for developing nanoelectronic devices. In this regard, lithium niobate (LNO) is a promising candidate as previous studies have shown the capability to significantly enhance its DWC by making use of head-to-head and tail-to-tail DW configurations, and DW inclination angles under voltage treatments. However, understanding of the temporal and temperature-dependent stability of the enhanced DWC is lacking, limiting further steps of device implementation. For this, we performed a series of conductive atomic force microscopy and macroscopic electrometer measurements on single crystalline LNO samples. We show a characteristic conductance trend during voltage-induced enhancement which provides insights into the temporal stability of DWC. Moreover, our temperature-dependent measurements between 100 K and 300 K reveal the transport mechanism along the walls, pointing to the role of bound polarons. This is confirmed by the calculation of the activation energy. These results provide key insights into the stability of DWC in LNO for applications in practical devices.

KFM 14.6 Wed 11:25 H5

Electron scattering signatures of ferroelectric domains — •Ursula Ludacka[1], Jiali He[1], Emil Frang Christiansen[1], Shuyu Qin[2], Zewu Yan3[3,4], Edith Bourret[4], Antonius van Helvoort[1], Joshua Agar[2], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Department of Materials Science and Engineering, Lehigh University, Bethlehem, PA 18015, USA — [3]ETH Zurich, Zurich, Switzerland — [4]Lawrence Berkeley National Laboratory, Berkeley, USA

The emergence of ferroelectricity originates from polar displacements of lattice atoms, connotating a one-to-one correlation between electronic and structural properties at the atomic level. An established approach that allows for determining associated structural variations is scanning electron diffraction (SED). In SED, a focused electron beam is scanned over the specimen, probing diffracted electrons at each position of the raster scan. The corresponding patterns represent unique fingerprints of the probed areas, containing structural information. We demonstrate the potential and opportunities of this innovative 4D-STEM approach using improper ferroelectric $ErMnO_3$, an ideal model system as its basic ferroelectric properties and atomic-scale structure are well understood. In the ferroelectric state, the Er ions exhibit characteristic up-up-down and down-down-up patterns, corresponding to ferroelectric 180° domains with positive and negative polarization, respectively. These shifts cause different Bragg scattering conditions for the electrons and, hence, specific diffraction patterns that we utilize for domain imaging assisted by machine learning algorithms.

KFM 14.7 Wed 11:45 H5

Oxygen vacancies nucleate domain walls in ferroelectrics — •Urko Petralanda[1], Mads Kruse[1], Hugh Simons[2], and Thomas Olsen[1] — [1]CAMD, Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark — [2]Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

Domain walls are topological defects which emerge spontaneously in ferroelectrics [1]. At charged domain walls (CDW), free charge from the bulk is promoted to the conduction band through a band-bending mechanism, to compensate their local bound charge [2]. This creates highly conductive embedded mobile 2D nanosheets, suitable for nanoelectronics related applications [2]. Oxygen vacancies are believed to play a role in helping CDW overcome their strong electrostatic interaction. In this work [3], by means of density functional theory calculations in $BaTiO_3$ we clarify the screening mechanism of CDW charge in both pristine and oxygen vacancy aided cases, and we propose that, beyond the commonly accepted view of oxygen vacancies as CDW stabilizers, they can actually ignite the formation of CDW. We explain the experimentally observed difference in electronic conductivity of the positively and negatively charged CDW in $BaTiO_3$, as well as the generic prevalence of CDW in ferroelectrics. Such a vacancy driven CDW formation implies that specific charged domain wall configurations may be realized by bottom-up design.

[1] G. Catalan et al, Rev. Mod. Phys. 84, 119 (2012)
[2] T. Sluka et al, Nat. Commun. 4, 1808 (2013).
[3] U Petralanda et al, Phys. Rev. Lett. 127, 117601 (2021)

KFM 15: Materials for Energy Storage (joint session KFM/CPP)

Chair: Prof. Dr. Theo Scherer (KIT, Karlsruhe)

Time: Wednesday 9:30–12:05 Location: H7

KFM 15.1 Wed 9:30 H7

Hybrid CuCo2O4 nanosheets as binder-free supercapacitor electrodes — •Zidong Wang[1,2], Yude Wang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]School of Materials and Energy, Yunnan University, 6500504 Kunming, Peoples Republic of China

CuCo2O4 is one kind of pseudocapacitive materials and it has a high theoretical capacitance, but it suffers from poor electrical conductivity. In this work, CuCo2O4 nanosheets were directly grown on a conductive skeleton to significantly enhance the conductivity and at the same time reduce the agglomeration of CuCo2O4 nanosheets. In addition, the hybrid nanosheet structures also expand the interface and provide more active electrochemical sites, facilitating kinetic processes and electrochemical reactions. The as-prepared CuCo2O4 nanosheets on a conductive skeleton were studied as binder-free electrode and exhibited outstanding electrochemical performance with the specific capacitance of 1595 F g*1 at a current density of 1 A g*1 and 85.1% capacitance retention after 4600 cycles. These results indicated that hybrid CuCo2O4 nanosheets has great application potential as binder-free electrode in supercapacitors.

KFM 15.2 Wed 9:50 H7

Investigation of K-ion Intercalation and Conversion in Layer Transiton Metal Disulfide anode: The case of MoS2 and WS2 — •Yulian Dong, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Two-dimensional transition metal dichalcogenides (2D-TMDs) have a unique layered structure characterized by weak interlayer van der Waals interaction and strong in-plane covalent bonding. The structure allows the intercalation of guest species in the interlayer space, which

shows impressive properties in potassium-ion batteries (PIBs). Thus, various 2D TMDs, including sulfides (MoS2, SnS2, WS2) and selenide (MoSe2 and VSe2), have been studied as potential anode materials for PIBs. This work compares the intercalation and conversion of K in MoS2 and WS2. Intercalation and conversion process is observed during potassium in MoS2 in a voltage range of 3.0-0.5V and 0.5-0.01V, respectively. By controlling cut-off voltage, the investigation demonstrated high capacities derived from the conversion, but it destroys the 2D diffusion pathways leading to an unstable cycling span. While the K+ storage in WS2 is governed by the intercalation reaction rather than the conversion reaction. It exhibited a low capacity decay rate at both low and high current densities as well as great rate capability.

KFM 15.3 Wed 10:10 H7

Elucidation of the Pore Formation Mechanism in Hard-Carbon Microspheres — •Martin Wortmann[1], Waldemar Keil[2], Michael Westphal[1], Elise Diestelhorst[3], Jan Biedinger[1], Bennet Brockhagen[3], Günter Reiss[1], Claudia Schmidt[2], Klaus Sattler[4], and Natalie Frese[1] — [1]Bielefeld University, Bielefeld, Germany — [2]Paderborn University, Paderborn, Germany — [3]Bielefeld University of Applied Sciences, Bielefeld, Germany — [4]University of Hawaii, Honolulu, USA

Micro-spherical hydrochar can be carbonized by pyrolysis to produce hard-carbon microspheres with excellent electrochemical properties for the application as anode material in batteries. In this contribution, a temperature-resolved study of the chemical and morphological evolution of saccharide-derived hydrochar during pyrolysis up to 1000°C is presented. By combining a wide range of characterization methods all aspects of the structural transition are examined. The chemical processes occurring both in the bulk and at the surface of the carbon spheres are shown to affect the transition from an amorphous-polymeric to a nanocrystalline carbon-structure. The study focuses on the pore formation mechanism, which is driven by the aggregation of nanometer-sized oxygen-rich clusters at the sphere surface, which disintegrate in a narrow temperature range, leaving behind a mesoporous structure. The revealed molecular mechanisms provide key insights into the pyrolysis of carbonaceous materials.

KFM 15.4 Wed 10:30 H7

Hydrogenation of Pd nanoparticles at the nanoscale with in-situ TEM — •Svetlana Korneychuk[1,2], Stefan Wagner[1], Georgian Melinte[2], Darius Rohleder[3], Philipp Vana[3], and Astrid Pundt[1] — [1]IAM-WK, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]INT, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Institute of Physical Chemistry Georg-August-University Göttingen, Göttingen, Germany

Palladium-based nanomaterials play an important role in hydrogen technology. Extreme affinity of palladium to hydrogen is very attractive for various applications. Besides catalysis, Pd nanoparticles can assist in hydrogen delivery into other materials for hydrogen storage through a spill-over process. Pd-based materials are also used as hydrogen purification membranes and hydrogen detectors. The hydrogenation and dehydrogenation process of Pd nanoparticles is hence of high interest in the applications mentioned above. Nanoscale systems reveal significant thermodynamic deviations from the bulk due to higher surface to volume ratio, absence of grain boundaries, different behavior of defects and mechanical stress. In this work, we investigate the behavior of Pd nanoparticles and formation of PdHx in real time with in-situ H2-gas TEM. Many applications require operation at elevated temperatures. With the special gas holder from Protochips it is possible to reach pressures up to 1 atmosphere and study the particles at elevated temperatures with the limit of 1000°C. We can observe the local phase change at different temperatures and pressures with the help of spectroscopic and diffraction techniques at the nanoscale.

15 min. break

KFM 15.5 Wed 11:05 H7

Mild-temperature solution-assisted encapsulation of phosphorus into ZIF-8 derived porous carbon as lithium-ion battery anode — •Chengzhan Yan[1], Shun Wang[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany. — [2]Key Laboratory of Carbon Materials of Zhejiang Province, Institute of Materials and Industrial Technologies, Wenzhou University, Wenzhou, Zhejiang, 325027, China.

The high theoretical capacity of red phosphorus (RP) makes it a promising anode material for lithium-ion batteries (LIBs). However, the large volume change of RP during charging/discharging imposes an adverse effect on the cyclability, and the rate performance suffers from its low conductivity. Herein, a facile solution-based strategy is proposed to incorporate phosphorus into the pores of MOF-derived carbon hosts under a mild temperature. With this method, the blocky RP is etched into the form of polyphosphides anions (PP, mainly P5-), making it easily diffuse into the pores of porous carbon hosts. Especially, the indelible crystalline surface phosphorus could be effectively avoided, which is generated in the conventional vapor condensation encapsulation method. Moreover, highly-conductive ZIF-8 derived carbon hosts with any pore smaller than 3 nm are efficient for loading PP and these pores can well alleviate the volume change. Finally, the composite of phosphorus encapsulated into ZIF-8 derived porous carbon exhibits a significantly improved electrochemical performance as LIBs anode.

KFM 15.6 Wed 11:25 H7

Study on Li Ion Diffusion in $Li_xV_2O_5$ using First Principle Calculations and Kinetic Monte Carlo Simulations — •Fabian Dietrich[1], Eduardo Cisternas[1], Marcelo Pasinetti[2], and Gonzalo Dos Santos[2,3] — [1]Universidad de La Frontera, Temuco, Chile — [2]Universidad Nacional de San Luis, CONICET, San Luis, Argentina — [3]Universidad de Mendoza, Mendoza, Argentina

We study the Li diffusion in $Li_xV_2O_5$ ($0 < x \leq 1$) - a potential cathode material for Lithium ion batteries. Different diffusion pathways in this material in dependence on the Li ion concentration are investigated by applying first-principles calculations. The results are used to obtain the corresponding diffusion coefficients by employing two complementary methodologies: Kinetic Monte Carlo (KMC) simulations and a statistical thermodynamics approach. The KMC simulations for two different crystal planes give new evidence that the diffusion occurs mainly along the [010] direction, while the corresponding diffusion coefficients show a temperature dependence obeying the Arrhenius' Law. The necessity of the consideration of concentration-dependent barrier heights in the KMC simulations are demonstrated by looking at the significant changes of the concentration-dependence of the diffusion coefficients. The simulated diffusion coefficients of the combined approach show a good quantitative agreement with experimental data reported previously.

KFM 15.7 Wed 11:45 H7

NMR studies of sintering effects on the lithium ion dynamics in $Li_{1.5}Al_{0.5}Ti_{1.5}(PO_4)_3$ — •Philipp Seipel[1], Edda Winter[1], Michael Vogel[1], Tatiana Zinkevich[2], Sylvio Indris[2], Bambar Davassuren[3], and Frank Tietz[3] — [1]AG Vogel, Institute for Condensed Matter Physics, Technische Universität Darmstadt, Germany — [2]Karlsruhe Institut of Technology, IAM-ESS, Karlsruhe, Germany — [3]Forschungszentrum Jülich GmbH, IEK-1, Jülich, Germany

Various NMR methods are combined to study the structure and dynamics of $Li_{1.5}Al_{0.5}Ti_{1.5}(PO_4)_3$ samples, which were obtained from sintering at various temperatures between 650 °C and 900 °C and show high bulk conductivities up to 5 mS/cm. We use ^{7}Li NMR to study the transport mechanism in these glass ceramics [1]. Analysis of ^{7}Li spin-lattice relaxation and line-shape changes indicates the existence of two species of lithium ions with clearly distinguishable jump dynamics, which can be attributed to crystalline and amorphous sample regions. An increase of the sintering temperature leads to higher fractions of the fast lithium species with respect to the slow one, but hardly affects the jump dynamics in either of the phases. ^{7}Li field-gradient diffusometry reveals that the long-range ion migration is limited by the sample regions featuring slow transport. The high spatial resolution available from the high static field gradients of our setup allows us to observe also the lithium ion diffusion inside the small (< 100 nm) LATP crystallites, yielding a high self-diffusion coefficient of D=2 x 10^{-12} m^2/s at room temperature. [1]Winter et al., ZPCH, DOI:10.1515/zpch-2021-3109

KFM 16: Oxide Semiconductors (joint session HL/KFM)

Time: Wednesday 9:30–12:30 Location: H33

KFM 16.1 Wed 9:30 H33

Heavily doped Zinc Oxide with plasma frequencies in the telecommunication wavelength range — •Alexander Koch[1], Hongyan Mei[2], Jura Rensberg[1], Martin Hafermann[1], Jad Salman[2], Chenghao Wan[2,5], Raymond Wambold[2], Daniel Blascke[3], Heidemarie Schmidt[3], Jürgen Saalfeld[4], Sebastian Geburt[4], Mikhail Kats[2,5,6], and Carsten Ronning[1] — [1]Institute for Solid State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Department of Electrical and Computer Engineering, University of Wisconsin Madison, Madison, Wisconsin 53706, USA — [3]Leibniz Institute of Photonic Technology, 07745 Jena, Germany — [4]Innovavent GmbH, 37077 Göttingen, Germany — [5]Department of Materials Science and Engineering, University of Wisconsin Madison, Madison, Wisconsin 53706, USA — [6]Department of Physics, University of Wisconsin Madison, Madison, Wisconsin 53706, USA

We demonstrate high doping of ZnO by a combination of Ga ion implantation using a focused ion beam (FIB) system and post-implantation laser and flash lamp annealing. While ion implantation allows for the incorporation of impurities with nearly arbitrary concentrations, the additional optical annealing processes enable dopant activation close to the solid-solubility limit of Ga in ZnO. By this means, we achieved highly-doped ZnO:Ga with free-carrier concentrations of $9.5 \cdot 10^{20}$ cm^{-3}, which results in a plasma wavelength shorter than the telecommunication wavelength of 1.55 μm. Thus, ZnO:Ga is a very promising plasmonic material for optical applications in the near-infrared spectral region.

KFM 16.2 Wed 9:45 H33

Side-by-side display of optical and resistive H_2S gas sensing properties of pristine and gold functionalized ZnO nanowires — •Angelika Kaiser[1], Tanja Mauritz[1], Joachim Bansmann[3], Ulrich Herr[1], and Klaus Thonke[2] — [1]Institute of Functional Nanosystems, University Ulm, 89081 Ulm, Germany — [2]Institute of Quantum Matter, Semiconductor Physics Group, University Ulm, 89081 Ulm, Germany — [3]Institute for Surface Chemistry and Catalysis, University Ulm, 89081 Ulm, Germany

We investigate the mechanism of hydrogen sulfide (H_2S) gas sensing in pristine and gold functionalized zinc oxide (ZnO) nanowires (NW), two potent nanomaterial systems with an enlarged surface-area-to-volume ratio for medical breath analysis in the sub-ppm regime through the "electronic nose" approach. Pristine ZnO NWs (ZnO(NM)) are grown by high-temperature chemical vapor deposition (CVD) and functionalized with gold (Au) nanoparticles by magnetron sputtering (ZnO(Au)). The sensor response is studied by photoluminescence (PL) and electrical conductivity measurements of as-grown ZnO NWs and open gate ZnO NW ChemFET structures. A systematical side-by-side comparison of PL-intensity-time measurements and current-time measurements reveal a two-step detection process between 1 ppm of H_2S and ZnO(NM)/ZnO(Au) NWs. Temperature series hints at underlying gas adsorption/desorption processes. Additional X-ray photoelectron spectroscopy (XPS) confirms the beneficial gas-sensitive affinity between Au functionalization and H_2S gas, which leads to a significant improvement of the sensitivity for H_2S detection.

KFM 16.3 Wed 10:00 H33

Growth window of α-Ga_2O_3 on m-plane sapphire by pulsed laser deposition — •C. Petersen, S. Vogt, M. Kneiss, H. von Wenckstern, and M. Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Due to its high bandgap of 4.6-5.3 eV and high predicted breakdown field of 8 MV/cm [1], much attention is drawn to the wide bandgap semiconductor Ga_2O_3 for applications in high-power devices. However, besides the well-studied thermodynamically stable monoclinic β-phase of Ga_2O_3, the metastable α-polymorph with corundum structure is gaining scientists' interest. Since it is isostructural to Al_2O_3, miscibility over the entire composition range of α-$(Al_xGa_{1-x})_2O_3$ can be achieved [2] and the growth on cost-effective sapphire substrates becomes feasible. Thereby m-plane sapphire facilitates the growth of the corundum phase [3] and allows for thin films with electron mobilities as high as 65 cm^2(Vs)$^{-1}$ [4]. We present phase-pure α-Ga_2O_3 thin films grown on m-plane sapphire over a wide temperature range of 565 °C up to 750 °C with high cristallinity and surface roughnesses as low as 0.7 nm (RMS). We further demonstrate that for oxygen partial pressures above 0.001 mbar the formation of the monoclinical β-phase and spinel-defective γ-phase occurs and provide a corresponding phase diagram. Resulting samples were investigated employing X-ray diffraction, reciprocal space maps and atomic force microscopy. [1] Higashiwaki, Sc. Sci. Tech., 034001, 2016. [2] Hassa, pss-b, 2000394, 2020. [3] Kneiß, jmr, 4816-4831, 2021. [4] Akaiwa, pss-a, 1900632, 2020.

KFM 16.4 Wed 10:15 H33

Simulation of Switching Processes Inside Bilayer Valence Change Memory Cells by a Drift-Diffusion Model — •Nils Sommer[1], Stephan Menzel[1], and Rainer Waser[1,2] — [1]Peter Grünberg Institut 7, Forschungszentrum Jülich, Germany — [2]Institut für Werkstoffe der Elektrotechnik 2, RWTH Aachen, Germany

Valence change memory (VCM) cells are promising candidates for future nonvolatile storage devices [1]. VCM cells are characterized by their ability to switch between at least two stable resistance states by applying suitable bias voltages. A special structure of VCM cells are bilayer cells consisting of two semiconducting oxide layers, with one oxide serving as a tunnel barrier. Experiments show that a change in resistance of the cell can be caused by the exchange of oxygen between the two oxide layers [2]. However, the processes taking place are not yet well understood. We use a drift-diffusion model to simulate the movement of oxygen inside the semiconductor to gain a better understanding of the exchange process between the layers. We investigate the internal electric fields acting as a driving force on the oxygen, as well as the oxygen diffusion process that causes it to return to an equilibrium state. We show that an oxygen exchange deforms the shape of the tunnel barrier and by this changing the resistance of the cell. Further, we show that the change in resistance depends on the permittivity of the oxides.

[1] R. Waser, R. Dittmann, G. Staikov, K. Szot, Adv. Mater. 2009, 21, 2632 [2] A. Gutsche, S. Siegel, J. Zhang, S. Hambsch, R. Dittmann, Frontires in Neuroscience,2021, 15, 661261

KFM 16.5 Wed 10:30 H33

Phonons, Isotope Effects, and Point Defects in β-Ga2O3 — •Benjamin M. Janzen[1], Piero Mazzolini[2,3], Roland Gillen[4], Andreas Falkenstein[5], Vivien F. S. Peltason[1], Hans Tornatzky[1], Daniel Cierpinsky[1], Andrea Ardenghi[2], Manfred Martin[5], Janina Maultzsch[4], Roberto Fornari[2,3], Zbigniew Galazka[6], Oliver Bierwagen[2], and Markus R. Wagner[1] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V, Germany — [3]Department of Mathematical, Physical and Computer Sciences, University of Parma, Italy — [4]Chair of Experimental Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [5]Institute of Physical Chemistry, RWTH Aachen University, Germany — [6]Leibniz-Institut für Kristallzüchtung, Berlin, Germany

We present a combined experimental and theoretical study of lattice vibrations in a homoepitaxial β-Ga2O3 thin film grown by MBE with different oxygen isotopes (16O, 18O). Using polarized first- and second order micro-Raman spectroscopy, we identified all 15 first-order Raman modes of β-Ga2O3. In combination with density functional perturbation theory calculations, we identify the atomistic origins (Ga-Ga, Ga-O or O-O) of all Raman active phonon modes in β-Ga2O3 by quantifying the isotopically-induced relative frequency shifts of the individual Raman modes and investigate the presence of point defects on specific lattice sites.

KFM 16.6 Wed 10:45 H33

Epitaxial ZnO thin films and NWs — •Maximilian Kolhep[1], Margit Zacharias[1], and Jürgen Bläsing[2] — [1]Laboratory for Nanotechnology, Department of Microsystems Engineering (IMTEK), University of Freiburg, Freiburg 79110, Germany — [2]Otto-von-Guericke-University Magdeburg, Institute of Physics, Magdeburg, Germany

Due to its high piezoelectric coefficient and direct band gap of 3.37 eV, ZnO and especially ZnO nanowires are of interest for numerous future applications. We demonstrate the epitaxial growth of ZnO on Si(111) substrates using an AlN buffer layer by atomic layer deposi-

tion (ALD). ALD is a promising technique as it allows the deposition of extremely thin films with precise thickness control and excellent conformality over large areas. The crystalline quality of ZnO thin films determined by XRD increases with increasing deposition temperature and an additional post-annealing step. These thin films have a great potential as a substrate for the subsequent catalyst-free and epitaxial growth of ZnO NWs by CVD. The influence of growth parameters on the morphology of ZnO NWs will be discussed.

15 min. break

KFM 16.7 Wed 11:15 H33

Investigation of $CuBr_xI_{1-x}$ thin films and CuI bulk material — •Michael Bar[1], Evgeny Krüger[1], Steffen Blaurock[2], Stefan Merker[2], Holger von Wenckstern[1], Harald Krautscheid[2], and Marius Grundmann[1] — [1]Universität Leipzig, Felix-Bloch Institute, Germany — [2]Universität Leipzig, Institute of Inorganic Chemistry, Germany

Oxide based wide-bandgap materials with suitable transparency in the visible range are typically unipolar, such that heterostructures are needed for complementary devices. The search for a suitable p-type candidate has led to copper iodide (CuI), which unites transparency in the visible spectral range with exceptional hole mobility, therefore sharing and yet complementing typical properties of oxides. Fabrication methods include sputtering, spin coating and molecular beam epitaxy. [1,2] We present structural, electrical and optical properties of CuI bulk material, and thin films which were grown by pulsed laser deposition (PLD). Furthermore, alloyed thin films of $CuBr_xI_{1-x}$ were deposited with a segmented target PLD approach and investigated using x-ray diffraction, transmission and photoluminescence measurements. This PLD approach allows for deposition of thin films in the full composition range using only a single target without the need of sintering. [3] A systematic shift of lattice constants as well as the excitonic features can be observed as function of alloy composition.

[1] C. Yang *et al.*, Proc. Natl. Acad. Sci. USA, **113**(46), 12929, (2016).
[2] S. Inagaki *et al.*, Appl. Phys. Lett., **116**(19), 192105, (2020).
[3] H. Wenckstern *et al.*, Phys. Stat. Sol. (b), **257**(7), 1900626, (2020).

KFM 16.8 Wed 11:30 H33

A Koopman's compliant exchange correlation potential for semiconductors — •Michael Lorke[1], Peter Deak[2], and Thomas Frauenheim[2] — [1]Institute for Theoretical Physics, University of Bremen, Germany — [2]BCCMS, University of Bremen, Germany

Density functional theory is the workhorse of theoretical materials investigations. Due to the shortcoming of (semi-)local exchange correlation potentials, hybrid functionals have been established for practical calculations to describe surfaces, molecular adsorption, and defects. These functionals operate by mixing between semi-local and Hartree-Fock exchange semi-emprically. However, their parameters have to be optimized for every material separately. To treat materials with a more physics driven approach and without the need of parameter optimization is possible with many-body approaches like GW, but at an immense increase in computational costs and without the access to total energies and hence geometry optimization.

We propose a novel exchange correlation potential[1] for semiconductor materials, that is based on physical properties of the underlying microscopic screening. We demonstrate that it reproduces the low temperature band gap of several materials. Moreover it respects the required linearity condition of the total energy with the fractional occupation number, as expressed by the generalized Koopman's theorem. We also show that this novel functional can be used as a kernel in linear response TDDFT to reproduce excitonic effects in optical spectra

[1] Physical Review B 102 (23), 235168 (2020)

KFM 16.9 Wed 11:45 H33

The role of defects in polaron hopping transport in epitaxial BiVO4 for solar water splitting — •Malte Luca Weber, Viktoria Franziska Kunzelmann, and Ian Sharp — Walter Schottky Institute, TUM, Am Coulombwall 4, 85748 Garching, Germany

Use of green hydrogen as a fuel, energy storage medium, and reactant in chemical industry is one of the key strategies on the way to a sustainable economy. In this regard, solar driven water splitting using semiconductor photoelectrodes is a promising approach for sustainable production of hydrogen. Among various investigated semiconductor photoelectrodes, BiVO4 offers several desirable characteristics, including favourable band edge energetics, high carrier separation efficiency, and potential for stable operation under photoelectrochemical conditions. However, the material is characterised by very low carrier mobilities due to self-trapping formation of small polarons. Here, the effect of intentionally introduced defects on charge carrier mobility is investigated. Using a novel solution-based synthesis technique, high-quality epitaxial BiVO4 thin films were grown on YSZ (001). Post-synthetic vacuum annealing enables tuneable introduction of tuneable concentrations of oxygen vacancy defects. Optical characterisation by photothermal deflection spectroscopy clearly indicates an increase of the sub-bandgap absorption for an increasing defect concentration, leaving unaltered the bandgap. Temperature-dependent electrical conductivity measurements indicate a thermally-activated hopping behaviour, which is characterised by higher conductivities and lower hopping behaviours with increasing native point defect concentrations.

KFM 16.10 Wed 12:00 H33

Conduction channels in polycrystalline copper iodede thin films — •Tillmann Stralka — Universtität Leipzig, Felix Bloch Institute for Solid State Physics, Linnéstr. 5, 04103 Leipzig, Germany

The search for high-performance, transparent p-type conductive materials has been a major challenge for decades [1]. Copper iodide (CuI) or alloys based on CuI [2] could offer a solution, since CuI does outperform all other known p-type TCMs, concerning transmittance in the visible spectrum as well as electrical conductivity at room temperature [3]. In this contribution polycrystalline CuI thin films, grown by sputtering, are investigated. Hereby we try to understand and differentiate the contribution of grains and grain boundaries (GBs) to electrical transport. Extended structural defects such as GBs lead to a depletion of majority charge carriers in their vicinity and even a localised inversion (two dimensional electron gas) within GBs was reported [4]. To acquire morphological (grain and GBs) and electrical properties with a high spatial resolution we employ current probe atomic force microscopy and Kelvin probe force microscopy. We evaluate these measurements with a novel approach that offers the possibility to correlate topographic and electrical properties over a whole series of scans in dependence on an externally applied voltage [5], measuring temperature, probe force, plasma treatment and degradation over time.

[1] M. Grundmann et al., J.Phys.D.Apps.Phys., 49(213001), 2016 [2] T. Jun et al., Adv. Mater., 30(1706573), 2018 [3] C. Yang et al., PNAS 113(412929), 2016 [4] M. Kneiß et al., Adv. Mater. Interfaces, 5(6), 2018 [5] I. Visoly-Fisher et al., Adv. Funct. Mater., 16(649), 2016

KFM 16.11 Wed 12:15 H33

First-Principles Studies of Defects in Bismuth Vanadate — •Nicklas Österbacka[1], Francesco Ambrosio[2], and Julia Wiktor[1] — [1]Chalmers University of Technology, Gothenburg, Sweden — [2]University of Salerno, Fisciano, Italy

Bismuth vanadate, a transition-metal oxide semiconductor with a bandgap of 2.4 eV, has shown great promise as a water-splitting photocatalyst. Its practical performance remains limited due to slow hole transfer, high charge recombination rates, and low conductivity, however. An atomistic understanding of the relationship between the material's structure and its properties is key to solving these issues. To this end, we have performed first-principles calculations on the native defects of bismuth vanadate, revealing their structural complexity and highlighting the importance of taking charge localization into account for this class of materials. Additionally, we show that oxygen vacancy-induced distortions in the material complicates phase identification of synthesized samples by making powder X-ray diffraction ambiguous.

KFM 17: Focus Session: Surfaces and Interfaces of (Incipient) Ferroelectrics (joint session O/KFM)

Ferroelectricity is a property of materials that allows spontaneous, switchable electric polarization. Recently, many surface-related applications have been proposed where ferroelectric or incipient-ferroelectric materials exhibit superior properties. These include catalysis, electron-hole separation in light harvesting, unique electronic properties such as a negative capacitance in heterostructures of ferroelectric materials, to name just a few. While (incipient) ferroelectrics clearly perform well in the aforementioned applications, there is very limited fundamental understanding of the processes involved on the surfaces of these materials.

Organizers: Martin Setvin (Charles University, Prague), Chiara Gattinoni (London South Bank University), and Michele Reticcioli (University of Vienna)

Time: Wednesday 15:00–18:30 Location: H3

Topical Talk KFM 17.1 Wed 15:00 H3

In search of electrostatic happiness at surfaces — •Nicola Spaldin — Materials Theory, ETH Zurich

We review the concept of surface charge in ionic insulators, first, in the context of the polarization in ferroelectric materials (traditionally discussed in the ferroelectrics community) and, second, in the context of layers of charged ions (traditionally discussed in the surface science community). In both cases, the surface charge leads to an electrostatic instability if it is not compensated, which is usually detrimental for the development of electronic devices based on ferroelectrics, but favorable for applications such as catalysis where surface reactivity is desirable.

Using the prototypical multiferroic bismuth ferrite, BiFeO3, as an example, we show how the spontaneous ferroelectric polarization and the charged ionic layers can in fact combine to yield stable, uncharged "happy" (100) surface geometries. Switching the polarization causes these (100) surfaces considerable electrostatic distress, which must be compensated by the introduction of charged point defects or adsorbates. We demonstrate that the relative happiness or unhappiness of the surfaces enables a cycle of alternating charged then neutral adsorbates on polarization switching, which can be exploited for water remediation and water splitting.

We close with a proposal that these physics can induce polarization in thin films of certain usually non-polar materials, and give a recipe for determining likely candidates.

In collaboration with Chiara Gattinoni, Ipek Efe and Marta Rossell

Topical Talk KFM 17.2 Wed 15:30 H3

Synthesis and Characterisation of Ultra-thin Aurivillius Phase Multiferroics — •Lynette Keeney — Tyndall National Institute, University College Cork, Lee Maltings Complex, Dyke Parade, Cork, Ireland, T12 R5CP

Multiferroic materials, possessing simultaneous ferroelectric and ferromagnetic memory states, have been road-mapped as promising multistate architectures for memory scaling beyond current technologies. In recent years, my team reported the design of such a novel room temperature multiferroic material with an Aurivillius phase structure that could ideally be suited to future fabrication of revolutionary memory devices. Electrostatic strain and elastic energy variations close to defect regions increase the extent of magnetic partitioning and also influence the formation of exotic charged domain walls and polar vortices. This further initiates technology prospects in ultra-compact data storage, energy-efficient neuromorphic computing and ultrahigh speed data processing. As miniaturisation of electronic devices continues, a crucial requirement is the enhancement of their functional properties at very small dimensions. In this presentation, I will discuss how direct liquid injection chemical vapour deposition allows for frontier-development of ultra-thin films at fundamental thickness. Via a two-dimensional layer-by-layer growth mode, films equating to half of one unit-cell (2.5 nm) of the Aurivillius structure are grown. The persistence of stable ferroelectricity, even when pushed to ultra-thin thicknesses, demonstrates the recent progress in the optimisation of Aurivillius phase materials for utilisation in future miniaturised multiferroic-based devices.

KFM 17.3 Wed 16:00 H3

Influence of Nb dopants on the polarization and screening on cleaved $SrTiO_3$(001) surfaces — •Igor Sokolović[1], Alexander Hoheneder[1], Jesus Redondo[2], Dominik Wrana[2], Michael Schmid[1], Ulrike Diebold[1], and Martin Setvín[2] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Faculty of Physics and Mathematics, Charles University, Prague, Czech Republic

The incipient ferroelectric $SrTiO_3$ can turn ferroelectric even at room temperature under the application of strain, and this quantum phase transition can be utilized to cleave $SrTiO_3$ single crystals that otherwise posses no preferable cleavage planes [1]. This cleaving procedure creates truly bulk-terminated $SrTiO_3$(001) surfaces that come the closest to being pristine [2]. In this talk, I will present how the SrO- and TiO_2-terminated surface domains of opposite polarity can be influenced by the small changes in the amounts of Nb doping. The cleaved $SrTiO_3$(001) surfaces with varying Nb doping levels were systematically studied with atomic resolution using noncontact atomic force microscopy (ncAFM) and scanning tunneling microscopy (STM). It was observed that Nb doping does not affect the magnitude of the strain-induced polarization, yet still significantly affects the morphology, the electronic structure, and the domain-wall structure on cleaved $SrTiO_3$(001) surfaces. Beside demonstrating the interplay between the domain distribution and electrostatic screening, these results show how the properties of these heterogeneous surfaces can be tuned.

[1] Sokolović *et al.*, Phys. Rev. Mater. 3, 034407 (2019)
[2] Sokolović *et al.*, Phys. Rev. B 103, L241406 (2021).

KFM 17.4 Wed 16:15 H3

Polaronic Properties of the weakly-polar $SrTiO_3$(001) Surface — •Florian Ellinger[1], Michele Reticcioli[1], Igor Sokolović[2], Ulrike Diebold[2], Martin Setvín[3], and Cesare Franchini[1,4] — [1]University of Vienna — [2]Technische Universität Wien — [3]Charles University Prague — [4]Università di Bologna

The $SrTiO_3$(001) surface shows ferroelectric-like distortions on the bulk-like termination, an out-of-plane dipole moment, and so-called "weak polarity". Recent experiments propose that these effects are compensated by Sr-adatoms and -vacancies, stabilizing the unreconstructed surface. [1]

We investigate the 1×1 $SrTiO_3$(001) surface with TiO_2- and SrO-terminations by means of density functional theory (DFT) simulations. Our calculations confirm the experimental interpretation and show that these polarity-compensating surface defects introduce additional charge. Adsorbing Sr-adatoms and doping with Nb leads to excess electrons in the crystal, facilitating the formation of electron-polarons. On the other hand, by creating Sr-vacancies on the surface we introduce excess holes to the system, which can localize as hole-polarons. For both kinds of polarons we analyze their general properties, e.g., the preferred localization site or stability. Further, we compare results of different structural phases of this crystal to achieve a comprehensive understanding of mentioned physical phenomena.

[1] Sokolović et al., *Incipient ferroelectricity: A route towards bulk-terminated $SrTiO_3$*, Phys. Rev. Materials 3, 034407 (2019)

KFM 17.5 Wed 16:30 H3

Ferroelectric domain imaging in barium titanate using infrared-visible sum-frequency generation microscopy — •Dorothee Mader[1], Daniel Lourens[2], Maarten Kwaaitaal[2], Richarda Niemann[1], Sören Wasserroth[1], Sandy Gewinner[1], Marco De Pas[1], Wieland Schöllkopf[1], Martin Wolf[1], Andrei Kirilyuk[2], Sebastian F. Maehrlein[1], and Alexander Paarmann[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Radboud Universiteit, Nijmegen, The Netherlands

Phonons exhibit a mostly unexplored leverage on the mechanisms and

dynamics of domain formation in ferroics. Here, a new method is employed combining resonant phonon excitation and ferroelectric domain imaging of barium titanate (BTO) using infrared-visible (IR-VIS) sum-frequency generation (SFG) microscopy [1]. BTO is a non-centrosymmetric perovskite oxide with a strong ferroelectric polarization in its tetragonal phase. Typically, BTO samples exhibit a multi-domain structure. In this contribution, SFG microscopy is shown to naturally provide domain contrast due to the polarization-induced local variation of the nonlinear susceptibility. Additionally, our spectral analysis of the SFG response reveals the domain-selective phonon resonances for all high-frequency phonons in the IR spectral range of 500-800 cm^{-1}. By locally mapping phonon resonances in domains and domain walls, this approach may enable in-depth understanding of the underlying physics of domain formation and its dynamics. [1] R. Niemann et al., Appl. Phys. Lett. 120, 131102 (2022).

Topical Talk KFM 17.6 Wed 16:45 H3

Water-oxidation catalysis on surfaces of ferroelectrics — •Ulrich Aschauer[1], Nathalie Vonrüti[1], Zhenyun Lan[2], Didrik R. Småbråten[1], Tejs Vegge[2], and Ivano E. Castelli[2] — [1]University of Bern, Bern, Switzerland — [2]Technical University of Denmark, Kgs. Lyngby, Denmark

Surfaces of ferroelectrics have unique properties for catalysis since the binding strength of reaction intermediates can be modulated by switching the ferroelectric polarization. This could allow to overcome the limitations of the Sabatier principle and enable dynamical catalysts operation. In this talk, we will focus on the interplay between screening charge transfer to surfaces, the adsorbate coverage and the (photo)electrochemical water-oxidation activity of ferroelectric surfaces. We will compare different ferroelectric materials such as $BaTiO_3$, strained $LaTiO_2N$ and the hexagonal improper ferroelectric oxynitride $InSnO_2N$. Our results indicate that ferroelectric switching can indeed provide an economically interesting route to enhance the catalytic activity but that material-specific intricacies of the surface adsorbate coverage need to be understood and controlled to exploit the full potential of ferroelectric switching in (photo)electrocatalysis.

KFM 17.7 Wed 17:15 H3

The polar $KTaO_3$ (001) surface: Electronic structure and CO adsorption — Zhichang Wang[1], Michele Reticcioli[2], Zdenek Jakub[1], Michael Schmid[1], Gareth Parkinson[1], Ulrike Diebold[1], Cesare Franchini[2], and •Martin Setvin[3] — [1]TU Wien, Vienna, Austria — [2]University of Vienna, Vienna, Austria — [3]Charles University, Prague, Czech Republic

Polar surfaces offer intriguing physical and chemical properties applicable in electronics or catalysis. Cleaving the $KTaO_3$ perovskite along its polar (001) plane provides a well-defined, bulk-terminated surface with KO and TaO_2 terminations [1]. As-cleaved surfaces exhibit a high concentration of in-gap states; these electrons predominantly reside at the TaO_2-terminated parts of the surface. These electrons can affect surface chemistry, as is demonstrated for CO molecules. CO has two adsorption configurations on the TaO_2 termination, and the CO differs in how it couples to the excess electrons. DFT calculations indicate that CO preferentially couples to electron bipolarons.

The work was supported by FWF project P32148-N36, by GACR 20-21727X and GAUK Primus/20/SCI/009.

[1] M. Setvin, M. Reticcioli, F. Poelzleitner et al., Science 359, 572 (2018)

KFM 17.8 Wed 17:30 H3

Polarons and ferroelectricity: tip-induced phenomena on oxide perovskite surfaces — •Dominik Wrana[1], Igor Sokolović[2], Jesus Redondo[1], Pavel Kocán[1], Aji Alexander[1], Llorenç Albons[1], and Martin Setvin[1] — [1]Department of Surface and Plasma Science, Charles University, Prague, Czech Republic — [2]Institute of Applied Physics, TU Wien, Vienna, Austria

In this talk, I will present the similarities and differences between two representative perovskite oxide surfaces: $KTaO_3$(001) and $BaTiO_3$(001), showcasing the manifestation of the (incipient-) ferroelectricity on the atomic and electronic structure. Both surfaces were prepared by cleaving single crystals in situ and characterized by means of qPlus nc-AFM at temperatures ranging from 4K to 100K.

Bulk-terminated $KTaO_3$(001) develops two alternating domains of KO and TaO_2 [1]. Excess electrons injected from the AFM tip form quasiparticles called polarons (charges coupled with lattice distortions) which can be further shaped into 1D or 2D structures by emerging electric fields.

Different mechanism applies in the case of $BaTiO_3$(001), where at low temperatures titanium atoms can easily break the symmetry causing a spontaneous polarization. Hence, a biased tip allows for reversible manipulation of individual atoms on the surface: writing and erasing polarized ferroelectric domains.

[1] Setvin, Martin, et al. Science 359.6375 (2018): 572-575

KFM 17.9 Wed 17:45 H3

Optimisation and miniaturisation of naturally-layered multiferroic thin films — •Lynette Keeney — Tyndall National Institute, University College Cork, Lee Maltings Complex, Dyke Parade, Cork, Ireland, T12 R5CP

Multiferroic materials, possessing simultaneous ferroelectric and ferromagnetic memory states, are road-mapped as promising multistate architectures for memory scaling beyond current technologies. In recent years, my team reported the design of such a novel room temperature multiferroic material with an Aurivillius phase structure that could ideally be suited to future fabrication of revolutionary memory devices. In this presentation, I will discuss how electrostatic strain and elastic energy variations close to bismuth oxide interfaces and defect regions are key to promoting magnetic cation partitioning and multiferroic behaviour. These also influence the formation of exotic charged domain walls and polar vortices, further initiating technology prospects in ultra-compact data storage. As miniaturisation of electronic devices continues, a crucial requirement is the enhancement of their functional properties at very small dimensions. Direct liquid injection chemical vapour deposition allows for frontier-development of ultra-thin films at fundamental thickness. Via a two-dimensional layer-by-layer growth mode, films equating to half of one unit-cell (2.5 nm) of the Aurivillius structure are grown. The persistence of stable ferroelectricity, even when pushed to ultra-thin thicknesses, demonstrates the recent progress in the optimisation of Aurivillius phase materials for utilisation in future miniaturised multiferroic-based devices.

Topical Talk KFM 17.10 Wed 18:00 H3

Spin-orbitronics and superconductivity in KTaO3 twodimensional electron gases — •Srijani Mallik[1], Gerbold Ménard[2], Guilhem Saiz[2], Hugo Witt[1,2], Sara Varotto[1], Luis M. Vicente-Arche[1], Julien Bréhin[1], Annika Johansson[3], Börge Göbel[4], Raphaël Salazar[5], Ingrid Mertig[4], Lara Benfatto[6], Nicolas Bergeal[2], and Manuel Bibes[1] — [1]Unité Mixte de Physique CNRS/Thales, Palaiseau, France — [2]LPEM ESCPI, Paris, France — [3]MPI, Halle, Germany — [4]Martin-Luther-Universitat Halle-Wittenberg, Germany — [5]Synchrotron SOLEIL, France — [6]Sapienza University of Rome, Italy

Similar to SrTiO3 (STO) recent research has shown that KTaO3 (KTO) may also harbor a 2DEG at interfaces with several oxide materials. Due to the presence of Ta (5d element), it is expected that the Rashba spin-orbit coupling in KTO 2DEGs should be larger than in STO 2DEGs. Further, (110) and (111)-oriented KTO 2DEG show superconductivity at temperature a factor of ca. 10 higher than in STO 2DEGs. In this talk we will show that 2DEGs can be generated by the simple deposition of Al metal on KTO single crystals. We will report their electronic band structure by angle-resolved photoemission spectroscopy, evidencing a peculiar Rashba splitting. We will show that this Rashba state can be harnessed to achieve very efficient spin-charge interconversion. Finally, we will present microwave impedance spectroscopy measurements of the superconducting condensate and discuss the nature of superconductivity in these systems.

KFM 18: Focus Session: Diamond and related dielectric materials

This focus session contains basic diamond research due to optical and dielectric properties for applications in low and high power electronics. High frequency and high microwave power applications are discussed. The use of diamond material in GHz up to THz range is the main purpose of this session.

Organizer: Prof. Dr. Theo Scherer (KIT, Karlsruhe)

Time: Wednesday 15:00–16:50 Location: H5

Invited Talk KFM 18.1 Wed 15:00 H5

Deep understanding of advanced optical and dielectric materials for fusion diagnostic applications — •Anatoli I. Popov[1], E Kotomin[1], V Kuzovkov[1], A Lushchik[2], and Theo A Scherer[3] — [1]Institute of Solid State Physics, University of Latvia, 8 Kengaraga str., LV-1063 Riga, Latvia — [2]Institute of Physics, University of Tartu, W. Ostwald Str. 1, 50411, Tartu, Estonia — [3]Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

In this talk, I will give a short overview of the most interesting results obtained in the framework of two EUROfusion Enabling Research projects - Advanced experimental and theoretical analysis of defect evolution and structural disordering in optical and dielectric materials for fusion applications (AETA) (2019-2020) and Investigation of defects and disorder in nonirradiated and irradiated Doped Diamond and Related Materials for fusion diagnostic applications (DDRM) Theoretical and Experimental analysis (2021-2023).

In a series of joint works by ISSP UL (Latvia), UT (Estonia), and KIT (Germany), radiation damage of some promising functional materials (Al2O3, MgAl2O4, SiO2, and diamond) from the priority list of the EUROfusion consortium was studied under neutron, proton, heavy-ion. Their optical, dielectric, vibrational & magnetic properties were carefully studied. Based on this study, we developed new theoretical methods able to evaluate and predict some important properties of these materials as well as their radiation damage evolution under extreme reactor conditions.

KFM 18.2 Wed 15:30 H5

Physics of natural and artificial diamond gemstones — •Theo Scherer — Karlsruhe Institut of Technology (KIT-IAM-AWP)

Diamond gemstones were very well appreciated in the antique world. Independent on the purpose of jewelry, diamond is a crystalline solid state material with excellent physical and chemical properties as a high Young modulus or a very high thermal conductivity. By doping the material with boron, electrical conductivity can be observed. This is important for electronic devices. In this talk the wide range of production of gemstones and technical applications like high frequency high power microwave transmission diamond windows for nuclear fusion power plants will be presented. Different diamond classifications, cuts and colors by impurities will be shown. A comparison of natural diamonds and artificial produces ones are topic of the discussion.

KFM 18.3 Wed 15:50 H5

Basic considerations for fracture toughness measurements of MPA CVD diamond to be used in nuclear fusion — •Gaetano Aiello, Theo Scherer, Andreas Meier, Sabine Schreck, and Dirk Strauss — Karlsruhe Institute of Technology, Institute for Applied Materials, D-76344 Eggenstein-Leopoldshafen, Germany

In nuclear fusion, Microwave Plasma Assisted (MPA) Chemical Vapour Deposition (CVD) polycrystalline diamond is the only material allowing for transmission of high power microwave beams (1-2 MW) in long-pulse gyrotron operations. The reason lies in the combination of extraordinary thermal, mechanical and optical properties of diamond, which is used in the shape of disks having thickness of 1 to 2 mm for windows. Being diamond a brittle material, failure to fracture is the main failure mode. Accordingly, an appropriate mechanical characterization is required as diamond plays a major safety role in fusion machines. Due to limited body of work in literature, fracture toughness measurements have to be first carried out for this material and then a design criterion for structural integrity assessment has to be applied. In this work, the preliminary activities aiming to define the optimum experimental measurement method of fracture toughness for thin diamond samples are shown and discussed. An outlook to the next steps is also given.

KFM 18.4 Wed 16:10 H5

Development diamond based Kinetic Inductance Detectors — •Francesco Mazzocchi, Dirk Strauss, and Theo Scherer — Karlsruhe Institute Of Technology

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 18.5 Wed 16:30 H5

Characterization of - A survey of electrical and dielectric properties — •Theo Scherer — Karlsruhe Institute of Technology (KIT-IAM-AWP)

p-Boron-doped polycrystalline CVD diamond samples were produced and delivered by the German company Diamond Materials in Freiburg (Germany). In a first step, main properties of this candidates for diagnostic and/or heating windows in future nuclear fusion reactors were investigated. By a special measurement technique, it was possible to determine the Boron doping concentration in Diamond by measurement of the resistive properties by using the van der Pauw method. So prepared, an irradiation campaign with neutrons and/or heavy ions on these samples will follow. The second material investigated, was r-plane single crystalline sapphire. For the first characterization the dielectric properties of a 3*-wafer in dependency of the frequency in a FABRY-PEROT resonator setup was performed. Also, this is the preparation for the next irradiation experiments in this project.

KFM 19: Ferroics – Domains and Domain Walls 2

Chair: Dr. Jan Schultheiß (Augsburg University, NTNU Trondheim)

Time: Wednesday 15:00–16:00 Location: H7

KFM 19.1 Wed 15:00 H7

Phase Field Simulations of the Dipolar Interaction in Hexagonal Manganites — •Aaron Merlin Müller, Amadé Bortis, Manfred Fiebig, and Thomas Lottermoser — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

We introduce a phase-field method that allows simulation of dipolar interaction in thin-film hexagonal manganites and investigate its effect on the unconventional ferroelectric vortex domain pattern of the material. Dipolar interactions are assumed to have negligible influence because of the improper nature of the ferroelectric order. Hence, dipolar interactions are commonly neglected when modeling such systems. Efficiently incorporating dipolar interactions of out-of-plane-oriented dipoles in phase-field methods is challenging as they represent a nonlocal Coulomb contribution to the free energy. In addition, the Coulomb interaction of a polarization field diverges at zero distance, unlike for atomistic dipole models. In our work, we show that including the dipolar interaction in the phase-field method results in more regular shaped domains in comparison to simulations that ignore the dipolar interaction, with lower variance in domain size. The ferroelectric domains of our revised approach resemble the experimentally observed patterns more closely. Hence, our work gives insights on the often neglected effects of dipolar interaction and the resulting depolarizing field on ferroelectric domains in an important class of improper ferroelectric materials.

KFM 19.2 Wed 15:20 H7

Dynamics of the electrocaloric effect in ferroelectric materials — •Jan Fischer, Daniel Hägele, and Jörg Rudolph — Ruhr-Universität Bochum, Faculty of Physics and Astronomy, Experimental Physics VI (AG), Germany

The electrocaloric effect (ECE) in ferroelectrics is a promising candidate for energy efficient cooling technologies. The ECE leads to a reversible adiabatic temperature change ΔT of a ferroelectric material upon a change of an external electric field. The reliable determination of the adiabatic ΔT is, however, experimentally challenging and most studies use either indirect methods which are prone to artifacts, or comparably slow direct methods. The dynamics of the ECE has therefore not been systematically studied so far. Here, we introduce a direct and contactless method to study the full dynamics $\Delta T(t)$ of the ECE with μK temperature resolution and μs temporal resolution via the infrared emission of the sample. The simultaneous recording of transients for $\Delta T(t)$, applied electric field $E(t)$, and induced polarization $P(t)$ gives the opportunity to correlate the caloric properties with the dielectric properties thus opening perspectives for a fundamental understanding of the ECE also in complex materials like relaxor ferroelectrics. Our techniques allows also for high-frequency measurements as needed for adiabatic measurements in thin films.[1,2] We will discuss several examples ranging from bulk materials to thin films.

[1] J., Döntgen, *et al.*, Applied Physics Letters 106, 3 (2015)
[2] J., Döntgen, *et al.*, Energy Technology 6, 8 (2018)

KFM 19.3 Wed 15:40 H7

Interfacial Stabilization of Homochiral Ferroelectric Domain Walls in $BiFeO_3$ — •Elzbieta Gradauskaite[1], Quintin N. Meier[2], Natascha Gray[1], Marco Campanini[3], 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

Chirality is a concept central to all molecular interactions in biological systems. In the last decade its importance was also highlighted in condensed-matter physics, where spin textures at the homochiral ferromagnetic domain walls were shown to enable their deterministic current-driven motion. Nevertheless, only a few reports on polar chirality exist to this date, prompting increased research efforts on this important issue. Here, we report the stabilization of net chirality in $BiFeO_3$ ferroelectric films grown on a fully in-plane-polarized ferroelectric layer of the Aurivillius phase. By introducing an in-plane-polarized epitaxial buffer we create polarization continuity and provide a symmetry breaking at the interface with the out-of-plane polarized $BiFeO_3$. Scanning probe microscopy uncovers the stabilization of conceptually novel 251° domain walls in $BiFeO_3$. Their unusual chirality is likely associated with the ferroelectric analog to the Dzyaloshinskii-Moriya interaction in magnets. Thus, we demonstrate a simple design combining perpendicular polar anisotropies for the effective stabilization of homochiral textures in ferroelectric thin films.

KFM 20: Perovskite and Photovoltaics 2 (joint session HL/CPP/KFM)

Time: Wednesday 15:00–18:15 Location: H34

KFM 20.1 Wed 15:00 H34

Electronic structure analysis of the interface of a TiO_2 electron-transport layer with a perovskite $CsPbI_3$ photovoltaic absorption layer — •Amirhossein Bayani[1], Julian Gebhardt[1], and Christian Elsässer[1,2] — [1]Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstrasse 11, 79108 Freiburg, Germany — [2]Freiburg Materials Research Center (FMF), Albert-Ludwigs-University Freiburg, 79104 Freiburg, Germany

Lead-based hybrid perovskite halides are currently the most promising light absorbing materials to supplement or even replace Si in next generation solar cells. With intensive research of the bulk material properties in recent years, a strong interest emerges in studying the interfaces to the contact layers in order to reach the final boost of solar efficiency in devices. Here, we study the interface of $CsPbI_3$ with TiO_2 as model interface for a perovskite with an electron transport layer. In particular, we investigate the rutile-TiO_2(001)[001] / $CsPbI_3$(001)[100] interface using self-energy corrected density functional theory. By this state-of-the art modeling technique, we analyze the alignment of work-functions and investigate the band alignment at the interface.

KFM 20.2 Wed 15:15 H34

Influence of the Ionic Liquid $BMIMBF_4$ on the film formation and optoelectronic properties of $MAPbI_3$ — •Simon Biberger, Konstantin Schötz, Philipp Ramming, Nico Leupold, Ralf Moos, Anna Köhler, Helen Grüninger, and Fabian Panzer — University of Bayreuth, Bayreuth, Germany

Today, metal halide perovskite solar cells (PSCs) are one of the most promising emerging photovoltaic technologies. However, their still limited stability is a main hurdle for their successful commercialization. In the past, various approaches have been developed to improve the long-term stability and performance of PSCs. Here ionic liquids (IL) as additives have attracted much attention as they passivate defects and suppress ion migration. In this work, we investigate the effect of the IL $BMIMBF_4$ on the film formation and optoelectronic properties of the model halide perovskite $MAPbI_3$. By multimodal in situ optical spectroscopy, we investigate the formation of the perovskite film during solution processing via one-step spin coating and a solvent engineering approach and how the film formation alters when the IL is added to the precursor solution. We find that the IL does not impact the formation of perovskite-solvent complexes, but the perovskite growth rate decreases with increasing IL content in the precursor solution. Additionally, we reveal that the IL already interacts with precursor materials and changes the evolution of the PbI_4^{2-} properties. Thus, our work provides important insights into how decisive ILs impact the sensitive interconnection between precursor properties, film formation process and final optoelectronic functionality of perovskite thin films.

KFM 20.3 Wed 15:30 H34

Transversal halide motion enables sharp optical absorption profiles in halide perovskites — •Sebastián Caicedo-Dávila,

Christian Gehrmann, Xiangzhou Zhu, and David A. Egger — Department of Physics, Technical University of Munich, Garching, Germany

Despite their strong vibrational anharmonicity, halide perovskites (HaPs) exhibit favorable optoelectronic properties, which facilitate their outstanding performance in solar cells, comparable to high-quality inorganic semiconductors. In this contribution, we explore the mechanisms and consequences of dynamic structural flexibility in $CsPbBr_3$ using first-principles molecular dynamics based on density-functional theory. We show that large Br displacements occur on planes that are transversal to the Pb-Br-Pb bonding axis. This *transversality* is concurrent with vibrational anharmonicity, results in short-ranged disorder correlations, and sharpens the joint-density of states rise at finite temperature. Finally, we contrast these results to the case of PbTe, which shares key properties with $CsPbBr_3$ but cannot exhibit any *transversality*, to show that this system features wider band-edge distributions and longer-ranged disorder correlations. These findings are relevant for connecting the structural flexibility and bonding of the halide perovskite structure with the sharp optical absorption of these materials.

KFM 20.4 Wed 15:45 H34

Investigating underlying mechanisms of K doping on stability of single- and mixed-cation perovskite solar cells with experimental and computational informed modelling — Saied Mollavali, Mohammad Moaddeli, and •Mansour Kanani — Department of Materials Science and Engineering, School of Engineering, Shiraz University, Shiraz, Iran

Recent studies revealed that the interstitial occupancy of potassium in single/mixed-cation based perovskite structures could hinder the ion migration mechanisms near interfaces, and therefore leads to a better structural stability. However, the underlying stability enhancement mechanisms and probable side effects of additional K atoms in corporate with other organic/inorganic constituents, with a long-range electronic bonding character, is not clear completely. In this study, the effect of doping K on the structural, morphological, electronic, and optical properties of different perovskite structures is investigated experimentally and computationally. The beneficial effect of interstitial K atom on long-range bonding of I atoms with organic molecules is observed. Furthermore, no degradation from additional K is detected for specific range of doping. This result opens a new insight on constructive impact of inorganic dopant on stability issue in perovskite solar cells. SEM, XRD, Photoluminescence and optical absorbance analysis were performed on the perovskite layer. The one layer-based experimental data incorporation with DFT based results were informed into the SCAPS-1D solar cell simulator package to predict cell efficiency, systematically.

KFM 20.5 Wed 16:00 H34

Revealing efficiency losses due to mobile ions in perovskite solar cells — •Sahil Shah, Jarla Thiesbrummel, and Jonas Diekmann — University of Potsdam, Germany

Perovskite semiconductors are distinct from most other semiconductors due to a large number of mobile ions in the active layer (e.g., iodide and methylammonium ions and vacancies, and others). Thus, ion dynamics have a critical impact on the performance and stability of perovskite-based applications.

In this work, we will show how the ionic density and induced losses change with device degradation under elevated temperatures and continuous light illumination. This is investigated via a simple and newly developed method *fast-hysteresis* which is a JV scan at a faster rate (~1000 Vs-1) which prevents the perturbation of mobile ions and we get the true ion free potential of the device. The fast-hysteresis measurements are corroborated by transient charge extraction and capacitance measurements as well as numerical simulations, which provide important insights into the dynamics of free electronic charges and mobile ions. We will then demonstrate how the mobile ions affect a range of commonly used mixed cation metal halide perovskite compositions and how the ionic losses vary with the charge transport layer.

Overall, the proposed methods quantify the ion-induced field screening, shed light on the complex device degradation process and PCE losses allow for a better understanding of several key phenomena in perovskite solar cells, and open up a large range of future experiments.

KFM 20.6 Wed 16:15 H34

Dissecting Ultrafast Polarization Responses in Lead Halide Perovskites via the THz-induced Kerr Effect — •Maximilian Frenzel[1], Marie Cherasse[1,2], Joanna Urban[1], Feifan Wang[3], Bo Xiang[3], Leona Nest[1], Lucas Huber[3], Martin Wolf[1], X.-Y. Zhu[3], and Sebastian F. Maehrlein[1] — [1]Fritz Haber Institute of the Max Planck Society, Department of Physical Chemistry, Berlin, Germany — [2]LSI, CEA/DRF/IRAMIS, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau, France — [3]Columbia University, Department of Chemistry, New York City, USA

The microscopic origin of the surprising optoelectronic properties of lead halide perovskite (LHP) semiconductors is still under debate. One hypothesis is that the highly polar and anharmonic lattice of LHPs influences their optoelectronic properties through dynamic charge carrier screening. We therefore study the ultrafast polarization response of the hybrid LHP $MAPbBr_3$ when exposed to transient electric fields in the form of intense, single-cycle THz pulses. By probing the THz-induced Kerr effect (TKE), we observe strong THz polarizability and complex ultrafast polarization dynamics. We perform 4-wave-mixing simulations, which show that it is crucial to account for anisotropic and dispersive light propagation for the correct interpretation of the measured TKE signals. Finally, we unveil a coherent phonon response in $MAPbBr_3$, which we assign to the inorganic cage and conclude to be the dominating polarizable mode in this material. This finding highlights the role of the inorganic lattice for dynamic carrier screening and the related mechanism of charge carrier protection.

30 min. break

KFM 20.7 Wed 17:00 H34

Calculating the temperature-dependent band gap of the halide perovskite $CsPbBr_3$ — •Stefan Seidl, Christian Gehrmann, Xiangzhou Zhu, Sebastian Caicedo Davila, and David A. Egger — Department of Physics, Technical University of Munich, Garching, Germany

Theoretical calculations based on density functional theory (DFT) can predict thermal effects in the electronic structure by considering important phenomena, such as thermal lattice expansion and electron-phonon coupling. The latter can be calculated using a Monte-Carlo (MC) sampling approach that is formally rooted within the harmonic approximation, which has recently been shown to yield accurate temperature-dependent band gaps for inorganic semiconductors [1]. A complementary approach to predict thermal effects in the electronic structure is first-principles molecular dynamics (MD), which can account for vibrational anharmonicity that is an important effect for certain technologically relevant materials. Here, we assess the temperature-dependent band gap of the halide perovskite $CsPbBr_3$ in the cubic and orthorhombic phases employing the two different methods, MC and MD, and compare our findings with experimental results. This includes a discussion about the role of anharmonicity and the contributions from spin-orbit coupling and thermal lattice expansion.

[1] F. Karsai et al, New J. Phys. 20, 123008 (2018)

KFM 20.8 Wed 17:15 H34

Electronic structure prediction of hybrid organic-inorganic metal halide perovskites using cost-effective DFT-1/2 method — Mohammad Moaddeli und •Mansour Kanani — Department of Materials Science and Engineering, School of Engineering, Shiraz University, Shiraz, Iran

Hybrid organic-inorganic metal halide perovskites (OIHPs) have attracted much attention in the last decade because of tunable photovoltaic performance and low fabrication cost. Regarding the tunable parameters for controlling the fundamental properties of OIHPs, recent computational and data-driven based approaches can accelerate new material prediction procedure significantly. Density functional theory (DFT) is considered as fundamental block of many multiscale, high-throughput and data-driven approaches typically. However, because of complexity of electronic orbital in OIHP as well as high sensitivity of regarding properties to atomistic configuration, employing conventional computational approaches faces many obstacles or needs very expensive corrections. Underestimation of routine functionals used in DFT calculations push people apply expensive approaches such as hybrid functionals and GW approximation. Here, DFT-1/2 method with a normal computational cost has been used for determining not only the band gap but also the true form of valence and conduction bands of OIHPs. The results showed that, the method could preserve the known Rashba band splitting in the conduction band of mixed-cation perovskites, which is the source of longer carrier lifetime behavior.

KFM 20.9 Wed 17:30 H34

Phonon Signatures for Polaron Formation in an Anharmonic Semiconductor — •Feifan Wang[1,2], Weibin Chu[3], Jin Zhao[3], and X.-Y. Zhu[1] — [1]Columbia University, New York, NY, 10027 USA — [2]Dept. of Materials, ETH Zurich, Switzerland — [3]University of Science and Technology of China, Hefei, Anhui 230026, China

Polaron formation, in which charge carriers are dressed by a cloud of lattice distortions, is partially responsible for the long carrier lifetimes and diffusion lengths in the lead halide perovskite (LHP), a superior optoelectronic material. Considerations of ferroelectric-like phonon anharmonicities of this system lead to the recent proposal of ferroelectric large polarons, which attributes efficient charge-carrier screening to the extended ordering of dipoles associated with inversion-symmetry-breaking unit cells. Here, we study electron-phonon coupling in Bi_2O_2Se, a semiconductor which bears resemblance to LHPs in ionic bonding, band transport with long carrier diffusion lengths, and dynamical phonon disorder as revealed by low-frequency Raman spectroscopy. Using coherent phonon spectroscopy, we show the strong coupling of an anharmonic phonon mode to photo-excited charge carriers, while the Raman excitation of this mode is symmetry-forbidden in the ground-state. Density functional theory calculations verify that the phonon mode originates from the symmetry reduction after charge injection and indicate the local dipole ordering induced by photo-excited electrons. This study provides an initial attempt to generalize the proposed charge-carrier screening model to account for the outstanding optoelectronic properties of defect-tolerant semiconductors.

KFM 20.10 Wed 17:45 H34

Tuning Perovskite Crystallization in the Hybrid Route — •Mohamed Mahmoud, Patricia Schulze, Andreas Bett, and Oussama Er-raji — Fraunhofer ISE

In 2009, perovskite solar cells were discovered in the solid-state that can be used not only as a single junction absorber but also in tandem configuration thanks to their bandgap tunability. It is a combination of organic and inorganic lead halide materials and they have the advantage of a strong absorption edge, defect tolerance and potential cheap production due to easy production methods such as spin coating or slot-die coating as a highly scalable production method. In the industry, double-sided textured silicon (DSTS) is commonly produced to overcome the reflection losses at surfaces. Spin coating of perovskite on top of DSTS resulted in low conformality which resulted in shunts and non-working solar cells. To overcome this issue, the hybrid route was developed, in which inorganic materials are co-evaporated using the thermal vapour deposition technique and then organic materials are spin-coated. By doing that, the high conformality of the thin film on top of the c-Si is achieved. However, the resulting perovskite grain size is in the nanometer scale. To increase the grain size - which results in higher short circuit current, lower grain boundaries and thus a more stable device - thermodynamics of the crystallization process need to be studied. In this work, using the thermodynamics fundamentals of crystallization, we tune the grain size of perovskite deposited via the hybrid route. In addition, we study the consequences of different grain sizes on the efficiency of the solar cell and especially on the stability.

KFM 20.11 Wed 18:00 H34

Dynamic nuclear spin polarization in lead halide perovskites — •Natalia Kopteva[1], Dennis Kudlacik[1], Marek Karzel[1], Mladen Kotur[1], Dmitri Yakovlev[1], Oleh Hordiichuk[2], Olga Nazarenko[2], Dmitry Dirin[2], Maksym Kovalenko[2,3], and Manfred Bayer[1] — [1]Experimentelle Physik 2, TU Dortmund, 44221 Dortmund, Germany — [2]Laboratory of Inorganic Chemistry Department of Chemistry and Applied Biosciences, ETH Zürich, CH-8093 Zürich, Switzerland — [3]Laboratory for Thin Films and Photovoltaics Empa-Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland

Lead halide perovskites are promising for applications in spintronics due to the nanosecond coherence time of the resident carriers [1]. The primary source of losing spin coherence is the interaction with the fluctuating nuclear spin environment [2]. Optically oriented carrier spins polarize nuclei, which create an Overhauser field. Due to the different strengths of the hyperfine interaction with the nuclear spins, the electron and hole experience different magnitude and directions of the Overhauser field. To study the degree of nuclear spin polarization and fluctuation, we investigate the interaction of resident and optically created carrier spins with nuclei using the Hanle effect in the tilted magnetic field in bulk formamidinium caesium lead iodine bromide.

[1] V. V. Belykh et al., Nat. Commun. 10, 673 (2019)
[2] I. A. Merkulov et al., Phys. Rev. B 65, 205309 (2002)

KFM 21: Functional semiconductors for renewable energy solutions (joint session HL/KFM)

Time: Wednesday 15:00–18:30 Location: H36

KFM 21.1 Wed 15:00 H36

A facile freeze-thaw ultrasonic assisted circulation method of graphite flakes prepared by anode graphite from spent lithium-ion batteries — •Yu Qiao[1,2], Zhonghao Rao[3,4], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]School of Electrical and Power Engineering, China University of Mining and Technology, 221116, Xuzhou, China — [3]School of Energy and Environmental Engineering, Hebei University of Technology, 300401, Tianjin, China — [4]Hebei Key Laboratory of Thermal Science and Energy Clean Utilization, Hebei University of Technology, 300401, Tianjin, China

Lithium-ion batteries (LIBs) have been widely employed in fast-growing mobile devices, stationary storage devices and electric vehicles. However, limited by particular service life, the booming increase in LIBs production will result in a large retirement wave. As the most common anode material in LIBs, waste graphite has also developed into a mode of high production capacity with the retirement of spent LIBs. Anode graphite (AG) of spent LIBs has the characteristics of large layer spacing and ease of being intercalated due to the reduced interlamination force after repeated charge and discharge cycles. This study presents a facile freeze-thaw ultrasonicassisted circulation method to prepare two-dimensional low-layer graphite flakes (GFs) using AG from spent LIBs. The results indicate that the freeze-thaw ultrasonic-assisted circulation method is feasible for preparing two-dimensional laminar materials.

KFM 21.2 Wed 15:15 H36

How could the heating process reduce the crystal damage of semiconductors? — •Khalid Lahmidi, Jale Schneider, Andreas Brand, Sebastian Roder, and Andreas Bett — Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany

Laser material processing can no longer be imagined away from the production chains in semiconductor industries. While being a precise, fast and wear-free processing tool, high intensity laser irradiation can also induce damage within the material, e.g. crystal damage, compromising the device quality. However, this damage can partly be healed or even prevented by an accompanying (laser) heating process.

In our laser lab, we built up a flexible laser heating setup with a spatial light modulator (SLM) as the core element. The setup allows to locally heat work pieces with different beam shapes with an intensity up to 220 W/cm* employing a cw-infrared laser source. Current research focuses on the temperature distribution in dependence of beam shape and beam dwell time on a specific position. Comsol based simulations support the experiments. Eventually, the heating beam will be overlaid to the process beam in use cases such as laser contact opening at lowered ablation thresholds or laser metal bonding for solar cell manufacturing. The damage after laser process with and without heating will be analyzed via microscopy.

KFM 21.3 Wed 15:30 H36

Energy landscape of the Boron and Indium single-atom defects in Silicon calculated by DFT — •Aaron Flötotto, Wichard Beenken, and Erich Runge — Institut für Physik, Technische Universität Ilmenau, Weimarer Str. 32, 98693 Ilmenau, Germany

The III group elements Boron and Indium form not only substitutional defects, which are important as electron acceptors, but also interstitial defects. Different configurations are possible for a single impurity

atom: (i) the impurity atom on an interstitional site, (ii) a substitutional impurity near a single interstitial Si atom, or (iii) the impurity and one Si atom form a pair of interstitials around an empty lattice point. We calculated within DFT the stable configurations of these defects for the Si:B and the Si:In system. We utilized the Nudged Elastic Band algorithm for finding minimal paths between these energetic minima in order to explore the energy landscape and to derive transition probabilities. The results are discussed with respect to the dynamical model suggested by K. Lauer et al. [1] for the explanation of PL-spectra of In-doped Si. [1] Lauer, K.; Möller, C.; Schulze, D. & Ahrens, C.; AIP Adv. 5 (2015) 017101

KFM 21.4 Wed 15:45 H36

Effects of Defects on the Optoelectronic Properties of Ta_3N_5 Thin Films — •Lukas M. Wolz, Gabriel Grötzner, Laura I. Wagner, Ian D. Sharp, and Johanna Eichhorn — Walter Schottky Institut, Technische Universität München

For photoelectrochemical energy conversion, metal nitride semiconductors have the potential to overcome several limitations associated with the more intensively investigated class of metal oxides. Among these materials, Ta_3N_5 is especially promising, possessing a bandgap of ∼2.2 eV and effective long-range charge transport. However, the (opto)electronic and photoelectrochemical properties of Ta_3N_5 photoelectrodes are often dominated by defects, such as oxygen impurities, nitrogen vacancies, and low-valent Ta cations. To identify the impact of such defects on the material properties, we prepare Ta_3N_5 via two different synthetic routes. As precursor, Ta_xN_y and Ta_xO_y thin films were deposited by magnetron sputtering and were subsequently annealed at high temperatures in NH_3 to form Ta_3N_5. Both films are homogenous and reveal the formation of phase-pure orthorhombic Ta_3N_5. Compared to nitride-derived Ta_3N_5, the oxide-derived films are characterized by higher structural disorder as well as higher oxygen and lower nitrogen concentrations. Despite these higher defect concentrations, the oxide-derived Ta_3N_5 films exhibit improved stability under photoelectrochemical operation conditions, though both films show similar photoelectrochemical performance. The improved understanding of defect properties and their impact on PEC stability provides a path to tailored optimization of photoelectrode properties.

KFM 21.5 Wed 16:00 H36

Investigation of various quenching materials on the P-line — •Dominik Bratek, Katharina Peh, Kevin Lauer, Aaron Flötotto, Dirk Schulze, and Stefan Krischok — Institut für Physik, Technische Universität Ilmenau, Weimarer Str. 32, 98693 Ilmenau, Germany

Solar-grade Si shows degradation effects and a lowering of the charge carrier lifetimes after illumination [1]. For In implanted Si this effect was shown to be connected to the P-line in photoluminescence spectra [2]. This P-line can furthermore be influenced by applying a strong quenching after an anneal. The intensity of the P-line increases by several orders of magnitude depending on the cooling rate [3]. In this contribution we investigate the influence of four different quenching liquids on the P-line. From an experimental point of view we discuss the applicability of each used liquid in consideration of P-Line intensity and probe integrity. [1] C. Möller and K. Lauer, Physica Status Solidi (RRL) 7, 461 (2013). [2] K. Lauer, C. Möller, D. Schulze, and C. Ahrens, AIP Advances 5, 017101 (20125). [3] M. L. W. Thewalt, U. O. Ziemelis, and P. R. Parsons, Solid State Communications 39, 27 (1981).

KFM 21.6 Wed 16:15 H36

Simulation of the reaction kinetics of the A_{Si}-Si_i-defect — •Kevin Lauer[1,2], Katharina Peh[2], Wichard Beenken[2], Erich Runge[2], and Stefan Krischok[2] — [1]CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany — [2]TU Ilmenau, Institut für Physik und Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany

Light-induced degradation (LID) is a severe problem for silicon photosensitive devices like solar cells and photo detectors. LID reaction kinetics may be explained by the A_{Si}-Si_i-defect model. [1] This model consists of seven states. The transitions between these states are assumed to be first order equilibrium reactions, which can be mathematically treated by a system of linear differential equation. [1] This is numerically solved and compared to the LID cycle using well-known together with some estimated reaction constants.

[1] K. Lauer, C. Möller, C. Tessmann, D. Schulze, and N. V. Abrosimov, "Activation energies of the In_{Si}-Si_i defect transitions obtained by carrier lifetime measurements", physica status solidi (c), vol. 14, no. 5, p. 1600033, 2017.

30 min. break

KFM 21.7 Wed 17:00 H36

Exploring Zirconium-doped Tantalum Nitride as a Photoanode for Solar Energy Conversion — •Oliver Brune, Laura I. Wagner, Verena Streibel, and Ian D. Sharp — Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Solar water splitting could pave the way to carbon-free hydrogen production as it allows for direct transformation of sunlight into chemical energy. While the oxygen evolution reaction is a crucial step in generating green hydrogen, there remains a lack of semiconductor photoanode materials that can simultaneously fulfill three key requirements: long-term chemical stability, high photocarrier extraction efficiencies, and appropriate bandgap for harvesting solar radiation. Nevertheless, among the various materials that have been investigated, the transition metal nitride Ta3N5 offers significant promise as an efficient n-type photoanode. Building upon this established material, we use reactive co-sputtering and subsequent ammonia annealing to introduce Zr into Ta3N5, with the aim of investigating how the ternary nitride character of Zr-Ta-N(O) enables tuning of key semiconductor properties. Using a range of complementary characterization methods, we show that synthesis parameters and Zr content have a significant influence on the crystal structure, morphology, and optoelectronic properties of this ternary compound. Based on these insights, we optimize the composition and synthesis processes to achieve a highly stable and efficient photoanode material, which is a key requirement for solar water splitting.

KFM 21.8 Wed 17:15 H36

Defect-Engineered Atomic Layer Deposited TaO_x Protection Layers for Photoelectrochemistry — •Tim Rieth, Clara Scherm, and Ian Sharp — Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Photoelectrochemical (PEC) energy conversion provides a viable route to the generation of chemical fuels from solar light. In this approach, charge carriers generated within a semiconductor light absorber immersed in an electrolyte are used to drive water splitting or carbon dioxide reduction reactions. A particularly relevant PEC configuration uses photovoltaic absorbers coated with transparent and conductive protection layers that prevent chemical corrosion of the semiconductor components. However, ensuring that the protection layer simultaneously fulfills the criteria for chemical stability, electronic conductivity, and optical transparency remains a challenging task. Here, we utilize plasma enhanced atomic layer deposition (PE-ALD) to create defect engineered and ultra-thin tantalum oxide (TaO_x) protection layers for PEC applications. In addition to their optical transparency, the TaO_x films form continuous coatings on the photoabsorber and provide improved chemical stability compared to titanium dioxide. A sufficiently high film conductivity is obtained by intentionally introducing electronic defects from hydrogen plasma sub-cycles during the ALD process. The demonstrated defect engineering mechanism and achieved TaO_x protection layers represent an advance towards efficient and stable PEC devices.

KFM 21.9 Wed 17:30 H36

Exploring novel ternary nitride semiconductor photoabsorbers for solar energy conversion applications — •Laura I. Wagner[1], Elise Sirotti[1], Johanna Eichhorn[1], Chang-Ming Jiang[1], Matthias Kuhl[1], Verena Streibel[1], David Egger[2], and Ian D. Sharp[1] — [1]Walter schottky Institut und TUM, München, Germany — [2]TUM, München, Germany

Solar water splitting offers the possibility to harvest the sunlight and store it in the chemical bonds of hydrogen. Exploratory research has revealed several possible photoanode materials, but until now no material meets the core requirements for photochemical stability, carrier extraction efficiency, and moderate band gap in the visible range. In this context, transition metal nitride semiconductors are underexplored and offer promise as new photoanode materials candidates. As a non-equilibrium synthesis approach, reactive magnetron co-sputtering enables the synthesis of novel ternary nitride photoabsorbers. In this work, a new ternary metal nitride photoanode material, cubic bixbyite-

type ZrTaN3, is presented. We observe the reactively sputtered ZrTaN3 thin films to exhibit an optical bandgap at 2.4 eV and n-type behavior. Most importantly, the resulting polycrystalline films exhibit appreciable photoactivity when implemented as a photoanode in a photoelectrochemical cell. Benefiting from the tunability of cation (Ta,Zr) ratio of reactive sputtering and anion (N,O) ratio with post annealing treatments, the solid solution of ZrxTa2-xN3(O) offers a large parameter space to tune and optimize optoelectronic properties for various applications, including for PEC applications.

KFM 21.10 Wed 17:45 H36

Electrical transport across catalyst/defect-engineered titania corrosion protection layer interfaces for light-driven CO2 reduction — •Julius Kühne, Oliver Bienek, Tim Rieth, and Ian D. Sharp — Walter Schottky Institute and Physics Department, Technical University of Munich, Am Coulombwall 4, 85748 Garching, Germany

Producing value-added products via light-driven CO2 reduction represents a promising approach to sustainably address increasing CO2 emissions and meet the growing global energy demand. However, such solar fuels systems require passivating layers to chemically protect semiconductor light absorbers from harsh reaction environments. Despite great progress in the development of atomic layer deposited (ALD) protection layers, the factors governing efficient charge injection into the catalytic component are not yet well understood. Here, the charge transport characteristics between various defect-engineered TiO2 protection layers grown with ALD and metal catalyst layers including Ag, Au, Pt, Ni and Ti are analyzed. This work aims to get a deeper understanding of the interface between catalyst and protection layer in terms of contact resistivity, carrier transport, and interface kinetics. Additionally, results of EC and PEC measurements are compared to assess the stability and activity of these systems under CO2 reduction conditions in a two-compartment cell with ion exchange membrane. The selectivity of selected catalyst layers is evaluated by gas chromatography of the reaction products, thereby enabling a quantification of their overall performance characteristics.

KFM 21.11 Wed 18:00 H36

Finite supercell charge correction for electronic transitions in defects including electronic and ionic screening — •Christoph Freysoldt[1], Baoying Dou[1], Stefano Falletta[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf — [2]Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Charged point defects play an important role in the function of (opto)electronic devices. Theoretical investigations have proven valuable to understand quantitatively their stability, electrical and optical properties, and hence their beneficial or detrimental role in device performance. Electronic transitions involving localized defect states have recently moved into the focus. Similar to formation energies, also the transition energies suffer from artifacts due the long-range Coulomb interactions and the artificial periodicity in supercell models of defects. While the initial charge state is subject to full electronic and ionic screening, the changes upon the transition are screened by electrons only. Yet, the required charge corrections cannot be derived by cleverly combining traditional corrections for formation energies of initial and final state. I will present an overview of how these artifacts can be understood and corrected for. I will show applications for vertical transitions and non-radiative carrier capture.

KFM 21.12 Wed 18:15 H36

Influence of Sr concentration on atomic, magnetic, and electronic structure of Ruddlesden-Popper oxide $La_{2-x}Sr_xCo_{1-y}Fe_yO_4$ — •Dina I. Mazitova[1], Debalaya Sarker[1,2], and Sergey V. Levchenko[1] — [1]Moscow, Russia — [2]UGC-DAE CSR, Indore, India

Ruddlesden-Popper oxides were demonstrated to be promising catalysts for oxygen evolution reaction. There are numerous attempts in the literature to find descriptors for predicting a catalytic activity. However, the descriptors may depend on the distribution of ions of different types in these multi-component systems.

We calculated atomic, electronic, and magnetic structure of $La_2Co_{0.5}Fe_{0.5}O_4$, $LaSrCo_{0.5}Fe_{0.5}O4$ (LSCFO), and $Sr_2Co_{0.5}Fe_{0.5}O_4$ for different distributions of iron and cobalt using all-electron DFT in GGA and GGA+U approximations. Our calculations show that the favorable distribution of transition metal cations depends on the amount of Sr substituted in the A site. The electronic and magnetic structures depend strongly on the Fe/Co distribution. For example, GGA-RPBE calculations in LSCFO showed charge-ordered ferromagnetic structure in the Co layer and antiferromagnetic structure in the Fe layer when Co and Fe layers interchange with one another, but for uniform distribution of iron and cobalt ions, LSCFO becomes ferromagnetic.

KFM 22: Members' Assembly

Annual KFM Meeting with elections of the spokespersons.

Time: Wednesday 17:00–18:00 Location: H5

All members of the Crystalline Solids and their Microstructure Division are invited to participate.

KFM 23: Skyrmions 2 (joint session MA/KFM)

Time: Thursday 9:30–12:45 Location: H37

KFM 23.1 Thu 9:30 H37

Complementary investigations of magnetic textures in the antiskyrmion compound $Mn_{1.4}PtSn$ with REXS and LTEM — M. Winter[1,2,3,4], M. Rahn[4], D. Wolf[3], S. Schneider[2], M. Valvidares[5], •C. Shekar[1], P. Vir[1], B. Achinuq[6], H. Popescu[7], N. Jaouen[7], G. Van der Laan[8], T. Hesjedal[6], B. Rellinghaus[2], and C. Felser[1] — [1]MPI CPfS, Dresden, Germany — [2]DCN, TU Dresden, Germany — [3]IFW Dresden, Germany — [4]IFMP, TU Dresden, Germany — [5]ALBA Synchrotron, Barcelona, Spain — [6]Clarendon Laboratory, University of Oxford, UK — [7]Synchrotron SOLEIL, Saint-Aubin, France — [8]Diamond Light Source, UK

The Heusler compound $Mn_{1.4}PtSn$ is known to host multiple non trivial magnetic textures like antiskyrmions (aSks). It's phase diagram depends not only on temperature and sample shape, but also on strength and orientation of an external magnetic field as well as on the history of its application. In order to better understand the formation of aSks, we have conducted complementary experiments of resonant elastic x-ray scattering (REXS) and Lorentz transmission electron microscopy (LTEM) on an identical lamella of $Mn_{1.4}PtSn$. Our complementary approach allows for the first time to directly relate the REXS patterns to the underlying magnetic phase as determined from LTEM. Along this approach, LTEM has proven an ideal pre-characterization tool to navigate the high-dimensional parameter space and subsequently take advantage of the better control of magnetic field directions, temperature as well as of energy resolved measurements as provided by REXS. Part of this work is gratefully supported by DFG within SPP 2137.

KFM 23.2 Thu 9:45 H37

Doping control of magnetic anisotropy for stable antiskyrmion formation in schreibersite (Fe,Ni)3P with S4 symmetry — Kosuke Karube[1], Licong Peng[1], •Jan Masell[1,2], Mamoun Hemmida[3], Hans-Albrecht Krug von Nidda[3], István Kézsmárki[3], Xiuzhen Yu[1], Yoshinori Tokura[1,4], and Yasujiro Taguchi[1] — [1]RIKEN CEMS, Wako, Japan — [2]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [3]University of Augsburg, Augsburg, Germany — [4]University of Tokyo, Tokyo, Japan

Recently, growing attention has also been paid to antiskyrmions emerging in non-centrosymmetric magnets with D2d or S4 symmetry. [1] In

these magnets, complex interplay among anisotropic Dzyaloshinskii-Moriya interaction, uniaxial magnetic anisotropy, and magnetic dipolar interactions generates a variety of magnetic structures. We control the uniaxial magnetic anisotropy of schreibersite (Fe,Ni)3P with S4 symmetry by doping and investigate its impact on the stability of antiskyrmions. With magnetometry, supported by ferromagnetic resonance spectroscopy, Lorentz transmission electron microscopy, and micromagnetic simulations, we quantitatively analyze the stability of antiskyrmion as functions of uniaxial anisotropy and demagnetization energy, and demonstrate that subtle balance between them is necessary to stabilize antiskyrmions.

[1] K. Karube, L. C. Peng, J. Masell, X. Z. Yu, F. Kagawa, Y. Tokura, and Y. Taguchi, Nat. Mater. 20, 335-340 (2021) [2] The authors, Adv. Mater. 34 (11), 2108770 (2022)

KFM 23.3 Thu 10:00 H37

Magnetic and Morphological Phases in the 2D van der Waals Magnet FexGeTe2 — •Kai Litzius[1], Max Birch[1,5], Lukas Powalla[2,3,5], Sebastian Wintz[1], Fabian Alten[1], Michael Miller[1], Markus Weigand[4], Klaus Kern[2,3], Marko Burghard[2], and Gisela Schütz[1] — [1]Max-Planck-Institute for Intelligent Systems, 70569 Stuttgart, Germany — [2]Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany — [3]Institut de Physique, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany — [5]These authors contributed equally to the work

Recently, observations of magnetic skyrmions in 2-dimensional (2D) itinerant ferromagnets opened many possibilities for technological implementation of 2D van der Waals structures in spintronics. However, the stability of the different magnetic states and morphological phases in FexGeTe2 remains an unresolved issue. In this work, we utilize real-space imaging to determine magnetic phase diagrams of exfoliated FexGeTe2 films. Our findings show besides complex, history-dependent magnetization states also that changes in the crystalline structure significantly alter the magnetic behavior. Ultimately, the choice of material and a proper nucleation mechanism result in the stabilization of a variety of (meta-) stable magnetic configurations, including skyrmions. These findings open novel perspectives for designing van der Waal heterostructure-based devices incorporating topological spin textures.

KFM 23.4 Thu 10:15 H37

Antiskyrmions in B20-type FeGe — •Nikolai S. Kiselev[1], Fengshan Zheng[2,3], Luyan Yang[2], Vladyslav M. Kuchkin[1], Filipp N. Rybakov[4,5], Stefan Blügel[1], and Rafal E. Nikolai[2] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Le Brandst. 1 — [3]Spin-X Institute, School of Physics and Optoelectronics, State Key Laboratory of Luminescent Materials and Devices, Guangdong-Hong Kong-Macao Joint Laboratory of Optoelectronic and Magnetic Functional Materials, South China University of Technology, Guangzhou 511442, China — [4]Department of Physics and Astronomy, Uppsala University, SE-75120 Uppsala, Sweden — [5]Department of Physics, KTH-Royal Institute of Technology, SE-10691 Stockholm, Sweden

We report the highly reproducible observations of statically stable antiskyrmion [1] – skyrmion antiparticle in thin plates of B20-type FeGe chiral magnet where only skyrmions were observed earlier. Using Lorents TEM and electron holography, we showed that skyrmions and antiskyrmions could coexist in a wide range of fields and temperatures. These findings are entirely consistent with micromagnetic simulations and prior theoretical studies of two-dimensional systems [2]. The mechanism of antiskyrmion stability, nucleation, and annihilation with ordinary skyrmions is discussed in detail.

[1] F. Zheng et al., Nat. Phys. (2022) accepted.

[2] V. M. Kuchkin, N. S. Kiselev, Phys. Rev. B 101, 064408 (2020).

KFM 23.5 Thu 10:30 H37

Asymmetric magnetization reversal in perpendicularly magnetized micro stripes induced by exchange-bias effect and Dzyaloshinskii-Moriya interaction — •Sapida Akhundzada[1], Piotr Kuświk[2], Christian Janzen[1], Arno Ehresmann[1], and Michael Vogel[1] — [1]Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Kassel, Germany — [2]Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

In a systematic study, the magnetization reversal in exchange-biased Ti/Au/Co/NiO/Au micro stripes with perpendicular magnetic anisotropy is characterized using high-resolution magneto-optical Kerr microscopy. Thereby, the remagnetization process is observed to be asymmetric with respect to the two branches of the hysteresis loop, being quantified as a higher nucleation density formed along one field branch with decreasing structure width. Additionally, a local asymmetry in the domain nucleation and domain wall movement within the stripe geometry is observed. The influence of the exchange bias effect and the Dzyaloshinskii-Moriya interaction is investigated by field-cooling and the application of additional in-plane magnetic fields during the magnetization reversal process. XMCD and XMLD experiments reveal the corresponding domain texture in the ferromagnetic and antiferromagnetic layers. These experiments show how the interplay between chiral Dzyaloshinskii-Moriya interaction and the unidirectional anisotropy modify the magnetic domain texture and the resulting magnetization reversal in microstructures.

KFM 23.6 Thu 10:45 H37

Magnetic skyrmion braids — •Nikolai S. Kiselev[1], Fengshan Zheng[2], Filipp N. Rybakov[3], Dongsheng Song[2], András Kovács[2], Haifeng Du[4], Stefan Blügel[1], and Rafal E. Dunin-Borkowski[2] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Department of Physics, KTH-Royal Institute of Technology, Stockholm, SE-10691 Sweden — [4]The Anhui Key Laboratory of Condensed Matter Physics at Extreme Conditions, High Magnetic Field Laboratory, Chinese Academy of Science (CAS), Hefei, Anhui Province 230031, China

In cubic chiral magnets, the magnetization of skyrmions resembles a string-like or filamentary texture. Skyrmion strings are naturally expected to interwind and form complex three-dimensional superstructures by analogy to elastic strings. We found that skyrmion strings in cubic crystals of chiral magnets can form braids – statically stable configurations where skyrmion strings wind around one another [1]. This finding is confirmed by direct observations of skyrmion braids in B20-type FeGe using transmission electron microscopy. The theoretical analysis predicts that the discovered phenomenon is general for a wide family of chiral magnets and can be observed in thick plates and bulk crystals.

[1] F. Zheng, et al., Nature Commun. 12, 5316 (2021).

KFM 23.7 Thu 11:00 H37

Tunable ellipticity of Bloch skyrmions in antiskyrmion-hosting materials — Sebastian Schneider[1,2], •Jan Masell[1,3], Fehmi S. Yasin[1], Licong Peng[1], Kosuke Karube[1], Yasujiro Taguchi[1], Darius Pohl[2], Bernd Rellinghaus[2], Yoshinori Tokura[1,4], and Xiuzhen Yu[1] — [1]RIKEN CEMS, Wako, Japan — [2]TU Dresden, Dresden, Germany — [3]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [4]University of Tokyo, Tokyo, Japan

Magnetic skyrmions are usually stabilized and studied in materials with isotropic Dzyaloshinskii-Moriya interaction (DMI). In materials with D2d or S4 symmetry, however, the sign of the DMI is exactly opposite in two orthogonal directions such that it favors antiskyrmions instead of skyrmions. [1,2] Yet, uniaxial anisotropy and dipolar interactions can also help stabilizing skyrmions in such materials which, as a consequence of the anisotropic DMI, are rendered elliptical. We quantify the elliptical distortion of skyrmions in an S4 symmetric material as function of magnetic field and temperature using LTEM holography. Our micromagnetic simulations and simple analytical modelling explain the experimentally observed behavior and provide a technique to quantitatively estimate the DMI.

[1] K. Karube, L. C. Peng, J. Masell, X. Z. Yu, F. Kagawa, Y. Tokura, and Y. Taguchi, Nat. Mater. 20, 335-340 (2021) [2] K. Karube, L. C. Peng, J. Masell, M. Hemmida, H.-A. Krug von Nidda, I. Kézsmárki, X. Z. Yu, Y. Tokura, and Y. Taguchi, Adv. Mater. 34 (11), 2108770 (2022) [3] In preparation.

KFM 23.8 Thu 11:15 H37

Long-range non-collinearity and spin reorientation in the centrosymmetric hexagonal magnet NiMnGa — •Parul Devi[1], Sanjay Singh[2], Thomas Hermannsdörfer[1], and Joachim Wosnitza[1,3] — [1]Dresden High Magnetic Field Laboratory, HZDR, Germany — [2]Institut für Festkörper und Materialphysik, TU Dresden, Germany — [3]School of Materials Science and Technology, Indian

Institute of Technology (BHU), Varanasi-221005, India

The recent discovery of biskyrmions and skyrmions in globally centrosymmetric crystals has raised questions about the role of the Dzyaloshinskii-Moriya interactions (DMI) in causing the topologically stable spin vortex textures, since DMI vanishes in such crystal structures. Here, we present a detailed crystal and magnetic structure investigation of the non-collinear hexagonal magnetic material NiMnGa exhibiting biskyrmions [1]. We show an investigation on the nature of the phase transitions, evidence of magnetoelastic coupling and anomalous thermal expansion in hexagonal, centrosymmetric NiMnGa using combined studies of magnetization and high-resolution synchrotron x-ray powder diffraction data. Magnetization data exhibits spin reorientation transition * 200 K. By means of powder neutron diffraction data, we investigate the change of the magnetic structure in NiMnGa. This study will help to understand the origin of biskyrmions in the absence of Dzyaloshinskii-Moriya interaction in magnetic materials.

[1] Yu et al., Nat. Comm. 5, 3198 (2014).

KFM 23.9 Thu 11:30 H37

Zero-field skyrmionic states and in-field edge-skyrmions induced by boundary tuning — •Jonas Spethmann, Elena Y. Vedmedenko, Roland Wiesendanger, André Kubetzka, and Kirsten von Bergmann — Universität Hamburg, Hamburg, Germany

When magnetic skyrmions are moved via currents, they do not strictly travel along the path of the current, instead their motion also gains a transverse component. This so-called skyrmion Hall effect can be detrimental in potential skyrmion devices because it drives skyrmions towards the edge of their hosting material where they face potential annihilation. To mitigate this problem it was proposed to create a potential well within the skyrmion hosting material and thereby guide the skyrmions along a desired pathway[1]. Here we have experimentally modified a skyrmion model system–an atomic Pd/Fe bilayer on Ir(111)[2]–by growing a self-assembled ferromagnetic Co/Fe bilayer adjacent to it. Employing spin-polarized scanning tunneling microscopy, we demonstrate that this ferromagnetic rim has an immediate effect on the spin spiral ground state of the Pd/Fe bilayer, stabilizes skyrmions and target states in zero field and prevents skyrmion annihilation at the film edge. Furthermore we show that in applied magnetic fields the Co/Fe gives rise to edge-skyrmions pinned to the Pd/Fe island rim. Finally we have performed spin dynamics simulations to investigate the role of different magnetic parameters in causing these edge effects.

[1] I. Purnama *et al., Scientific Reports* **5**, 10620 (2015).
[2] N. Romming *et al. Science* **341**, 636-639 (2013).

KFM 23.10 Thu 11:45 H37

Real-space determination of the isolated magnetic skyrmion deformation under electric current flow — Fehmi S. Yasin[1], •Jan Masell[1,2], Kosuke Karube[1], Akiko Kikkawa[1], Yasujiro Taguchi[1], Yoshinori Tokura[1,3], and Xiuzhen Yu[1] — [1]RIKEN CEMS, Wako, Japan — [2]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [3]University of Tokyo, Tokyo, Japan

The effect of electric current on topological magnetic skyrmions, such as the current-induced deformation of isolated skyrmions, is of fundamental interest. The deformation has consequences ranging from perturbed dynamics to modified packing configurations. [1] We measure the current-driven real-space deformation of isolated, pinned skyrmions within CoZn at room temperature. We observe that the skyrmions are surprisingly soft, readily deforming during electric current application into an elliptical shape with a well-defined deformation axis. We find that this axis rotates towards the current direction, in agreement with our simply Thiele-based theoretical analysis. We quantify the average eccentricity and how the skyrmion size expands during current application. This first evaluation of in-situ electric current-induced skyrmion deformation paints a clearer picture of spin-polarized electron-skyrmion interactions and may prove essential when designing spintronic devices.

[1] J. Masell, D.R. Rodrigues, B.F. McKeever, and K. Everschor-Sitte, Phys. Rev. B 101, 214428 (2020). [2] Under review.

KFM 23.11 Thu 12:00 H37

Magnetocrystalline anisotropy in cubic chiral magnets — •Vivek Kumar[1], Andreas Bauer[1], Schorsch Michael Sauther[1], Michelle Hollricher[1], Markus Garst[2], Marc Andreas Wilde[1], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany

Magnetocrystalline anisotropy plays an important role in the stabilization, orientation and manipulation of exotic spin textures like skyrmions in cubic chiral magnets [1-3]. Here, we report the determination of the fourth and sixth order anisotropy constants of MnSi as a function of temperature and field using the cantilever torque magnetometry option in a physical property measurement system. Torque curves were recorded by rotating the single-crystalline spherical sample in the field polarized state. This allows us to extract anisotropy constants by fitting the experimental data to the theoretical expressions of torques belonging to the symmetry class ($P2_13$). In addition, we discuss technical issues in measurement related to sample shape and geometry. The present technique is used to obtain the anisotropy constants of other cubic chiral magnets including Cu_2OSeO_3, $Mn_{1-x}Fe_xSi$ and $Fe_{1-x}Co_xSi$ series.

[1] Chacon *et al.*, Nat. Phys. **14**, 936 (2018).
[2] Bauer *et al.*, Phys. Rev. B **95**, 024429 (2017).
[3] Adams *et al.*, Phys. Rev. Lett. **121**, 187205 (2018).

KFM 23.12 Thu 12:15 H37

Change of electronic Chern number induced by phase shifts in multiple-Q textures — •Pascal Prass[1], Fabian R. Lux[1], Duco van Straten[2], and Yuriy Mokrousov[1,3] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Germany — [2]Institute of Mathematics, Johannes Gutenberg University Mainz, Germany — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany

A multiple-Q spin texture is given by the superposition of multiple spin spirals and gives rise to a periodic array of topological spin structures, such as skyrmions. Using the emergent magnetic field formalism [1] the topological Hall current in the texture is proportional to the real-space winding number of its spin vector field. In recent articles [2,3], it was illustrated how tuning the relative phase shifts of the spin waves as well as the textures' net magnetization leads to topological phase transitions in the spin texture, i.e. integer jumps of its winding number. Combining these ideas implies the existence of significant discontinuous jumps in the topological Hall current and its associated Chern numbers in the underlying electronic spectrum. In this work, we directly investigate the spin textures' electronic band topology to determine the relationship between its real-space winding number and quasi-momentum space Chern numbers. Understanding the electronic behaviour during these transitions will have far-reaching implications for developing tunable topological Hall devices. [1] T. Schulz et al. Nat. Phys. 8, 301-304 (2012). [2] K. Shimizu et al. arXiv:2201.03290 (2022). [3] S. Hayami et al. Nat. Commun. 12, 6927 (2021).

KFM 23.13 Thu 12:30 H37

Audio Recognition with Skyrmion Mixture Reservoirs — •Robin Msiska[1], Jake Love[1], Jonathan Leliaert[2], Jeroen Mulkers[2], George Bourianoff[3], and Karin Everschor-Sitte[1] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]Ghent University, Ghent, Belgium — [3]Senior Principle Engineer, Intel Corp. (Retired)

Physical reservoir computing is an information processing scheme that enables energy efficient temporal pattern recognition to be performed directly in physical matter [1]. Previously, random topological magnetic textures have been shown to have the characteristics necessary for efficient reservoir computing [2] and allowed for simple pattern recognition with two input channels [3].

We propose a skyrmion mixture reservoir computing model with multi-dimensional inputs. Through micro-magnetic simulations, we show that our implementation can solve audio classification tasks at the nanosecond timescale to a high degree of accuracy. Due to the quality of the results shown and the low power properties of magnetic texture reservoirs, we argue that skyrmion magnetic textures are a competitive substrate for reservoir computing.

Funding from the Emergent AI Centre (Carl-Zeiss-Stiftung), DFG (320163632), FWO-Vlaanderen and computer resources by VSC (Flemish Supercomputer Center) are gratefully acknowledged.

[1] G. Tanaka et al., Neural Networks 115, 100 (2019). [2] D. Prychynenko et al., Physical Review Applied 9, 014034 (2018) [3] D. Pinna et al., Phys. Rev. Applied 14, 054020 (2020)

KFM 24: New Methods and Developments: Spectroscopies, Diffraction and Others (joint session O/KFM)

Time: Thursday 10:30–12:30 Location: H6

Topical Talk KFM 24.1 Thu 10:30 H6

Element and Structure Analysis of Surfaces Using Positrons — •Christoph Hugenschmidt — Forschungs-Neutronenquelle Heinz Maier-Leibnitz (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

With the advent of bright low-energy positron beams novel analysis tools have been developed exploiting the unique properties of positron matter interaction such as repulsive crystal potential or positron trapping in surface states [1]. Positron annihilation is established for defect spectroscopy and the characterization of the free volume in amorphous matter. By applying a slow positron beam, however, defects near the surface can be specifically addressed, e.g. for the determination of the oxygen vacancy concentration in $YBa_2Cu_3O_{7-x}$ [2]. The positron counterparts of reflection high-energy electron diffraction (RHEED) and electron induced Auger-electron spectroscopy (AES) intrinsically exhibit superior surface sensitivity. In contrast to electrons, positrons show total reflection for small glancing angles. It was demonstrated that with reflection high-energy positron diffraction the structure of the topmost and the immediate subsurface atomic layer of surfaces are revealed with outstanding accuracy. The main advantages of positron annihilation induced AES are the missing secondary electron background and its topmost layer sensitivity for element analysis allowing, e.g. the *in-situ* observation of the Ni adatom migration from the Pd surface into the bulk [3]. [1] C. H.; Surf. Sci. Reports 71 (2016) 547; [2] M. Reiner et. al.; Phys. Rev. B 97 (2018) 144503; [3] S. Zimnik et. al.; Surf. Sci. 664 (2017) 61

KFM 24.2 Thu 11:00 H6

Active sample manipulation with electrostatic beams: a different way of bridging the high-voltage gap — •Francesco Guatieri, Kilian Brenner, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Lichtenbergstr. 1, 85748 Garching, Germany

Most electrostatic positron beams used to perform surface studies are accelerated to the desired implantation energy by floating the target to a high electrostatic potential relative to ground. The presence of tens on kilovolts of electric potential makes the use of instrumentation attached directly to the sample inconvenient. The conventional solution to this hurdle consists in wiring insulated connections from the sample to a high-voltage galvanic decoupling placed outside of the experimental chamber far away from the sample holder. This solution carries limitations on the kind and amount of electrical connections employed. We will present, instead, a novel approach to in-operando sample manipulation that we have developed to be used at the Doppler broadening spectrometer installed on the NEPOMUC positron source, which implements the galvanic insulation in situ and removes many of the limitations imposed by conventional solutions.

KFM 24.3 Thu 11:15 H6

Advanced Kernel-Based NMR Cryoporometry Characterization of Mesoporous Solids — •Henry R.N.B. Enninful, Daniel Schneider, Richard Kohns, Dirk Enke, and Rustem Valiullin — Leipzig University, Leipzig, Germany

NMR cryoporometry is a pore space characterization technique for industrial and natural materials such as catalysts, gas storage materials, cartilage, bones, rocks and many more. While gaining wide use, the fundamental phenomena underlying solid-liquid phase transitions in geometrically disordered porous materials is still not fully understood. This may lead to inaccurate pore size distributions from the NMR cryoporometry technique.

In this work, we have developed a new approach to NMR cryoporometry. Herein, it takes account of cooperativity effects in pores, the existence of a variable non-frozen layer (NFL) thickness between the frozen core and pore wall and the effect of curvature on thermal fluctuations in pores which hitherto are missing in the current approach. In the first place, we compile a family of transition curves characterizing the phase state in pores with different pore sizes, so called kernels. Thereafter, we apply a general framework for predicting phase equilibria in a collection of pores. Specifically, the proposed kernel-based approach is coupled with the serially-connected pore model (SCPM) to be able to predict phase behavior in independent pore systems as well as in pore networks. We demonstrate the new approach by applying it to ordered porous materials such as MCM-41 and SBA-15. Consequently, a more accurate pore size distribution (PSD) is obtained.

KFM 24.4 Thu 11:30 H6

Development of an electron spin resonance spectrometer in ultra-high vacuum for surface spins — •Juyoung Park[1,2], Franklin H. Cho[1,2], Jisoo Yu[1,2], Luciano Colazzo[1,2], Yejin Jeong[1,2], Junjie Liu[3], Arzhang Ardavan[3], Giovanni Boero[4], Andreas Heinrich[1,2], and Fabio Donati[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea — [2]Ewha Womans University, Seoul, Republic of Korea — [3]The Clarendon Laboratory, Department of Physics, University of Oxford, Oxford, UK — [4]Ecole Polytechnique Fédérale de Lausanne, Laboratory for Microsystems, Lausanne, Switzerland

We present the development of an electron spin resonance (ESR) spectrometer operating in ultra-high vacuum (UHV) for studying surface-adsorbed molecular and atomic spin systems. Such surface spin systems are promising platforms for potential applications in quantum computing and information processing [Science 366, 509 (2019)]. Our spectrometer is capable of both continuous-wave and pulsed ESR measurement in the temperature range of 2.5 K to 300 K. The surface-sensitivity is attained using a surface-type microwave resonator with its resonance frequency in the X-band. The spectrometer is connected to a home-built in-situ preparation chamber which allows us to prepare and characterize surfaces with low-energy electron diffraction and Auger electron spectroscopy. We demonstrate that we are sensitive down to a monolayer of molecular film using organic radicals such as α,γ-Bisdiphenylene-β-phenylallyl, and metal phthalocyanine complexes such as vanadyl phthalocyanine.

KFM 24.5 Thu 11:45 H6

Unsupervised machine learning-assisted analysis of multidimensional ARPES data — •Steinn Ymir Agustsson[1], Mohammad Ahsanul Haque[2], Fatemeh Zardbani[2], Davide Mottin[2], Panagiotis Karras[2], and Philip Hofmann[1] — [1]Institute of Physics and Astronomy, Aarhus University, Denmark — [2]Institute of Computer Science, Aarhus University, Denmark

In recent years, the size and complexity of experimental data sets has been dramatically growing in many fields of science. For photoemission spectroscopy, the development of novel detectors and multidimensional measurement modes (e.g., including a time dependence or spatial dependence), has lead to orders of magnitude more data being produced. Even after a necessary upgrade of the data management system, it remains highly challenging to visualize and superficially interpret the data fast enough to feed back into decisions about what to measure in an ongoing experimental run. A promising approach to address this is the application of machine learning tools. These have shown promising results when applied to data reduction and feature detection tasks in many fields of science. We have developed an unsupervised clustering method which is able to distinguish differences between ARPES spectra obtained from different spatial locations in nanoARPES measurements. This enables quick and automatic identification and classification of regions with different spectral features, allowing to invest more time in the collection of significant data.

KFM 24.6 Thu 12:00 H6

ViPErLEED: A modern all-in-one LEED I(V) package — •Alexander M. Imre[1], Florian Kraushofer[1,2], Florian Doerr[1], Tilman Kisslinger[3], Michael Schmid[1], Ulrike Diebold[1], Lutz Hammer[3], and Michele Riva[1] — [1]TU Wien, Vienna, Austria — [2]TU Munich, Munich, Germany — [3]FAU Erlangen-Nürnberg, Erlangen, Germany

Many surface science groups use Low-Energy Electron Diffraction (LEED) for quick, qualitative analysis of surface periodicity. Analysis of the beam intensities as a function of electron energy [LEED $I(V)$] is sensitive to surface atom positions at the picometer scale. Thus, comparison with calculated intensities can verify or reject structural models. Despite this, LEED $I(V)$ is currently rather unpopular, largely because the available software solutions are not sufficiently user-friendly. To greatly lower the barrier of entry into the field, we present

the Vienna Package for TensErLEED (ViPErLEED) which provides a truly all-in-one package for LEED $I(V)$. ViPErLEED includes a freely available design for electronics that enable upgrading existing LEED setups for LEED $I(V)$ use. With sophisticated image acquisition and processing methods, as well as an automated spot-tracking tool for curve extraction, we greatly simplify the most tedious parts of the experiment. For the calculation of intensities, the package includes a user-friendly front-end and an extensive overhaul to the established TensErLEED package that only requires a few standardized input files. We further describe automated symmetry detection, improvements to the structure search algorithm, and a Python API.

KFM 24.7 Thu 12:15 H6

On-surface GNR fabrication via electrospray deposition of monomers and polymers from solution — •Felix Baier[1], Christoph Dobner[1], Michael Beckstein[1], Mamun Sarker[2], Alexander Sinitskii[2], and Axel Enders[1] — [1]Universität Bayreuth — [2]University of Nebraska - Lincoln, USA

Strategies for depositing large organic molecules such as proteins, DNA or graphene nanoribbons (GNRs) are urgently needed because the conventional method of evaporation is impossible due to the size of the molecules. GNRs prepared in solution are of particular interest because they are longer compared to those synthesized on the surface and can be produced in large quantities. Since GNRs form crystallites, they cannot be brought onto the surface by direct contact printing and characterized using STM. Therefore, a new electrospray setup was developed for the deposition of GNR precursor molecules, large precursor polymers, and GNR from a solution. The instrument consists of a heatable stainless steel capillary to which a high voltage in the range -8 to 8 kV, with respect to the sample can be applied. The assembly is placed in a glovebox which ensures the cleanliness of the working process. The characterization of the deposits was done with STM under ultra high vacuum after sample transfer. The deposition of TPTP monomers from solution onto Au(111) brought comparable results as other, established approaches were cGNR were formed after direct contact printing in UHV. Larger polymers were also deposited and completely cyclized on the surface after deposition, forming promising GNRs that have not been studied anywhere before.

KFM 25: Poster

Time: Thursday 15:00–18:00 Location: P2

KFM 25.1 Thu 15:00 P2

Ferroelectric properties of $(Na_{0.5}Bi_{0.5})TiO_3$-$BaTiO_3$ perovskite ceramics modified by LiF additives — •Sobhan M. Fathabad[1], Vladimir V. Shvartsman[1], Ekaterina D. Politova[2], Galina M. Kaleva[2], and Doru C. Lupascu[1] — [1]Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg Essen, Essen, Germany — [2]Moscow

The system of $(Na_{0.5}Bi_{0.5})TiO_3$-$BaTiO_3$ solid solutions has attracted considerable interest due to its promising electromechanical, electrocaloric, and energy storage properties. In this work, the effect of LiF additive on the ferroelectric properties of $0.8(Na_{0.5}Bi_{0.5})TiO_3$-$0.2BaTiO_3$ ceramics is investigated. The samples were prepared by the conventional solid state synthesis technology. The LiF content varied from 0 to 15 mol

KFM 25.2 Thu 15:00 P2

Strain and defect location in the cross-section of laterally aligned SnO2 NWs — •Jasmin-Clara Bürger, Sebastian Gutsch, and Margit Zacharias — Laboratory for Nanotechnology, Department of Microsystems Engineering - IMTEK, University of Freiburg, Georges-Köhler-Allee 103, 79110 Freiburg, Germany

The 1D structure and the high surface-to-volume ratio of SnO2 nanowire-based devices allow for high sensitivities in gas- and biosensing. By their self-alignment towards the substrate edge and by the self-alignment of the SnO2 nanowire crystal lattice towards the atomic arrangement on the substrate surface[1], laterally aligned SnO2 NWs are superior to freestanding NWs as a basic structure for a single-NW-based sensor. However, up to now, only little is known about their crystal quality compared to the excellent material quality of freestanding NWs. Hence, here, laterally aligned SnO2 NWs on r-plane sapphire substrates were grown by the vapor-liquid-solid mechanism and morphologically analyzed by scanning electron microscopy. By focused-ion beam preparation, cross-sectional TEM lamellas of the laterally aligned SnO2 NWs on r-plane sapphire were prepared. For analysis of the NW defect density, post-processed strain maps were computed of atomically resolved TEM images. The theoretical background for the experimentally observed location of the lowest strain density close to the substrate-NW interface and the highest defect density close to the NW surface will be discussed.

[1] J.-C. Bürger et al., Cryst. Growth Des. (2021), 21 (1), 191-199

KFM 25.3 Thu 15:00 P2

Influence of sulfur doping on the creation yield of near-surface nitrogen vacancy centers and their charge state ratio — •Sven Graus[1], Ulrich Köhler[1], Tobias Lühmann[2], and Jan Meijer[2] — [1]Lehrstuhl für Experimentalphysik IV, Ruhr-Universität Bochum — [2]Felix-Bloch-Institut für Festkörperphysik, Angewandte Quantensysteme, Universität Leipzig

The negative charge state of nitrogen vacancy (NV) centers presents an extremely attractive candidate for a number of applications in quantum information technology and magnetometry. However, the implantation of near-surface NV centers shows a low yield and they have the tendency to convert into the neutral charge state. Recently, a significant increase in the creation yield of negative NV centers in the bulk of the diamond has been achieved by prior local doping of sulfur. We report on the in-situ implantation of sulfur and subsequent nitrogen implantation at energies of up to 5 keV while the sample is heated to temperatures of up to ∼800 °C under UHV conditions. Our setup presents a unique method for the implantation of near surface NV centers in small laboratories. First results on how these parameters influence the creation yield of negative NV centers close to the surface are presented.

KFM 25.4 Thu 15:00 P2

Improved thermoelectric properties of SnSe through forming a phase employing metavalent bonding — •Nan Lin, Yuan Yu, Oana Cojocaru-Miredin, and Matthias Wuttig — I.Physikalisches Institut IA, RWTH Aachen, Sommerfeldstraße 14, 52074 Aachen, Germany

SnSe only shows high ZT values above 750 K when the structure transforms from the asymmetrical Pnma phase to the higher symmetrical Cmcm phase. As a typical IV-VI compound bonded by p-state electrons, the Cmcm phase SnSe with an improved symmetry is expected to show the same chemical bonding with other rock-salt IV-VI compounds, which could be responsible for its excellent thermoelectric performance. Yet, it is challenging to stabilize the Cmcm phase at room temperature to characterize the bonding indicators. We successfully obtained the high-symmetry rock-salt SnSe phase by growing (SnSe)0.67(AgSbTe2)0.33, (SnSe)0.67(AgBiTe2)0.33, (SnSe)0.67(AgBiSe2)0.33, and (SnSe)0.5(AgSbSe2)0.5 alloys in a Bridgman oven. All cubic SnSe alloys show a unique portfolio of properties including a high optical dielectric constant, a large Born effective charge, and abnormal bond-breaking behavior in laser-assisted atom probe tomography. All these characteristics are indicative of the metavalent bonding mechanism while are not found in the pristine SnSe. Concomitantly, zT increases from near 0.1 for the Pnma SnSe to about 1.0 for all the Fm-3m SnSe phases. Our work demonstrates that metavalent bonding could be the origin of many special properties of SnSe including the excellent thermoelectric performance.

KFM 25.5 Thu 15:00 P2

Real space texture analysis using the 3D pair distribution function on a Pt thin film — •Sani Y. Harouna-Mayer[1,2], ZiZhou Gong[3], Martin v. Zimmermann[4], Ann-Christin Dippel[4], Simon J.L. Billinge[2], and Dorota Koziej[1,2] — [1]Institute for Nanostructure and Solid-State Physics, Center for Hybrid Nanostructures (CHyN), University of Hamburg, Hamburg, Germany — [2]The Hamburg Center for Ultrafast Imaging, Hamburg, Germany — [3]Department of Applied Physics and Applied Mathematics, Columbia University, New York, USA — [4]Deutsches Elektronen-Synchrotron

DESY, Hamburg, Germany

An approach is described for studying texture in nanostructured materials. It is demonstrated on a fiber textured polycrystalline Pt thin film. The approach uses 3D PDF methods to reconstruct the orientation distribution function (ODF) of the powder crystallites from a set of diffraction patterns taken at different tilt angles of the substrate with respect to the incident beam directly from the 3D PDF of the sample. A real space equivalent of the reciprocal space pole figure is defined in terms of interatomic vectors in the PDF and computed for various interatomic vectors in the Pt film. Further, it is shown how a valid isotropic PDF may be obtained from a weighted average over the tilt series. Finally, we describe an open source Python software package, FouriGUI, that may be used to help in studies of texture from 3D reciprocal space data, and indeed for Fourier transforming and visualizing 3D PDF data in general.

KFM 25.6 Thu 15:00 P2

An X-ray diffraction studies on AlCrVY(O)N thin films. — •Eric Schneider[1], Michael Paulus[1], Nelson Filipe Lopes Dias[1], David Kokalj[2], Dominic Stangier[2], and Wolfgang Tillmann[2] — [1]Fakultät Physik/DELTA TU Dortmund University, 44221 Dortmund, Germany — [2]Institute of Materials Engineering, Dortmund, Germany

The aim of this project is to gain a fundamental understanding of the dependence between deposition parameters, layer structure and oxidation behavior of AlCrVY(O)N coatings. For this purpose, the coating systems were deposited on a WC-Co composite substrate by DC sputtering and high-energy pulse magnetron sputtering (HiPIMS). In addition to this, individual process parameters such as BIAS voltage and substrate temperature are varied to determine their influence on the thin films structure. For the investigation of the samples we used synchrotron radiation at beamline BL9 of the synchrotron radiation source DELTA (Dortmund, Germany) to perform XRD measurements. The samples were heated in an heating cell to temperatures up to 1000°C to study their oxidation behavior. Depending on the process parameters, different oxidation behaviour and residual stresses present in the samples were observed. We thank DELTA for providing synchrotron radiation. This work was supported by the DFG via TO 169/21-1.

KFM 25.7 Thu 15:00 P2

Hydrostatic high-pressure cells for X-ray scattering applications — •Kevin Lehninger[1], Christian Sternemann[1], Michael Paulus[1], Bridget Murphy[1], Metin Tolan[1], and Lutz Feldmann[2] — [1]Fakultät Physik/DELTA TU Dortmund, 44221 Dortmund, Deutschland — [2]Fakultät Physik/Konstruktionsbüro TU Dortmund, 44221 Dortmund, Deutschland

Small angle and wide angle X-ray scattering (SAXS/WAXS) at moderate pressures are of increasing relevance for the study of e.g. protein denaturation and stimuli responsive materials, respectively. One of the experimental challenges here is the precise pressure control in the pressure range up to 10 kbar while separating the sample volume from the pressure transmitting medium. For this purpose, we present two dedicated hydrostatic high pressure cells designed for use at beamlines BL2 and BL9 of the DELTA synchrotron radiation source that use water for pressure transmission. The WAXS cell with an opening angle of 60 degrees allows a sample volume with a cross-sectional area of one square millimeter that can be exposed to a maximum pressure of 5000 bar. The sample volume is enclosed in a flexible capillary tube which is placed between two diamond windows and can have a maximum diameter of 1.5 mm. The SAXS cell can be operated up to a pressure of 10000 bar providing an opening angle 20 degrees. Here the sample volume is contained in a cylinder sealed by polyimide film which is screwed into the high pressure cell by a slide system.

KFM 25.8 Thu 15:00 P2

Entwicklung von Herstellungsverfahren für koordinatenbasierte 3D Mikro-Standarts — •Celina Hellmich[1], Sebastian Bütefisch[1], Thomas Weimann[1], Stefanie Kroker[1,2] und Matthias Hemmleb[3] — [1]Physikalisch-Technische Bundesanstalt Braunschweig, Bundesallee 100, 38116 Braunschweig, Deutschland — [2]Technische Universität Braunschweig, Institut für Halbleitertechnik, LENA Laboratory for Emerging Nanometrology, Hans-Sommer-Str. 66, 38106 Braunschweig, Deutschland — [3]point electronic GmbH Erich-Neuß-Weg 15 D-06120 Halle (Saale) Deutschland

3D-Normale vereinen die Eigenschaften der üblichen Normale und die Kalibrierfaktoren für alle Achsen und die Kopplungsfaktoren zwischen ihnen können in einem Mess- und Auswertungsschritt ermittelt werden können. Mit diesem alternativen Kalibrieransatz können geometrische Verlagerungen über 3D-Referenzstrukturen mit bekannten Objektkoordinaten bestimmt werden. Die derzeit verwendeten 3D-Normale werden mit FIB hergestellt. Jedes Normal ist daher eine kostenintensive Sonderanfertigung, die zudem eine zeitaufwändige Kalibrierung erfordert. Daher sollen waferbasierte Maskenprozesse zur Herstellung von 3D-Standarts entwickelt werden, mit denen viele Strukturen reproduzierbar hergestellt und an das jeweilige zu kalibrierende Gerät angepasst werden können. Erste Ergebnisse wurden durch den schrittweisen Aufbau von Siliziumoxidschichten in Kombination mit einem Trockenätzverfahren erzielt. Auf diese Weise können zweistufige Pyramidenstrukturen hergestellt werden, auf die der Marker für die Kalibrierung mit Hilfe von Lift-off aufgebracht werden kann.

KFM 25.9 Thu 15:00 P2

The Relation between Electrocaloric Effect and Non-Collinear Electric Fields: A Coarse-Grained Case Study of $BaTiO_3$ — •Lan-Tien Hsu[1,2], Frank Wendler[1], and Anna Grünebohm[2] — [1]Institute of Materials Simulation (WW8), Friedrich-Alexander University of Erlangen-Nürnberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Universitätsstr 150, 44801 Bochum, Germany

Ferroelectric perovskites are promising candidates for future electrocaloric cooling devices due to their adiabatic temperature changes in varying external electric fields.[1,2] Recently, the origin of the inverse electrocaloric effect (ECE) has been discussed.[2,3,4] In this work, we do coarse-grained molecular dynamic simulation using feram[5] to explore the phase stability and caloric responses of $BaTiO_3$ over a wide temperature range including fields in low-symmetry directions. We observe large inverse ECEs close to high-symmetry directions where the applied fields stabilize phases outside the zero-field coexistence temperature range. We believe this finding can provide general insights into the anisotropic nature of the ECE of ferroelectric perovskites.

[1] A. Torelló and E. Defay, Adv. Electron. Mater. (2022)
[2] A. Grünebohm, *et al.*, Energy Technol. **6** (2018)
[3] H. H. Wu and R. E. Cohen., J. Phys.: Condens. Matter **29** (2017)
[4] M. Marathe, *et al.*, Phys. Rev. B **96** (2017)
[5] T. Nishimatsu, *et al.*, Phys. Rev. B **78** (2008)

KFM 25.10 Thu 15:00 P2

Dielectric loss measurements of CVD diamond disks for ITER windows — •Sabine Schreck[1], Gaetano Aiello[1], Pablo Estebanez[2], Andreas Meier[1], Dirk Strauss[1], and Theo Scherer[1] — [1]Karlsruhe Institute of Technology, Institute for Applied Materials, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]F4E, Josep Pla 2, Torres Diagonal Litoral B3, 08019 Barcelona, Spain

Diamond disks manufactured by chemical vapor deposition (CVD) are essential elements of windows of the Electron Cyclotron Heating and Current Drive systems of fusion reactors like ITER. Diamond is selected as window material because of its high mechanical stability, high thermal conductivity and low dielectric loss. Only diamond disks with a low loss tangent guarantee a high transmission, i.e. a low absorption of microwave power in the disk. The latter results in moderate window temperatures and therefore in low thermal stresses. Hence, the measurement of the loss tangent is essential for the qualification of diamond disks for high-power windows. Dedicated measurement facilities (Fabry-Perot resonators) at KIT allow a high resolution measurement of the loss tangent at the disk centre (spherical set-up) as well as a mapping over the disk area to estimate its homogeneity (hemispherical set-up). Within a contract between F4E and KIT more than 60 diamond disks (D=70mm, t=1.11mm) produced similarly by MPA-CVD need to be qualified for their application in the ITER EC-system. The development of a dedicated test plan as well as initial results for the first disks delivered to KIT will be presented.

KFM 25.11 Thu 15:00 P2

X-ray emission spectroscopy at DELTA — •Nicola Thiering, Christian Albers, Robin Sakrowski, Michael Paulus, Metin Tolan, and Christian Sternemann — Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany

The analysis of the electronic and structural properties of transition metals is of enormous importance for a variety of research fields and applications. At beamline BL2 of the DELTA synchrotron radiation

source (Dortmund, Germany) we used a hardened white beam of a bending magnet for efficient excitation to conduct X-ray emission spectroscopy experiments. The emission spectra were measured using a von Hámos spectrometer equipped with four cylindrically bent analyzer crystals in combination with a Pilatus 100K area detector. In order to demonstrate the capabilities of this setup, we present Kα, Kβ, and valence-to-core spectra of selected transition-metal bearing compounds.

KFM 25.12 Thu 15:00 P2

Phase retrieval for X-ray in-line holographic imaging: beyond the homogeneous object assumption — •Jens Lucht[1], Simon Huhn[1], Leon Merten Lohse[1,2], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Universität Göttingen — [2]Deutsches Elektronen-Synchrotron DESY

X-ray lensless near-field holographic imaging offers high resolution 3d imaging with spatial resolution down to the nanometer scale with wide applicability in biomedical imaging and material sciences. To access quantitative images, phase retrieval has to be performed on the recorded Fresnel diffraction patterns. This constitutes an ill-posed inverse problem where several reconstruction methods have been developed. For high resolution synchrotron experiments, computationally efficient algorithms are needed. Widely employed is the computationally efficient contrast transfer function (CTF) method proposed by P. Cloetens two decades ago [P. Cloetens et al., Appl. Phys. Lett. 75, 2912 (1999)], besides more demanding nonlinear Fresnel propagation based methods. The CTF relies upon linearization of the Fresnel propagation. Notwithstanding its tremendous success, CTF-based methods often assume a homogeneous or low absorbing object as prior. We propose a CTF-based scheme that could relax these restriction to applicability while keeping reconstruction stability and computational requirements comparable. First experiments indicate very promising results.

KFM 25.13 Thu 15:00 P2

X-ray emission setup to study electronic structure of iron bearing compounds *in situ* at high pressure and high temperature — •Nicola Thiering[1], Christian Albers[1], Robin Sakrowski[1], Max Wilke[2], Johannes Kaa[1,4], Hlynur Gretarsson[3,5], Martin Sundermann[3,5], Metin Tolan[1,6], and Christian Sternemann[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, Dortmund, Germany — [2]Institut für Geowissenschaften, Universität Potsdam, Potsdam, Germany — [3]Deutsches-Elektronen-Synchrotron DESY, Hamburg, Germany — [4]European XFEL, Schenefeld, Germany — [5]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [6]Universität Göttingen, Göttingen, Germany

The determination of iron-bearing compounds' electronic structure under high pressure and temperature (HPHT) conditions is pivotal to understand the chemistry, physics and dynamics of the Earth's interior [1]. We present a setup for investigating the electronic structure of such compounds *in situ* at HPHT up to 80 GPa and 3000 K, achieved by using diamond anvils cells in combination with a double-sided laser heating setup [2,3] using (resonant) X-ray emission spectroscopy ((R)XES) and show results for α-Fe_2O_3 and $FeCO_3$. (R)XES spectra were acquired utilizing a wavelength-dispersive von Hámos spectrometer in combination with a Pilatus 100K area detector [4] at PETRA III. [1] B. Orcutt et al. Deep Carbon (2019) [2] C. Albers et al. PRB 105 085155 (2022) [3] G. Spiekermann et al. JSR, 27, 414 (2020) [4] C. Weis et al. JAAS 34, 384 (2019)

KFM 25.14 Thu 15:00 P2

X-ray off-axis holography using iterative phase retrieval and waveguide beam splitters — •Paul Meyer and Tim Salditt — Institute for X-ray Physics, Georg August University of Göttingen, Germany

Propagation based phase contrast imaging (PB-PCI) with hard X-rays has become a powerful technique to study weakly absorbing specimen. Iterative algorithms can for example make single cells in a hydrated environment visible by retrieving the phase shift induced by the sample [1].

As image contrast in PB-PCI data arises from phase curvature, the reconstruction of low-frequency signals is challenging. In practice, it often requires support constraints on the sample. This problem does not arise with off-axis holography. Here, information of the phase image is extracted through interference with an additional reference beam that can for example be generated by a beamsplitting waveguide [2].

We observed that introducing such a reference beam in simulations for PB-PCI accelerates convergence and improves accuracy of the iterative phase retrieval (RAAR). We aim to transfer the observed advantage to the practical application of off-axis holography at synchrotron imaging facilities.

[1] Krenkel et al. Three-dimensional single-cell imaging with X-ray waveguides in the holographic regime. Acta Cryst A 73, 282-292 (2017). [2] Fuhse et al. Waveguide-Based Off-Axis Holography with Hard X Rays. Phys. Rev. Lett. 97, 254801 (2006).

KFM 25.15 Thu 15:00 P2

Hierarchically Porous Carbon Derived from the Activation of Waste Chestnut Shells as High Performance Electrode Materials for Supercapacitor — •Ping Hong[1,2], Yude Wang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]School of Materials Science and Engineering, Yunnan University, Kunming, People's Republic of China

3D hierarchical porous carbon consisting of micropores, mesopores and macropores was successfully prepared through the activation of chestnut shell with potassium bicarbonate (KHCO3). The influence of KHCO3/chestnut shell ratio on the textural properties was carefully investigated. By optimizing the amount of KHCO3, 3D hierarchical porous carbon with high specific pore surface area (2298 m2 g-1) and high total pore volume (1.51 cm3 g-1) were achieved. When applying the as-prepared 3D hierarchical porous carbon as electrode materials for supercapacitors, a high specific electric capacity of 387 F g-1 was reached at a current density of 2 A g-1. The remarkable electrochemical performances are mainly attributed to the hierarchical porous structure with the high specific surface area and the eminent total pore volume. It suggests that this hierarchical porous carbon prepared by activated by using KHCO3 would have more promising foreground in the field of energy storage.

KFM 25.16 Thu 15:00 P2

Ni-SnO2 nanopore arrays as potassium-ion battery anodes — •Mo Sha, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Sodium-ion batteries (SIBs) represent an effective energy storage technology with potentially lower material costs than lithium-ion batteries. Here, we show the electrochemical performance of SIBs with electrode design at the nanoscale. Highly ordered three-dimensional (3D) self-supported Ni-TiO2 nanopore arrays (NiNPA@TiO2) with highly oriented nanoporous structures are fabricated using nanoimprited AAO templating technique and applied as nanostructured anodes for SIBs applications. Their large specific surface area can ensure a high capacity, and their highly oriented and stable nanoporous structure can facilitate ion transport. The NiNPA@TiO2 nanoarrays delivered a reversible capacity of 240 mAh g-1 after 100 cycles at the current density of 50 mAh g-1 and were able to retain a capacity of 105 mAh g-1 at the current density as high as 5 A g-1. Their large active sites, high ion accessibility, fast electron transport, and excellent electrode integrity were shown as great merits to obtain the presented electrochemical performance. Not limited to the SIBs electrodes, the highly ordered 3D heterostructured nanoarrays as a promising electrode design for other electrochemical energy conversion and storage devices.

KFM 25.17 Thu 15:00 P2

Enhanced efficiency of graphene-silicon Schottky junction solar cell through inverted pyramid arrays texturation — •Jiajia Qiu[1,2], Huaping Zhao[1], Wenhui Ma[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]State Key Laboratory of Complex Nonferrous Metal Resources Clean Utilization, Kunming University of Science and Technology, Kunming 650093, China

Nanostructures of silicon are gradually becoming hot candidate due to outstanding capability for trapping light and improving conversion efficiency of solar cell. In this work, silicon nanowires (SiNWs) and silicon inverted pyramid arrays (SiIPs) were introduced on surface of graphene-silicon (Gr-Si) solar cell through silver and copper-catalyzed chemical etching, respectively. The effects of SiNWs and SiIPs on carrier lifetime, optical properties and efficiency of Gr-SiNWs and Gr-SiIPs solar cells were systematically analyzed. The results show that the inverted pyramid arrays have more excellent ability for balancing antireflectance loss and surface area enlargement. The power conver-

sion efficiency (PCE) and carrier lifetime of Gr-SiIPs devices respectively increase by 62% and 34% by comparing with that of Gr-SiNWs solar cells. Finally, the Gr-SiIPs cell with PCE of 5.63% was successfully achieved through nitric acid doping. This work proposes a new strategy to introduce the inverted pyramid arrays for improving the performance of Gr-Si solar cells.

KFM 25.18 Thu 15:00 P2

Structural behavior of delithiated $Li_xNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (0<x<1) battery cathodes — •Tobias Hölderle[1,2], Peter Müller-Buschbaum[1,2], and Anatoliy Senyshyn[2] — [1]Lehrstuhl für funktionelle Materialien, Technische Universität München, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany

The development of portable electronic devices up to electric vehicles powered with lithium-ion batteries led to an increased demand for lithium-ion batteries with higher capacities, energy/power densities, and cycling life. One of the most encouraging and state of the art commercial cathode materials are mixed lithium Ni, Co, Al metal oxides, e.g. in the form of high nickel content $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) cathodes possessing high energy and power densities at lower costs. Besides advantages, NCA materials possess several essential drawbacks. For example, NCA cathode materials are known to suffer from poor thermal stability, pronounced capacity as well as power density fading, and antisite disorder in NCA materials [1]. In the current contribution, a systematic *ex-situ* neutron powder diffraction study on differently electrochemically delithiated NCA cathode materials is presented. A set of structural parameters was obtained using full-profile Rietveld refinement. The lithium occupations reflect the increasing state-of-charge whilst the occupations of transition metals do not change, indicating the absence of antisite defects (cation mixing) in the NCA material. [1] C. Xu, P. J. Reeves, Q. Jacquet and C. P. Grey, Adv. Energy Mater., 11, 2003404 (2021).

KFM 25.19 Thu 15:00 P2

Dense binary Fe-Cu sites promoting CO2 utilization to enable highly-reversible hybrid Na-CO2 battery — •Changfan Xu — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — School of Metallurgy and Environment, Central South University, Changsha 410083, China — Faculty of Metallurgical and Energy Engineering, Kunming University of Science and Technology, Kunming 650093, China

A well-defined morphology of nitrogen-rich graphitic carbon framework with dense bimetallic active sites (Fe-Cu-N-C) was facilely prepared by introducing Fe3+ and Cu2+ to regulate in-situ grown carbon nanotubes as an advanced catalyst toward hybrid Na-CO2 batteries. Through metal content-tuning and carbon architecture-altering, the Fe-Cu-N-C was proved to be dramatically more effective than Cu-N-C and Fe-N-C. As the cathodic catalyst of a hybrid Na-CO2 battery, Fe-Cu-N-C can facilitate the fast evolution and degradation of flocculent discharge products and achieve an excellent long-term cyclability up to 1550 cycles (over 600 h). The outstanding performance is attributed to the cross-linked conductive framework affording a highway for accelerating electron transport and Na+/CO2 diffusion. Besides, the synergistic effects among defect-rich interfaces, Fe/Fe3C nanocrystals, Fe-Nx, and Cu-Nx sites derived from nitrogen doping enhance the catalytic activity. The possible growth and decomposition mechanisms of NaHCO3 products were also presented and discussed.

KFM 25.20 Thu 15:00 P2

Dynamics of lithium-distribution in 18650-type LFP|C lithium-ion batteries during electrochemical cycling — •Dominik Petz[1,2], Peter Müller-Buschbaum[1,2], and Anatoliy Senyshyn[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]Lehrstuhl für Funktionelle Materialien, Technische Universität München, Garching, Germany

The electrochemical cycling of lithium-ion batteries is characterized by an active transport of lithium ions and electrons, which are exchanged between the cathode and anode materials. Ionic exchange influences structural and chemical properties of electrode materials, which, in turn, affects electrode dimensions and geometry, current density, temperature, pressure, reaction rate, etc. Such parameters are in general neither uniformly nor statically distributed and therefore serve as stabilizing factor for heterogeneous states in lithium-ion batteries, which are typically reflected in the lithium concentration distribution in the electrodes. In most of the studies reported in literature, the lithium distribution has typically been examined in static equilibrium (e.g. in fully charged state), neglecting the evolution of the distribution under real charging conditions like the influence of C-rates, etc.

In this work the evolution of the lithium-ion distribution in the graphite anode was investigated in-operando by spatially-resolved neutron powder diffraction. Neutron data were supplemented by diffraction studies with high-energy photons. The occurrence of lithium inhomogeneities on different length scales was observed and will be presented in the current contribution.

KFM 25.21 Thu 15:00 P2

Strong electron-phonon coupling in $EuPd_2Si_2$ — •Mai Ye[1], Mark Joachim Graf von Westarp[1], Sofia-Michaela Souliou[1], Marius Peters[2], Robert Möller[2], Kristin Kliemt[2], Cornelius Krellner[2], and Matthieu Le Tacon[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Institute of Physics, Goethe-University Frankfurt, 60438 Frankfurt am Main, Germany

Mixed-valence metal $EuPd_2Si_2$ exhibits a valence transition from Eu^{2+} to Eu^{3+} with the crossover temperature T_v around 140 K [Jpn. J. Appl. Phys. 50 (2011) 05FD03]. On cooling, the tetragonal crystal symmetry is unchanged, with the a-axis length decreasing and the c-axis length essentially unchanging [arXiv:2203.05136]. We study the phonon modes of this material by Raman spectroscopy to explore the effect of valence transition and electron-phonon coupling. The Raman-active A_{1g} phonon mode shows Fano-type asymmetric lineshape, indicating interaction between the phonon mode and underlying continuum of electronic excitations. This mode also exhibits large frequency hardening on cooling: the frequency at 25 K is around 30% larger than that at 300 K. Such a large frequency change cannot be solely explained by the change of lattice parameters, which is only 2%, and points to the role played by electron-phonon interaction. Moreover, the frequency and linewidth of other Raman-active phonon modes show anomalies at T_v. We also present Raman spectra of $EuPd_2(Si_{0.94}Ge_{0.06})_2$ for comparison.

KFM 26: Focus Session: Topological Devices (joint session TT/KFM)

The properties of topological phases of matter give rise to unique phenomena, such as edge or surface transport, spin-momentum locking, or topological protection against perturbations. Many years after their conception, several topological platforms have reached maturity, and research interests have shifted towards mesoscopic devices unveiling rich and new topological physics, driven in part by the perspectives of novel topological quantum computation. Within this Focus Session, recent examples of devices exploring or exploiting the topological properties of various phases of matter shall be discussed.

Organizers: Erwann Bocquillon, Oliver Breunig, Yoichi Ando (all Universität zu Köln)

Time: Thursday 15:00–18:30 Location: H10

Invited Talk KFM 26.1 Thu 15:00 H10

Supercurrents in HgTe-based topological nanowires — •Dieter Weiss — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg/Germany

Topological insulator (TI) nanowires in proximity to conventional superconductors constitute a tunable platform to realize topological superconductivity and Majorana zero modes [1]. Tuning is done by an axial magnetic flux ϕ transforming the system from trivial at $\phi = 0$

to topologically nontrivial when a magnetic flux quantum $\phi_0 = h/2e$ threads the wire's cross-section. Here, we investigate the evolution of the supercurrent in ballistic HgTe Josephson junctions as a function of axial magnetic flux ϕ and examine the periodicity of the supercurrent utilizing microwave irradiation and probing Shapiro steps. Suppressed odd Shapiro steps herald the existence of 4π-periodic supercurrents, a signature of topological superconductivity. Our data suggest that at small ϕ this 4π-periodic supercurrent is of trivial origin but that at magnetic fields above $\phi_0/2$, topological 4π-periodic supercurrents take over [2].

Work done in cooperation with Ralf Fischer, Wolfgang Himmler, Johannes Ziegler, Jordi Picó-Cortés , Gloria Platero, Milena Grifoni, Dmitriy A. Kozlov, N. N. Mikhailov, Sergey A. Dvoretsky , Michael Barth, Jakob Fuchs, Cosimo Gorini, Klaus Richter, and Christoph Strunk.

[1] A. Cook and M. Franz, PRB 84, 201105(R) (2011)
[2] R. Fischer et al., PRR 4, 013087 (2022)

Invited Talk KFM 26.2 Thu 15:30 H10

Majorana bound states and non-reciprocal transport in topological insulator nanowire devices — •Henry Legg — Department of Physics, University of Basel

I consider devices consisting of a three-dimensional topological insulator (TI) nanowire placed in proximity to an s-wave superconductor.

First, I will show that a non-uniform chemical potential induced, for instance, by gating enables the device to be brought into a topological superconducting phase at relatively weak magnetic fields with Majorana bound states (MBSs) present for an exceptionally large region of parameter space in realistic systems. I also consider the experimental challenges posed by the metallization effect that occurs as a result of bringing a TI nanowire into proximity with a superconductor.

Second, I will discuss non-reciprocal transport evidence for the subband splitting that is central to the proposal to achieve MBSs in TI nanowires. I will show that a giant magnetochiral anisotropy observed in the normal state of the TI nanowire provides strong evidence for the artificial breaking of inversion symmetry due to gating effects. Furthermore, I will argue that the superconducting diode effect can be used as measure of inversion symmetry breaking in the presence of a superconductor and to determine when the TI nanowire is in the region of parameter space where topological superconductivity is expected.

Invited Talk KFM 26.3 Thu 16:00 H10

Integration of topological insulator Josephson junctions in superconducting qubit circuits — •Tobias W. Schmitt[1], Malcolm R. Connolly[2,3], Michael Schleenvoigt[1], Chenlu Liu[2], Oscar Kennedy[3], José M. Chávez-Garcia[4], Anne Schmidt[1], Albert Hertel[1], Tobias Lindström[5], Sebastian E. de Graaf[5], Karl D. Petersson[4], Detlev Grützmacher[1], and Peter Schüffelgen[1] — [1]Peter Grünberg Institute & Jülich-Aachen Research Alliance, Forschungszentrum Jülich — [2]Blackett Laboratory, Imperial College London — [3]London Centre for Nanotechnology, University College London — [4]Center for Quantum Devices, University of Copenhagen — [5]National Physical Laboratory

Since the prediction of topological superconductivity in hybrid devices of topological insulators (TIs) and conventional s-wave superconductors (S), S-TI-S Josephson junctions have been studied intensively in electrical transport experiments. The integration of these Josephson junctions in superconducting qubit circuits allows to investigate them via circuit quantum electrodynamic techniques, which promises novel insights into their exotic characteristics. In this talk, I will present the implementation of transmon qubits with *in situ* fabricated S-TI-S Josephson junctions and outline fabricational challenges. I will further show results on coherent qubit control as well as temporal quantum coherence and discuss possible limitations on qubit coherence for the first generation of TI transmon devices [1]. An outlook on qubit improvements and developements towards the detection of topological superconductivity will be given.

[1] Nano Lett. 22, 7, 2595 (2022)

15 min. break

Invited Talk KFM 26.4 Thu 16:45 H10

Universal fluctuations of the induced superconducting gap in an elemental nanowire — Lauriane Contamin, Lucas Jarjat, William Legrand, Audrey Cottet, Takis Kontos, and •Matthieu Delbecq — Laboratoire de Physique de l'Ecole Normale Supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université Paris-Diderot, Sorbonne Paris Cité, Paris, France.

Proximity induced superconductivity in a normal conductor is a rich field of experimental and theoretical investigations. Lately it has been at the heart of the quest for realizing topological modes in hybrid superconductor-nanowire nanodevices. Yet it turns out that there was a lack of investigations in elemental systems. In this work we therefore investigate an ultra-clean carbon nanotube coupled to a superconducting lead. We observe for the first time a long standing prediction of random matrix theory (RMT) that mesoscopic fluctuations of the mini-gap in a conductor follow a universal distribution with a clear transition when time reversal symmetry is broken, as predicted by RMT. Interestingly, mesoscopic fluctuations of the minigap were precisely predicted to lead to ubiquitous nontopological edge states clustering towards zero energy. We do indeed observe ubiquitous and robust zero bias conductance peaks under magnetic field in our device that cannot host topological modes by design. The RMT predictions that are compatible with our observations are very general and should be present in any system showing disorder. It therefore calls for alternatives to transport measurement to identify Majorana modes in 1D systems with microwave photons in a cavity as a promising platform.

Invited Talk KFM 26.5 Thu 17:15 H10

Exploring the full potential of edge channel transport in HgTe based two-dimensional topological insulators — •Saquib Shamim[1,2], Wouter Beugeling[1,2], Pragya Shekhar[1,2], Jan Böttcher[3], Andreas Budewitz[1,2], Julian-Benedikt Mayer[3], Lukas Lunczer[1,2], Jonas Strunz[1,2], Johannes Kleinlein[1,2], Ewelina Hankiewicz[3], Björn Trauzettel[3], Hartmut Buhmann[1,2], and Laurens Molenkamp[1,2] — [1]Experimentelle Physik III, Physikalisches Institut, Universität Würzburg, Am Hubland, Würzburg, Germany — [2]Institute for Topological Insulators, Universität Würzburg, Am Hubland, Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany.

In this talk, I will discuss some of our recent results on HgTe-based two-dimensional topological insulators. Over the past few years, we have developed a chemical wet-etch technique to fabricate high-quality microstructures in HgTe quantum wells. Firstly, I will discuss some important achievements due to the wet-etch fabrication process: We fabricated quantum point contacts in topological HgTe quantum wells and investigated the interactions among helical edge channels. We also fabricated microstructures from (Hg,Mn)Te quantum wells and observed quantized conductance in these devices. Secondly, I will introduce a gate training method that allows us to approach conductance quantization in macroscopic devices. Finally, I will present recent magnetotransport results on (Hg,Mn)Te quantum wells and the emergence of quantum Hall plateaus at extremely low magnetic fields (˜ 50 mT).

KFM 26.6 Thu 17:45 H10

Quantum non-Hermitian topological sensors — •Florian Koch and Jan Carl Budich — Institute of Theoretical Physics, Technische Universität Dresden

Recent discoveries regarding the exceptional spectral and topological properties of non-Hermitian (NH) tight-binding models, e.g. their striking boundary-sensitivity, have triggered the quest for constructing novel sensors [1,2]. Here, using quantum master equations we promote the architecture of such sensing devices to a fully quantum-mechanical framework. Specifically, we study a setting of weakly-coupled bosonic modes arranged in an array with broken ring geometry that would realize a NH topological phase in the classical limit. Employing methods from quantum-information theory of Gaussian states, we show that a small coupling induced between the ends of the broken ring may be detected with a precision that increases exponentially in the number of coupled modes. Our findings pave the way towards designing quantum NH topological sensors (QUANTOS) that may observe with high precision any physical observable that couples to the boundary conditions of the device [3].

[1] J.C. Budich and E.J. Bergholtz, Phys. Rev. Lett. **125**, 180403 (2020).
[2] E.J. Bergholtz, J.C. Budich, and F.K. Kunst, Rev. Mod. Phys. **93**, 015005 (2021).
[3] F. Koch and J.C. Budich, Phys. Rev. Res. **4**, 013113 (2022).

KFM 26.7 Thu 18:00 H10

First magnetic field measurements of a topological insulator based Transmon Qubit — •Anne Schmidt[1], Tobias W. Schmitt[1], Chenlu Liu[2], Albert Hertel[1], Christian

Dickel[3], Michael Schleenvoigt[1], Malcolm R. Connolly[2,4], Yoichi Ando[3], Detlev Grützmacher[1], and Peter Schüffelgen[1] — [1]Peter Grünberg Institute & Jülich-Aachen Research Alliance, Forschungszentrum Jülich — [2]Blackett Laboratory, Imperial College London — [3]Institute of Physics II, University of Cologne — [4]London Centre for Nanotechnology, University College London

Hybrid topological insulator (TI) – superconductor (S) heterostructures are a promising platform for the realization of topologically protected quantum computation based on Majorana zero modes. This promises fewer physical qubits for creating a logical qubit compared to conventional superconducting qubits. Our full *in situ* device fabrication, which combines selective area growth of thin $(Bi,Sb)_2Te_3$ films and stencil deposition of superconductive Nb has already shown to create highly transparent S-TI interfaces. Recently, we have demonstrated that this fabrication process can readily be integrated into cQED structures as building block for a transmon qubit and performed coherence measurements at zero magnetic field. Here, we will expand these measurements to finite magnetic fields, as in-plane magnetic fields are a requirement for restoring the topological phase in confined $(Bi,Sb)_2Te_3$ nanostructures. We present initial results on the magnetic field dependence of the T_1 lifetime and the qubit's anharmonicity.

KFM 26.8 Thu 18:15 H10

Kondo interactions of quantum spin Hall edge channels with charge puddles — •Christopher Fuchs[1,2], Pragya Shekhar[1,2], Saquib Shamim[1,2], Lena Fürst[1,2], Johannes Kleinlein[1,2], Jukka I. Väyrynen[3], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Physikalisches Institut, Universität Würzburg, Würzburg, Germany — [2]Institute for Topological Insulators, Universität Würzburg, Würzburg, Germany — [3]Department of Physics and Astronomy, Purdue University, West Lafayette, USA

Quantum spin Hall edge channels are protected against backscattering by time-reversal symmetry. However, since the first observation of the quantum spin Hall effect in HgTe in 2007 it is known that reproducible fluctuations shape the quantization plateau when the chemical potential is tuned through the bulk gap. Here, those fluctuations are examined in high-quality micron-sized quantum well structures of HgTe at millikelvin temperatures. By performing temperature and gate-dependent measurements, we conclude that the observed conductance fluctuations indicate interactions of the edge channel electrons with individual charge puddles – microscopic fluctuations in the potential landscape commonly observed in narrow gap semiconductors – that act like Kondo correlated quantum dots. The resulting spin-flip backscattering gives rise to a distinct Kondo-like temperature dependence of the conductance fluctuations, which is backed up by theoretical modelling. Our results provide insight into the leading mechanism of decoherence of quantum spin Hall edge channels.

KFM 27: Perovskite and Photovoltaics 3 (joint session HL/CPP/KFM)

Time: Thursday 15:00–16:30 Location: H31

KFM 27.1 Thu 15:00 H31

Atomically Thin Sheets of Lead-Free 1D Hybrid Perovskites Feature Tunable White-Light Emission from Self-Trapped Excitons — •Philip Klement[1], Natalie Dehnhardt[2], Chuan-Ding Dong[3], Florian Dobener[1], Julius Winkler[2], Samuel Bayliff[4], Detlev M. Hofmann[1], Peter J. Klar[1], Stefan Schumacher[3,5], Sangam Chatterjee[1], and Johanna Heine[2] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Giessen, Germany — [2]Department of Chemistry and Material Sciences Center, Philipps-Universität Marburg, Marburg, Germany — [3]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Paderborn, Germany — [4]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK, USA — [5]College of Optical Sciences, The University of Arizona, Tucson, AZ, USA

One of the major current challenges in 2D materials' synthesis is the intentional design of building blocks to introducing superior chemical and physical properties. The limiting factor in this approach is the commonly-believed paradigm that in-plane covalent interactions are strictly necessary to form 2D materials, limiting the number of candidates. Here, we go beyond the paradigm that atomically thin materials require in-plane covalent bonding and report single layers of the one-dimensional organic-inorganic perovskite [C7H10N]3[BiCl5]Cl. Its unique 1D-2D structure enables single layers and the formation of self-trapped excitons which show white-light emission.

KFM 27.2 Thu 15:15 H31

Multiple spin-flip Raman scattering in bulk lead halide perovskites — •Marek Karzel[1], Dennis Kudlacik[1], Natalia E. Kopteva[1], Ina Kalitukha[2], Maksym V. Kovalenko[3], Dmitri R. Yakovlev[1], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]St. Petersburg, Russia — [3]Laboratory of Inorganic Chemistry, ETH Zürich, 8093 Zürich, Switzerland

Lead halide perovskites like FACs are promising competitors for conventional semiconductors in spintronics due to their highly efficient light absorption and emission properties. We study spin-flip Raman scattering (SFRS) of resident carriers and investigate possible carrier exchange interactions. The measurements are performed at low temperatures around 1.6 K and external magnetic fields up to 10 T in Faraday and tilted geometries. This method allows us to observe Raman shifts in high magnetic fields which according to [1] are attributed to the g-factors of resident electrons and holes. The SFRS efficiency significantly increases for resonant probing of the free exciton resonances. We conduct from our measurements, that the creation of the free exciton is the essential requirement for observation of multiple spin-flip Raman scattering.

[1] E. Kirstein et al., Adv. Mater. 34, 2105263 (2022).

KFM 27.3 Thu 15:30 H31

Stability Enhancement of perovskite nanoplatelets via crosslinking of ligands — •Maximilian Gruber, Ulrich Leo, Nina Henke, Patrick Ganswindt, Michael Lichtenegger, Connor Heimig, and Alexander Urban — Nanospectroscopy Group and Center for Nanoscience (CeNS), Nano-Institute Munich, Department of Physics, Ludwig-Maximiliäns-Universitat München, Königinstr. 10, 80539 Munich, Germany

In recent years lead halide perovskite nanoplatelets (NPL) have attracted a lot of attention due to low-cost production and excellent spectral tuning. Additionally, perovskite NPLs exhibit the benefit of exciton energy tunability via quantum confinement as well as large photoluminescence quantum yield. The high surface to volume ratio of the NPLs, however, makes them susceptible to degradation by water, air and ion migration.

One solution to these issues of degradation investigated here is a process called crosslinking. Hereby the exposure of a film of NPLs to a dose of electron radiation induces intermolecular bonds between the organic ligands attached to the individual nanocrystals, hence forming a protective matrix around a film of pristine perovskite NPLs.

Varying dosages of irradiation of three monolayer CsPbBr3 NPLs were investigated followed by an exposure to other halides, NPLs with a different halide composition as well as different solvents, showing a drastic increase in stability of the crosslinked compared to untreated NPLs. This enables the possibility of a future application of lead halide perovskite NPLs under ambient conditions.

KFM 27.4 Thu 15:45 H31

Enhancing the optical performance of perovskite nanoplatelets — •Stefan Martin[1], Carola Lampe[1], Nina Henke[1], Ioannis Kouroudis[2], Milan Harth[2], Alessio Gagliardi[2], and Alexander Urban[1] — [1]LMU Munich, Nanospectroscopy Group — [2]TU Munich

Lead halide perovskites have been drawing a lot of interest during the last few years due to their unique properties. Their excellent optical performance combined with easy and cost-efficient production are interesting for both light-emitting devices and solar cells. Perovskite nanoplatelets are furthermore convincing with high photoluminescence quantum yields and narrow emission linewidths tunable from 430 to 505 nm. The thickness of these nanoplatelets can be tuned with a

monolayer precision and determines the absorption and emission profile of the sample.

By using different machine learning approaches the synthesis parameters were investigated and optimized based on the emission spectrum. With this method, the emission properties of nanoplatelets with thicknesses reaching from 2 to 8 monolayers were enhanced. Additionally, the emission wavelengths can be finetuned using a post-synthetic enhancement treatment comprising a lead halide ligand solution. Depending on the time interval between synthesis and enhancement, a redshift of controllable extent can be introduced while further reducing the emission linewidth. With these strategies, a narrow and symmetric emission peak can be achieved at any desired wavelength. This is particularly interesting for the implementation in optoelectronic devices.

KFM 27.5 Thu 16:00 H31

Extensive study on sequential physical vapor deposition of mixed-cation perovskite (Cs,FA)PbI_3 — •Karl Heinze[1], Tobias Schulz[1], Roland Scheer[1], and Paul Pistor[2] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, von-Danckelmann-Platz 3, 06120 Halle (Saale), Germany — [2]Universidad de Pablo Olivade, Carretera de Utrera 1, 41013, Sevilla, Spain

Sequential deposition via physical vapor deposition (PVD) is underexplored, even though it offers precise adjustment of components and composition and a variety of routes to investigate the optimization of perovskite growth. We combine in situ XRD and in situ laser light scattering to monitor phase evolution of (Cs,FA)PbI3 during PVD. We study the influence of deposition sequence of the components PbI2, FAI and CsI on CsFAPbI3 growth. Noticeably, the sequence strongly influences the orientation of deposited components. Similarly, diffusion before and during annealing as well as resulting alpha phase share depend on the evaporation sequence. When depositing PbI2 first, conversion to the perovskite phase was not achieved, unless an over stoichiometric share of FAI was deposited. Depositing FAI first and PbI2 later resulted in a high probability of layer conversion to the perovskite phase without secondary phases being detected. A striking feature during our investigation was the absence of the delta phase during deposition and annealing, seemingly caused solely by the preparation method. We deliver important insight into this poorly investigated preparation path and provide a foundation for further research based on our detailed study of sequence-dependent crystalline growth.

KFM 27.6 Thu 16:15 H31

Ultrafast transient spectroscopy of Cu(In,Ga)Se_2 coupled to different buffer layers. — •Pirmin Schweizer, Ricardo Rojas-Aedo, Alice Debot, Philip Dale, and Daniele Brida — Department of Physics and Materials Science, University of Luxembourg, 162a avenue de la Faïencerie, L-1511 Luxembourg, Luxembourg

The dynamic parameters of photo-induced electron-hole pairs, such as recombination time and charge conductivity, play a major role in the efficiency of photovoltaic devices. Among thin film materials for photovoltaics, one of the most interesting is the p-type Cu(In,Ga)Se_2 alloy (CIGS) on which an n-type buffer layer is deposited, forming the initial part of the device p-n junction. The inter-material transport dynamics strongly depend on how the band structure is affected by the buffer layer, and also on the quality of the CIGS \ buffer layer interface which may contain defects. In our experiments we have compared the ultrafast transient reflectivity on CIGS epitaxially grown on a GaAs substrate. New Cd free buffer layers In_2S_3 and band offset tunable Zn(O,S), are compared to the most commonly used buffer layer, CdS. The transient reflection measurements allows for the extraction of the electronic transport dynamics at the interface with the buffer. This study allows us to draw conclusions about the pair formation capacity mediated by the transport properties between the CIGS and the buffer layer. The results can guide the development of Cd free buffer layers thus reducing the environmental impact caused by CdS in traditional CIGS solar cells.

KFM 28: Topological Insulators (joint session MA/KFM)

Time: Thursday 15:00–17:45 Location: H37

Invited Talk KFM 28.1 Thu 15:00 H37

Neutron scattering on magnetic topological materials: From topological magnon insulators to emergent many-body effects — •Yixi Su — Jülich Centre for Neutron Science JCNS at MLZ, Forschungszentrum Jülich, 85747 Garching, Germany

Recent theoretical predictions and experimental realizations of exotic fermions and topologically protected phases in condensed matter have led to tremendous research interests in topological quantum materials. Especially, magnetic topological materials, such as magnetic Dirac and Weyl semimetals, and intrinsic magnetic topological insulators etc., in which non-trivial topology of single-electron band structures and electronic correlation effects are often intertwined, have emerged as an exciting platform to explore novel phenomena. Here I will present our recent neutron scattering studies. In the Dirac semimetal EuMnBi2, the evidence for the possible impact of magnetism on Dirac fermions is obtained via a detailed neutron diffraction study of the spin-flop transition [1]. Based on our inelastic neutron scattering study and theoretical analysis of spin-wave excitations, the exotic topological magnon insulators, the bosonic analogs of topological insulators, have been experimentally realized in the two-dimensional van der Waals honeycomb ferromagnets CrSiTe3 and CrGeTe3 [2]. Furthermore, in the magnetic Weyl semimetal Mn3Sn, an unusual magnetic phase transition that is driven by emergent many-body effects is revealed via a combined neutron scattering study and band-structure calculations [3].

[1] F. Zhu, et al., Phys. Rev. Research 2, 043100 (2020). [2] F. Zhu, et al., Sci. Adv. 7, eabi7532 (2021). [3] X. Wang (unpublished)

KFM 28.2 Thu 15:30 H37

Tuning the magnetic gap of a topological insulator — •Marcus Liebmann[1], Philipp Küppers[1], Jannik Zenner[1], Stefan Wimmer[2], Gunther Springholz[2], Oliver Rader[3], and Markus Morgenstern[1] — [1]II. Phys. Inst. B, RWTH Aachen Univ., Germany — [2]Inst. Halbleiter- u. Festkörperphysik, Johannes Kepler Univ., Linz, Austria — [3]Helmholtz-Zentrum Berlin f. Mater. u. Energie, Germany

Mn-rich $MnSb_2Te_4$ is a ferromagnetic topological insulator with yet the highest Curie temperature $T_C = 45 - 50$ K. It exhibits a magnetic gap at the Dirac point of the topological surface state that disappears above T_C. We probe the gap size by scanning tunneling spectroscopy, varying in-plane magnetic field $B_{||}$ and temperature. We demonstrate shrinkage of the average gap size with $B_{||}$ revealing that the gap opening originates from out-of-plane magnetization. In line, the gap does not close completely up to $B_{||} = 3$ T as the magnetization is only partially rotated in-plane. In addition, we demonstrate significant spatiotemporal fluctuations of the gap size at temperatures as low as $T_C/2$, above which the remanent magnetization indeed decays. Thus, the gap is tightly bound to the out-of-plane magnetization, as expected theoretically but not demonstrated experimentally yet. The partial in-plane rotation at $B_{||} = 3$ T and the low temperature onset of fluctuations stress the important role of competing magnetic orders in the formation of the favorable ferromagnetic topological insulator in Mn-rich $MnSb_2Te_4$, providing insight into the complex magnetic gap opening that is decisive for quantum anomalous Hall devices.

KFM 28.3 Thu 15:45 H37

Local magnetic and electronic properties of the intrinsic magnetic topological insulator $MnBi_6Te_{10}$ — •Abdul-Vakhab Tcakaev[1], Volodymyr Zabolotnyy[1], Bastian Rubrecht[2], Laura Corredor[2], Jorge Facio[2], Laura Folkers[3], Anja Wolter[2], Anna Isaeva[2], and Vladimir Hinkov[1] — [1]Experimentelle Physik IV and R ontgen Research Center for Complex Materials (RCCM), Fakult at f ur Physik und Astronomie, Universit at W urzburg, Am Hubland, D-97074 W urzburg, Germany — [2]Leibniz IFW Dresden, Helmholtzstraße 20, D-01069 Dresden, Germany — [3]Faculty of Physics, Technische Universit at Dresden, D-01062 Dresden, Germany

The recent observation of novel phenomena in the intrinsic magnetic topological insulator $MnBi_2Te_4$, such as the quantum anomalous Hall effect and the topological magnetoelectric effect has prompted research of the higher-n members of the $(MnBi_2Te_4)(Bi_2Te_3)_n$ family. Here we combine x-ray absorption spectroscopy, and x-ray circular and linear

dichroism at the Mn $L_{2,3}$ edges, with density-functional (DFT) and multiplet ligand-field (MLFT) theory to investigate the ground state of Mn in $MnBi_6Te_{10}$ single crystals. Our magnetometry data reveal FM state with finite remanence consistent with the spectroscopy data. Our spectroscopy results together with DFT and *ab initio* MLFT calculations allow us to determine in full detail the local magnetic and electronic properties of the Mn ions in the bulk and near the surface, and deliver important microscopic physical parameters, including Mn 3*d*-shell occupation, the spin and orbital magnetic moments.

KFM 28.4 Thu 16:00 H37

Probing the Superconductor / Quantum Anomalous Hall Interface — •Anjana Uday[1], Gertjan Lippertz[1,2], Andrea Bliesener[1], Alexey Taskin[1], and Yoichi Ando[1] — [1]University of Cologne, Cologne, Germany — [2]KU Leuven, Leuven, Belgium

Recently, crossed Andreev conversion was reported in a hybrid quantum Hall (QH) / Superconductor (SC) system [1]. The evidence was based on the observation of a negative downstream resistance R_D in a three-terminal measurement of a Hall-bar device with respect to the grounded SC electrode. Similar experiments would be of great interest in the quantum anomalous Hall (QAH) / SC hybrid system, where superconductivity can be suppressed for control experiments by applying a magnetic field while keeping the 1D edge state unchanged. We fabricated Hall-bar devices from V-doped $(Bi_xSb_{1-x})_2Te_3$ thin films contacted with Nb electrodes having various widths. We found a finite positive R_D which increases with decreasing the widths of the SC electrode due to the QAH breakdown mechanism [2]. We also found a clear increase in R_D upon killing the superconductivity with a magnetic field for Nb electrodes narrower than 200 nm; this can be attributed to either non-local Andreev reflections on top of the breakdown-induced finite R_D or local Andreev reflections on the 2D normal metal/SC interface, which can be created by the charge transfer from the Nb electrode to the gapped VBST surface state. In both cases our observation implies a high transparency of the SC/QAH interface.

[1] G.-H. Lee et al., Nat. Phys. 13, 693-698 (2017)
[2] G. Lippertz et al., arXiv:2108.02081 (2021)

KFM 28.5 Thu 16:15 H37

Magnetotransport Properties of MnSb2Te4 — •Michael Wissmann[1,2,3], Joseph Dufouleur[2], Anna Isaeva[4], Bernd Büchner[2,3], and Romain Giraud[1,2] — [1]Université Grenoble-Alpes, CNRS, CEA, SPINTEC, F-38000 Grenoble, France — [2]Leibniz Institute for Solid State and Materials Research IFW Dresden, 01069 Dresden, Germany — [3]Institute of Solid State Physics, TU Dresden, 01069 Dresden, Germany — [4]Department of Physics and Astronomy, University of Amsterdam,1098 XH Amsterdam, Netherlands

The new family of intrinsically magnetic van-der-Waals layered topological insulators Mn(Bi,Sb)Te, with strong spin-orbit coupling, is of great interest to investigate the interplay between topology and magnetic order in electronic band structures. When introducing magnetism into a 3D topological insulator, this interplay can generate topological quantum states like the quantum anomalous Hall effect (QAH) or the axion insulator, which can be modified by tuning the magnetization.

Our recent studies consider the MnSb2Te4 compound, a ferromagnet with a perpendicular-to-plane anisotropy and a critical Curie-Weiss temperature as high as 50K. MnSb2Te4 has been controversially discussed to be a magnetic Weyl semimetal or a candidate to realize the axion insulator. We investigated the thickness-dependent properties of exfoliated nanoflakes using magneto-transport, revealing the change in important parameters such as the resistivity, the Curie temperature and the magnetic coercive field. The influence of both the intrinsic electrical doping and disorder in magnetic topological insulators is considered as well.

KFM 28.6 Thu 16:30 H37

Investigation of the magnetic and electronic properties of topological insulator/ferromagnet heterostructures — •Simon Marotzke[1,2], André Philippi-Kobs[1,2], Leonard Müller[1,3], Matthias Kalläne[2], Jens Buck[2], Wojciech Roseker[1], Nils Wind[3], Sanjoy Mahatha[4], Nils Huse[3], Gerhard Grübel[1,3], Martin Beye[1], and Kai Rossnagel[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Christian-Albrechts-Universität zu Kiel, Germany — [3]Universität Hamburg, Germany — [4]Thapar Institute of Engineering and Technology, Patiala, India

Heterostructures of the design Bi_2Se_3/X/Co/Pt, with X = None, Pt, B_4C or B_4C/Pt as separation layer between the topological insulator (TI) and the ferromagnetic overlayer are studied. By means of magneto-optical Kerr effect, the magnetic behaviour is characterised, showing that perpendicular magnetic anisotropy can be achieved in the overlayer and minutely tuned by changing layer properties. In X-ray photoemission spectroscopy measurements, two Bi phases are identified in the heterostructures. By systematically varying the photon energy, the depth, in which the two Bi phases are located, is analysed. Significant differences of the chemical properties at the interface to the TI are found for heterostructures consisting of Bi_2Se_3 with a metallic or insulating overlayer, respectively. Finally, a scheme to invert the heterostructures is presented, potentially enabling angle-resolved photoemission spectroscopy measurements on the TI's surface in future in order to study the influence of the magnetisation state on the TI's surface states.

KFM 28.7 Thu 16:45 H37

Current-induced breakdown of the quantum anomalous Hall effect — •Gertjan Lippertz[1,2], Andrea Bliesener[1], Anjana Uday[1], Lino M.C. Pereira[2], Alexey Taskin[1], and Yoichi Ando[1] — [1]University of Cologne, Cologne, Germany — [2]KU Leuven, Leuven, Belgium

The quantum anomalous Hall (QAH) effect is characterised by zero longitudinal resistivity and quantized Hall resistance without the need of an external magnetic field. However, when reducing the device dimensions or increasing the current density, an abrupt breakdown of the dissipationless state occurs. In this talk, the mechanism of breakdown will be adressed, and the electric field created between opposing chiral edge states will be shown to lie at its origin. Electric-field-driven percolation of two-dimensional charge puddles in the gapped surface states of compensated topological-insulator films is proposed as the most likely cause of the breakdown [1].

Moreover, it was recently reported that the interplay between the 1D chiral edge state and the 2D surface state can give rise to nonreciprocity in the longitudinal resistance [2]. In this talk, it will be shown that the onset of 2D conduction due to breakdown is sufficient to create the nonreciprocal effect, allowing for efficient switching between the dissipationless and nonreciprocal transport regime of the QAH state.

[1] G. Lippertz et al., arXiv:2108.02081 (2021)
[2] K. Yasuda et al., Nat. Nanotechnol. 15, 831-835 (2020)

KFM 28.8 Thu 17:00 H37

Thermal Hall Effect of Magnons in Collinear Antiferromagnets: Signatures of Magnetic and Topological Phase Transitions — •Robin R. Neumann[1], Alexander Mook[2], Jürgen Henk[1], and Ingrid Mertig[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Department of Physics, University of Basel, Basel, Switzerland

While chiral edge states of topological bosons lack clear hallmarks and are difficult to detect, topological electrons can directly be identified by means of the quantized transverse conductivity intrinsic to the quantum anomalous Hall effect. In this talk I consider magnons, the bosonic quanta of collective spin excitations, in a collinear antiferromagnet that is driven from its antiferromagnetic phase via a spin-flop phase to the field-polarized phase by an external magnetic field. Besides the magnetic phase transitions, topological phases occur in the spin-flop and field-polarized phases. To identify these phase transitions, the thermal Hall effect (THE), i. e. the transversal heat transport induced by a longitudinal temperature gradient, is studied across the phase transitions. It is demonstrated that the THE exhibits pronounced signatures of the phase transitions and the temperature tunes the sensitivity to these phase transitions oppositely, allowing for their distinction in transport experiments.

KFM 28.9 Thu 17:15 H37

Topology, Colossal Magnetoresistance, and Complex Magnetic Domains in Eu5In2Sb6 — •Marein Rahn[1,2], Murray N. Wilson[3], Priscila F. S. Thomas[2], Tom Lancaster[3], Filip Ronning[2], and Marc Janoschek[4,5] — [1]IFMP, TU Dresden, 01062 Dresden, Germany — [2]LANL, Los Alamos, New Mexico 87545, USA — [3]Department of Physics, Durham University, Durham, DH1 3LE, UK — [4]Laboratory for Neutron and Muon Instrumentation, Paul Scherrer Institute, CH-5232 Villigen, Switzerland — [5]Physik-Institut, U. Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

The axion insulating state is a paradigm of topological correlated matter which has been particularly difficult to demonstrate in real materials. Using neutron scattering, resonant elastic x-ray scattering, muon spin-rotation and bulk measurements, we demonstrate how the combination of co-planar glide symmetries and large Eu2+ magnetic mo-

ments in the Zintl phase Eu5In2Sb6 produces an unusual two-step ordering process. At 14 K, Eu5In2Sb6 first forms a complex non-collinear weak Ising-ferrimagnet, which we identify as a trivial insulator. Below 7.5 K, this phase is continuously displaced by a growing volume fraction of a compensated antiferromagnetic arrangement that may have axion insulating character. This discovery also implies the presence of a solitonic antiferromagnetic domain structure on the mesoscale, which demonstrably couples to charge transport and, due to the net magnetization of some domains, should be highly susceptible to manipulation. This may open up a platform to engineer interfaces of trivial and non-trivial insulators on the mesoscale.

KFM 28.10 Thu 17:30 H37

Invisible flat bands on a topological chiral edge — •Youjiang Xu, Irakli Titvinidze, and Walter Hofstetter — Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt am Main, Germany

We prove that invisible bands associated with zeros of the single-particle Green's function exist ubiquitously at topological interfaces of 2D Chern insulators, dual to the chiral edge/domain-wall modes. We verify this statement in a repulsive Hubbard model with a topological flat band, using real-space dynamical mean-field theory to study the domain walls of its ferromagnetic ground state. Moreover, our numerical results show that the chiral modes are split into branches due to the interaction, and that the branches are connected by invisible flat bands. Our work provides deeper insight into interacting topological systems.

KFM 29: Multiferroics and Magnetoelectric Coupling (joint session MA/KFM)

Time: Thursday 15:00–16:45 Location: H47

KFM 29.1 Thu 15:00 H47

Fast non-volatile electrical switching of the magnetoelectric domain states in the cubic spinel Co_3O_4 — •Maximilian Winkler, Somnath Ghara, Korbinian Geirhos, Lilian Prodan, Vladimir Tsurkan, Stephan Krohns, and Istvan Kezsmarki — Universität Augsburg, Augsburg, Deutschland

Here, we investigate the magnetoelectric effect of Co_3O_4 at temperatures far below the Neel-temperature of T_N = 30K. A large magnetoelectric coefficient of up to 14ps/m is achieved if the system is cooled through TN while magnetic and/or electric fields are applied. According to these poling procedures we provide a systematic analysis of how the magnetoelectric domain state can be controlled and even in situ switched by reversing the direction of either the electric or the magnetic field. The complete switching of the antiferromagnetic state is found to be faster than microseconds. Altogether, the control of the magnetoelectric domains and the fast switching dynamics makes the linear magnetoelectric coupling of Co_3O_4 highly interesting for spintronics.

KFM 29.2 Thu 15:15 H47

Contribution of charge and strain coupling in artificial multiferroic Fe3O4/PMN-PT heterostructures — •Patrick Schöffmann[1,2], Anirban Sarkar[2], Mai H. Hamed[2], Tanvi Bhatnagar-Schöffmann[3], Sabine Pütter[4], Philippe Ohresser[1], Brian J. Kirby[5], Alexander J. Grutter[5], Juri Barthel[6], Emmanuel Kentzinger[2], Annika Stellhorn[2], Martina Müller[7], and Thomas Brückel[2] — [1]Synchrotron SOLEIL, France — [2]Forschungszentrum Jülich GmbH, JCNS-2 and PGI-4, JARA-FIT, Germany — [3]Centre de Nanoscience et de Nanotechnologies, CNRS, Université Paris-Saclay, France — [4]Forschungszentrum Jülich GmbH, JCNS@MLZ, Germany — [5]NIST Center for Neutron Research, USA — [6]Forschungszentrum Jülich GmbH, ER-C-2, Germany — [7]Fachbereich Physik, Universität Konstanz, Germany

To be able to develop denser and faster data storage and computing solutions artificial multiferroic heterostructures are a promising approach, as they enable direct switching of magnetic states with voltage. We grow ferrimagnetic Fe3O4 thin films on ferroelectric PMN-PT substrates to study the effect of strain and polarisation induced by the substrate onto the magnetic properties of the film. We found that the coupling due to strain and charge is strongly dependent on the orientation of the sample in an external magnetic field as well as the substrate cut. We will present a simple model to explain the contribution of strain and charge for different substrate and magentic field orientations.

KFM 29.3 Thu 15:30 H47

Microscopic theory of the THz modes and their nonreciprocal directional dichroism in the antiferromagnet Fe2Mo3O8 — •Kirill Vasin[1,2], Alexey Nurmukhametov[2], Mikhail Eremin[2], Anna Strinic[1], Lilian Prodan[1], Vladimir Tsurkan[1], István Kézsmárki[1], and Joachim Deisenhofer[1] — [1]Augsburg University, Augsburg, Germany — [2]Kazan, Russia

In the present work, the transmission measurements of a polar dielectric Fe2Mo3O8 were performed by THz time-domain spectroscopy. The origin of the low-lying excitations is not clear, but they were assigned to electromagnons and magnons due to their appearance below TN.

Our microscopic model successfully describes the origin of the optical excitation spectrum in a broad frequency range from the THz to the near-infrared frequency range and the observed dichroism of the low-lying optical modes because of the on-site excitations of the Fe2+ ions in this material. We used the technic of the effective Hamiltonian, including the effects of the crystal field, superexchange interaction and spin-orbit coupling, to model the level schemes of Fe ions projected on the ground configuration of 3d6 electrons.

The directional dichroism in Fe2Mo3O8 can be described by the interference of magnetic and electric-dipole matrix elements, which depend on the applied magnetic field. Our modelled results agrees to the acquired experimental data.

KFM 29.4 Thu 15:45 H47

Magnetization reversal through an antiferromagnetic state — •Somnath Ghara[1], Evgenii Barts[2], Kirill Vasin[1], Dmytro Kamenskyi[1], Lilian Prodan[1], Vladimir Tsurkan[1], Maxim Mostovoy[2], Istvan Kezsmarki[1], and Joachim Deisenhofer[1] — [1]Experimentalphysik V, University of Augsburg, Augsburg, Germany — [2]University of Groningen, Groningen, The Netherlands

The polar magnet $Fe_2Mo_3O_8$ has recently attracted tremendous interests due its versatile properties, such as magnetoelectric effect and giant thermal hall effect. This compound has a polar hexagonal (space group $P6_3mc$) structure at room temperature and undergoes a collinear antiferromagnetic ordering of Fe^{2+} moments below T_N = 60 K, accompanied by a large electric polarization besides that of the structural origin. Upon application of (high) magnetic field, a metamagnetic transition from the antiferromagnetic to a ferrimagnetic state takes place. The ferrimagnetic state can also be stabilized by partially substituting Fe^{2+} ions by Zn^{2+} ions. The magnetic symmetry ($6m'm'$) of the ferrimagnetic state is compatible with a linear magnetoelectric effect. In this talk, I will show that at the coercive field of the isothermal reversal of a ferrimagnetic state in $Fe_{1.86}Zn_{0.14}Mo_3O_8$ the pristine antiferromagnetic state re-emerges as a metastable state. The reappearance of the antiferromagnetic state, supported by the theoretical calculations, is reflected in a large change of electric polarization and directly established by the reoccurrence of the characteristic low-energy THz excitation of the AFM state.

KFM 29.5 Thu 16:00 H47

Transfer of a domain pattern between ferroic orders — •Yannik Zemp[1], Ehsan Hassanpour[1], Yusuke Tokunaga[2], Yasujiro Taguchi[3], Yoshinori Tokura[3], Thomas Lottermoser[1], Manfred Fiebig[1], and Mads C. Weber[1,4] — [1]Department of Materials, ETH Zurich — [2]University of Tokyo — [3]Riken CEMS, Japan — [4]IMMM, Université Le Mans

In multiferroic materials with two ferroic orders, the order parameters and their respective domain patterns may be rigidly coupled or completely independent, with both of these cases having their merits. We show that in materials with three ferroic order parameters, unusual combinations of coupling and independence are possible. One such material is $Dy_{0.7}Tb_{0.3}FeO_3$. Here, an antiferromagnetic order of the rare earth ions (L) and a ferromagnetic order of the iron ions (M) induce an electric polarisation (P) and a trilinear coupling term

$M \cdot L \cdot P$ contributes to the free energy. This coupling term dictates that a reversal of one order parameter needs to be compensated by the product of the other two order parameters to minimise the free energy. Using this fact, we show that a domain pattern in M can be transferred to P while erasing it in the original order parameter, and vice versa, by the application of magnetic and electric fields. We measure the P and M patterns independently by optical second harmonic generation imaging and Faraday rotation microscopy, respectively. The third order parameter L acts as the "memory buffer" for the transfer. The presented work demonstrates the significance of exploration in multiferroics beyond a bilinear coupling.

KFM 29.6 Thu 16:15 H47

Magnetoelectric domains and topological defects in hexagonal manganites — •M. Giraldo, Q. N. Meier, A. Bortis, D. Nowak, N. A. Spaldin, M. Fiebig, M. C. Weber, and Th. Lottermoser — Department of Materials, ETH Zurich

Domains and domain walls reflect the different interdependence of magnetic and electric order in multiferroics. For example, in type-II multiferroics, magnetic and electric domain patterns are one-to-one linked, whereas in type-I multiferroics, magnetic and electric domain morphologies can be different, and their coupling no longer mandatory. We show – using experiment and theory – that multiferroics with separately emerging magnetic and electric order can have a strong bulk magnetoelectric coupling even though the leading magnetoelectric cross-coupling is symmetry-forbidden. We show, taking ErMnO3 as example, that the structural distortions that lead to the ferroelectric polarization also break the balance of the competing superexchange contributions. The resulting bulk coupling leads to novel types of topological defects, like magnetoelectric domain walls and multifold vortex-like singularities. We argue that the apparent independence of magnetic and electric orders in type-I multiferroics leads to uncommon phenomena, not open to the type-II class, which can open additional degrees of freedom for the future control of their magnetoelectric functionality [1].

[1] M. Giraldo, Q.N. Meier, A. Bortis et al. Magnetoelectric coupling of domains, domain walls and vortices in a multiferroic with independent magnetic and electric order. Nat Commun 12, 3093 (2021).

KFM 29.7 Thu 16:30 H47

Measuring Antiferromagnets with a SQUID Setup in Magnetically Shielded Environments — •Michael Paulsen[1], Jörn Beyer[1], Michael Fechner[2], Ralf Feyerherm[3], Klaus Kiefer[3], Bastian Klemke[3], Julian Lindner[3], and Dennis Meier[4] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg, Germany — [3]Helmholtz-Zentrum Berlin, Berlin, Germany — [4]Norwegian University of Science and Technology, Trondheim, Norway

Antiferromagnets possess zero net dipole magnetization. While predictions of higher order magnetizations have been made for Cr_2O_3, few confirmed measurements exist. In this contribution, we present low-temperature measurements gained on different systems with antiferromagnetic order in very low magnetic backgrounds using a dedicated SQUID setup. In particular, we discuss our results on exterior quadrupolar magnetic fields and relate the distinct quadrupolar magnetic signals to the microscopic spin arrangement in our model systems.

KFM 30: Skyrmions 3 (joint session MA/KFM)

Time: Friday 9:30–12:45 Location: H37

KFM 30.1 Fri 9:30 H37

Emergence of zero-field non-synthetic single and catenated antiferromagnetic skyrmions in thin films — •Amal Aldarawsheh[1,2], Imara Lima Fernandes[1], Sascha Brinker[1], Moritz Sallermann[1], Muayad Abusaa[3], Stefan Blügel[1], and Samir Lounis[1,2] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany — [3]Department of Physics, Arab American University, Jenin, Palestine

Antiferromagnetic (AFM) skyrmions are envisioned as ideal topological magnetic bits in future information technologies. In contrast to ferromagnetic (FM) skyrmions, they are immune to the skyrmion Hall effect, might offer potential terahertz dynamics [1] while being insensitive to external magnetic. Although observed in synthetic AFM structures [2], their realization in non-synthetic AFM films has been elusive. Here[3], we unveil their presence in a row-wise AFM Cr film deposited on PdFe bilayer grown on fcc Ir(111) surface. Using first-principles, we demonstrate the emergence of single and catenated AFM skyrmions, which can coexist with the rich inhomogeneous exchange field, including that of FM skyrmions, hosted by PdFe. Besides the identification of an ideal platform of materials for intrinsic AFM skyrmions, we anticipate the uncovered solitons to be promising building blocks in AFM spintronics. -Work funded by (BMBF-01DH16027) [1] Gomonay et al., Nat. Physics 14, 213 (2018). [2] Legrand et al., Nat. Materials 19, 34 (2020). [3] Aldarawsheh et al., ArXiv:2202.12090 (2022).

KFM 30.2 Fri 9:45 H37

Chiral standing spin waves in 3D skyrmion lattice — •Andrii Savchenko[1,2], Vladyslav Kuchkin[1], Filipp Rybakov[3,4], Stefan Blügel[1], and Nikolai Kiselev[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Donetsk Institute for Physics and Engineering, National Academy of Sciences of Ukraine, 03028 Kyiv, Ukraine — [3]Uppsala University, SE-75120 Uppsala, Sweden — [4]KTH Royal Institute of Technology, SE-10691 Stockholm, Sweden

The resonance excitations of the three-dimensional skyrmions lattice in the finite thickness plate of an isotropic chiral magnet were studied using spin dynamics simulations. We calculated the absorption spectra and resonance mode profile configurations for the cases of in-plane and out-of-plane excitations. These results differ from those predicted by the two-dimensional model and the model of the unconfined bulk crystal. In the case of in-plane excitation, absorption spectra dependencies on film thickness have the periodic zones with fading intensity. This effect can be explained by the formation of chiral standing spin waves, which, contrary to conventional standing spin waves, are characterized by the helical profile of dynamic magnetization of fixed chirality defined by the Dzyaloshinskii-Moriya interaction [1]. The chiral standing spin waves are localized in the inter-skyrmion area or the skyrmion core. Under out-of-plane excitation, the absorption spectrum also demonstrates the appearance of standing spin waves, which are localized in the skyrmion shell. 1. A.S. Savchenko et al, arXiv:2205.05466

KFM 30.3 Fri 10:00 H37

Generalization of the collective variables approach for skyrmion strings. — •Volodymyr Kravchuk[1,2] and Markus Garst[1] — [1]Karlsruhe Institute of Technology, Germany. — [2]Bogolyubov Institute for Theoretical Physics, Kyiv, Ukraine

In a bulk saturated chiral magnet, the skyrmion core penetrates the ferromagnet volume forming a string-like object [1]. Here we describe the small-amplitude dynamics of the string, applying the generalized collective variable approach. For the collective variables, we use the coordinate- and time-dependent string position defined as the first moment of topological charge calculated for the continuously stacked horizontal cross-sections perpendicular to the applied magnetic field. The simplest "plane-wave" solution corresponds to the helix-shaped deformation of the string. In a nonlinear regime, this solution is unstable due to the Lighthill criterion, that results in a self-modulation of the wave. Using a multiscale analysis both in space and time, we show that this modulation is captured by a non-linear Schroedinger equation of focusing type. Two classes of non-linear periodic waves of skyrmion string (so-called dc- and cn-waves) are analytically predicted and numerically verified. The separatrix soliton solution just corresponds to the solitary wave found previously [1]. The developed approach is generalized for the case of arbitrary meaning of the collective variables. The latter enables us to describe the string excitations of various symmetries, e.g. breathing and elliptical modes in a nonlinear regime.

[1] V. Kravchuk, U. Rößler, J. van den Brink, M. Garst, PRB, 102, 220408(R) (2020).

KFM 30.4 Fri 10:15 H37

Fermi-surface origin of helical single Q-state and skyrmion lattice in centrosymmetric Gd compounds — •Juba Bouaziz[1], Eduardo Mendive-Tapia[1], Stefan Blügel[1], and Julie Staunton[2] — [1]Forschungszentrum Jülich, Germany — [2]University of Warwick, Coventry CV4 7AL, United Kingdom

We show from first principles that cylindrical structures within the Fermi surface are the origin of the single-Q helical state in the $GdRu_2Si_2$ and Gd_2PdSi_3 intermetallic compounds. The geometry of the Fermi surface nesting describes the strength and sign of the underlying pairwise Ruderman-Kittel-Kasuya-Yosida interactions between the Gd moments as the main mechanism. These interactions are quasi-two-dimensional, isotropic within the Gd layers, and provide a transition temperature and helix period in very good agreement with experiment. Using atomistic spin-dynamical simulations, we investigate the effects of magnetic anisotropy and construct a general magnetic phase diagram that explains the stabilization of the $2Q$-skyrmion lattice observed in experiment with applied magnetic fields.

Funding: ERC Grant No. 856538 (project "3D MAGiC"), SPP 2137 "Skyrmionics" (Project No. BL 444/16), UK EPSRC Grant No. EP/M028941/1.

KFM 30.5 Fri 10:30 H37

Non-Abelian Vortices in Magnets — •Filipp Rybakov[1] and Olle Eriksson[1,2] — [1]Uppsala University, Sweden — [2]Örebro University, Sweden

The non-Abelian (non-commutative) topological states in ordered media may exhibit interesting physics emerging from purely topological arguments [1].

Here we show that non-Abelian vortices also can exist in magnets [2]. We give a topological classification of these vortices and reveal their connection with Abelian topological structures, such as usual vortices, merons, skyrmions. We analyze the potential of non-Abelian magnetic vortices for memory devices and emphasize their advantage, since they provide topological protection of all information, rather than individual bits, as in Abelian cases.

[1] N. D. Mermin, Rev. Mod. Phys. 51, 591 (1979).
[2] F. N. Rybakov and O. Eriksson, arXiv:2205.15264 (2022).

KFM 30.6 Fri 10:45 H37

Thermal properties of magnetic skyrmions — •Balázs Nagyfalusi[1], László Udvardi[2,3], and László Szunyogh[2,3] — [1]Wigner Research Center for Physics, Institute for Solid State Physics and Optics, Budapest, Hungary — [2]Budapest University of Technology and Economics, Budapest Hungary — [3]MTA-BME Condensed Matter Research Group, Budapest, Hungary

We have recently implemented metadynamics in Monte Carlo simulation code[1], which has been modified to use the topological charge Q of magnetic skyrmions as collective variable. The free energy can thus be determined as a function of Q and its equilibrium value can be explored as a function of temperature. The knowledge of the free energy $F(Q;T)$ also permits to evaluate the chemical potential μ of the skyrmions.

We investigated the thermal evolution of magnetic skyrmions in a $Pt_{95}Ir_5$/Fe bilayer on Pd(111) and an FePd bilayer on Ir(111) substrate in the presence of a normal-to-plane external magnetic field. The equilibrium number of skyrmions and the phase boundaries are in good agreement with previous studies[2,3]. For the former system we found that Q has a maximum around 60 K and below this temperature this number drops rapidly, while for the later system it freezes in as the skyrmion lattice is a ground state of the system. The slope of $\mu(T)$ also distinguishes the different ground states of the two system.

1. Nagyfalusi *et al.*, Phys. Rev. B 100, 174429 (2019)
2. Rózsa *et al.*, Phys. Rev. B 93, 024417 (2016)
3. Schick *et al.*, Phys. Rev. B 103, 214417 (2021)

KFM 30.7 Fri 11:00 H37

Constructing coarse-grained skyrmion potentials from experimental data with Iterative Boltzmann Inversion — •Jan Rothörl, Yuqing Ge, Maarten A. Brems, Nico Kerber, Raphael Gruber, Fabian Kammerbauer, Takaaki Dohi, Mathias Kläui, and Peter Virnau — Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 9, D-55099 Mainz, Germany

In an effort to understand skyrmion behavior like skyrmion lattice formation [1] or commensurability effects [2], skyrmions are often described as 2D quasi particles on a coarse-grained level evolving according to the Thiele equation. In particular, the interaction potentials are the key missing parameters for predictive modeling of experiments. We apply the Iterative Boltzmann Inversion technique commonly used in soft matter simulations to construct potentials for skyrmion-skyrmion and skyrmion-magnetic material boundary interactions from a single experimental measurement without any prior assumptions of the potential form. We find that the two interactions are purely repulsive and can be described by an exponential function for experimentally relevant micrometer-sized skyrmions. This captures the physics on experimental time and length scales that are of interest for most skyrmion applications and typically inaccessible to atomistic or micromagnetic simulations. [3]

[1] J. Zázvorka et al., Adv. Funct. Mater. 30, 2004037 (2020). [2] C. Song et al., Adv. Funct. Mater. 2010739 (2021) [3] Y. Ge et al., arXiv:2110.14333 [cond-mat.mtrl-sci] (2021)

KFM 30.8 Fri 11:15 H37

Development of a current solver for studying non-linear skyrmion dynamics — •Thorben Pürling[1,2], Daniele Pinna[3], Fabian Lux[4], Jonathan Kipp[1,3], Stefan Blügel[1,3], Abigail Morrison[2,5], and Yuriy Mokrousov[3,4] — [1]Department of Physics, RWTH Aachen University, Aachen, Germany — [2]Institute of Neuroscience and Medicine 6 and Institute for Advanced Simulation 6 and JARA BRAIN Institute I, Jülich Research Centre, Jülich, Germany — [3]Peter Grünberg Institute 1 and Institute for Advanced Simulation 1, Forschungszentrum Jülich and JARA, Jülich, Germany — [4]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany — [5]Computer Science 3 - Software Engineering, RWTH Aachen University, Aachen, Germany

Transport phenomena in skyrmionic textures have recently gained attention owing to possible applications in spintronics and in cognitive computing. While the reservoir computing aspect of skyrmions relies heavily on their nonlinear response properties, little is known about the real-space distribution of the current density that reflects the nontrivial structure of the local conductivity tensor of these complex objects. Here we report on the development of a method that provides the local current distribution for arbitrary spin textures under bias, and apply that method to study the current distribution of isolated skyrmions. We address the importance of diagonal and Hall components of the conductivity tensor for the current distribution and discuss possible relevance of our findings to reservoir computing applications.

KFM 30.9 Fri 11:30 H37

Atomistic spin simulations of electric-field assisted nucleation and annihilation of magnetic skyrmions — •Moritz A. Goerzen[1], Stephan v. Malottki[1,4], Grzegorz J. Kwiatkowski[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, Reykjavík, Iceland — [3]St. Petersburg, Russia — [4]Thayer School of Engineering, Dartmouth College, Hannover, USA

We demonstrate electric-field assisted thermally activated writing and deleting of magnetic skyrmions in ultrathin transition-metal films. We apply an atomistic spin model which is parameterised from density functional theory (DFT) calculations for a Pd/Fe bilayer on the Ir(111) surface for electric fields of $\mathcal{E} = 0, \pm 0.5$ V/Å. Based on harmonic transition-state theory [1,2], we calculate the transition rates for skyrmion nucleation and annihilation. Using these rates we quantify the probability for electric-field assisted deleting and writing of skyrmions by means of Master equations. The magnetic-field dependent skyrmion probability can be directly related to the free energy differences of the skyrmion and the ferromagnetic state and resembles a Fermi-Dirac distribution function. The obtained probability function at opposite electric fields is in striking agreement with experimental results [3].

[1] Bessarab *et al.*, Sci. Rep. **8**, 3433 (2018)
[2] von Malottki *et al.*, Phys. Rev. B **99**, 060409 (2019)
[3] Romming *et al.*, Science **341**, 636 (2013)

KFM 30.10 Fri 11:45 H37

Strain and electric field control of magnetic skyrmions in Fe3GeTe2 van der Waals heterostructures — •Dongzhe Li[1], Soumyajyoti Haldar[2], and Stefan Heinze[2] — [1]CEMES, Université de Toulouse, CNRS, 29 rue Jeanne Marvig, F-31055 Toulouse, France — [2]Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstrasse 15, 24098 Kiel, Germany

Magnetic skyrmions are topologically protected chiral spin structures with particle-like properties, which are often induced by the

Dzyaloshinskii-Moriya interaction (DMI). The recent discovery of truly two-dimensional (2D) magnetic materials opened up new opportunities for exploring magnetic skyrmions in atomically thin vdW materials. Here, using density functional theory and atomistic spin simulations, we predict the emergence of a large DMI in 2D vdW heterostructures where a 2D ferromagnetic metal Fe3GeTe2 monolayer is deposited on a nonmagnetic vdW layer. In particular, the DMI turns out to be highly tunable by strain and electric-field, leading to giant DMI comparable to that of ferromagnetic/heavy metal interfaces, which have been recognized as prototype multilayer systems to host skyrmion states. Our atomistic spin simulations further show that the efficient control of the DMI, the exchange coupling, and the magnetic anisotropy energy by strain, lead to the stabilization of isolated skyrmions.

KFM 30.11 Fri 12:00 H37

Resonant optical Hall conductivity from skyrmions — •Sopheak Sorn[1], Luyi Yang[2], and Arun Paramekanti[3] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department of Physics, Tsinghua University, Beijing, China — [3]Department of Physics, University of Toronto, Toronto, Canada

Metallic magnets hosting topological skyrmions exhibit the topological Hall effect, which arises from a real-space Berry-phase mechanism, and it has been used as an indirect signature of skyrmions in transport experiments. This talk will focus on the less explored impact of skyrmions on optical Hall conductivity which is studied using a two-dimensional model of conduction electrons coupled to a background skyrmion spin texture via an effective Hund's coupling. For a skyrmion crystal, a Kubo-formula calculation reveals a resonant feature in the optical Hall response at a frequency set by the Hund's coupling. A linear relation between the area under the Hall resonant curve and the skyrmion density is discovered numerically and is further elucidated in a gradient expansion analysis. The presence of the resonance is robust, persisting in a system with an isolated skyrmion and even in a three-site system hosting a trimer of noncoplanar spins, which implies the indispensable role of the local noncoplanarity. Our results suggest that the resonance can be used as a basis for a magneto-optical Kerr microscopy for visualizing skyrmions.

KFM 30.12 Fri 12:15 H37

Artificial neuron based on a magnetic biskyrmion — •Ismael Ribeiro de Assis, Börge Göbel, and Ingrid Mertig — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

Skyrmionics and neuromorphics are among the most promising fields of physics with the perspective of creating future devices and technologies. Magnetic skyrmions are extremely stable and can be moved by currents which has lead to the prediction of a skyrmion-based artificial neuron [1]: When a skyrmion is pushed by current pulses, it will eventually reach a designated location and can be detected electrically. This resembles the excitation process of a neuron that fires ultimately. However, a realistic refractory process has not been achieved, so far, for such a device. The skyrmion-based neuron would keep on firing when more current pulses are applied which renders this device not useful.

In this talk we suggest that a biskyrmion solves this major issue. The attractive interaction of the two partially overlapping skyrmions and their skyrmion Hall effects lead to a unique trajectory when they are driven by current pulses: The two subskyrmion move along opposite directions to the two designated detection areas where they reverse their direction of motion until they come back and eventually reestablish the biskyrmion. During the second period the skyrmion cannot fire again. Our suggested device resembles the response of a biological neuron better than all existing skyrmion-based devices so far.

[1] S. Li et al., Nanotechnology 28, 31LT01 (2017)

KFM 30.13 Fri 12:30 H37

Magnetoelastic surface states of skyrmion textures — •Lars Franke and Markus Garst — Institute for Theoretical Solid State Physics, Karlsruhe Institute for Technology, Germany

At the surface of chiral magnets uncompensated Dzyaloshinskii-Moriya interaction modifies the boundary conditions for the magnetization resulting in a so-called a surface twist. Consequently, skyrmions are expected to change their helicity from Bloch-like within the bulk of the chiral magnet to Néel-like close to the surface [1]. Resonant elastic X-ray scattering experiments [2] have confirmed this predicted change of helicity close to the surface, but the experimentally observed penetration depth was found to be an order of magnitude larger than theoretically expected. In order to account for this discrepancy, we investigate theoretically the influence of a magnetoelastic coupling on the surface twist. Analytical calculations are complicated by broken translational invariance and nontrivial boundary conditions at the surface. However, as in the uncoupled system the length scale for helicity variations is already encoded in the bulk equation. We demonstrate how to extract the length scale from a perturbative approach. The validity of these calculations is checked using micromagnetic simulations, extended with magnetoelastic coupling, of the complete surface state including boundary conditions.

[1] Three-dimensional skyrmion states in thin films of cubic helimagnets, F. N. Rybakov et al. Phys. Rev. B 87, 094424 (2013).

[2] Reciprocal space tomography of 3D skyrmion lattice order in a chiral magnet, S. Zhang et al. PNAS 201803367 (2018).

KFM 31: Electrical, Dielectrical and Optical Properties of Thin Films (joint session CPP/KFM)

Time: Friday 11:30–12:30 Location: H38

KFM 31.1 Fri 11:30 H38

Mechanical nanoscale polarization switching in ferroelectric polymer films — •Kathrin Dörr, Martin Koch, Diana Rata, and Robert Roth — MLU Halle-Wittenberg

Ferroelectric polymer films offer strong advantages like mechanical flexibility, biocompatibility, optical transparency and low-cost processing. However, their dielectric or piezoelectric performance is often inferior to that of oxide ferroelectric materials. Key to that is the electric dipolar order which is naturally lower in semicrystalline polymers than in crystalline ferroelectrics. We introduce the reorientation and alignment of the electric polarization in thin films utilizing the mechanical effect of an unbiased scanning force microscopy tip, providing a versatile tool for nanoscale domain writing [1]. Thin films (50 - 150 nm) of P(VDF-TrFE) (78:22) on graphite were prepared with dense (110)-oriented beta-phase lamellae randomly oriented in the film plane. Domain patterns with resolution down to 50 nm have been written with four (out of six possible) local polarization orientations. Written domains show excellent long-time stability. We discuss a ferroelastic origin of the mechanical polarization switching and make suggestions for how to utilize the domain patterns in thin film devices. [1] Adv. Electron. Mater. 2022, 2101416

KFM 31.2 Fri 11:45 H38

In-situ investigations of morphology degradation and oxidation level changes in EMIM DCA post-treated PEDOT:PSS thin films upon external influence — •Anna Lena Oechsle[1], Julian E. Heger[1], Nian Li[1], Shanshan Yin[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]ELETTRA, 34149 Basovizza TS, Italy — [3]MLZ, TU München, 85748 Garching

Nowadays thermoelectric generators are considered a promising technique for heat waste recovery as they enable a direct conversion of a temperature gradient into electrical power. Especially, organic thermoelectric polymers are attractive, owning some advantages like low cost, lightness and high mechanical flexibility, low or no toxicity, as well as a usually low thermal conductivity. In our work we show the positive effect of ionic liquid (IL) treatment on the thermoelectric properties, Seebeck coefficient and electrical conductivity, of semi-conducting PEDOT:PSS thin films. Furthermore with different in-situ experiments like GISAXS (grazing incidence small angle x-ray scattering), UV-Vis, and conductivity measurements we examine the inner film morphology and oxidation level changes upon operation at different ambient conditions.

KFM 31.3 Fri 12:00 H38

Improvement of TE properties of PEDOT:PSS films via DMSO addition and DMSO/salt post-treatment resolved

from a fundamental view — •Suo Tu[1], Ting Tian[1], Anna-Lena Oechsle[1], Shanshan Yin[1], Xinyu Jiang[1], Wei Cao[1], Nian Li[1], Manuel A. Reus[1], Lennart K. Reb[1], Shujin Hou[2], Aliaksandr S. Bandarenka[2], Matthias Schwartzkopf[3], Stephan V. Roth[3], and Peter Müller-Buschbaum[1,4] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]TU München, Physik-Department, Physik der Energiewandlung und -speicherung, 85748 Garching — [3]DESY, 22607 Hamburg — [4]MLZ, TU München, 85748 Garching

The combination of DMSO-solvent doping and physical-chemical DMSO/salt de-doping in a sequence has been used to improve the thermoelectric PEDOT:PSS films. The initial DMSO-doping treatment induces a distinct phase separation by facilitating the aggregation of the PEDOT molecules. At the same time, the subsequent DMSO/salt de-doping post-treatment strengthens the selective removal of the surplus non-conductive PSS chains. Substantial alterations in the oxidation level, chain conformations, PEDOT crystallites and their preferential orientation are observed upon treatment on the molecular level. At the mesoscale level, the purification and densification of PEDOT-rich domains enable the realization of inter-grain coupling by the formation of the electronically well-percolated network. Thereby, both electrical conductivity and Seebeck coefficient are optimized.

KFM 31.4 Fri 12:15 H38

Exciton dynamics in surface-mounted metal-organic frameworks: A femtosecond transient absorption study — •Vipilan Sivanesan[1], Martin Richter[1], Debkumar Rana[1], Ritesh Haldar[2], Christoph Wöll[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — [2]Institute of Functional Interfaces, Karlsruhe Institute of Technology, Germany

For the optimization of organic optoelectronic devices, it is important to understand the ultrafast electronically excited state dynamics in organic semiconductors after optical excitation. For instance, different molecular packing and relative orientations of the optically active chromophores can affect the excitonic coupling strength. This can be studied in crystalline molecular assemblies by integrating these chromophores into surface-mounted metal-organic frameworks (SURMOFs) as organic linkers. Varying the side-groups of the molecules enables to engineer the crystal structure to tune the excitonic coupling. To analyse the influence of this crystal engineering on the ultrafast dynamics we investigated thin films of chromophore functionalized Zn-SURMOF by means of femtosecond transient absorption.