

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 E 124, EMH 025, and EMH 225; Poster E)

Invited Talks

KFM 10.1	Tue	9:30–10:00	E 124	Exploring of the accumulation and thermal annealing of radiation defects in metal oxides via optical absorption, EPR and luminescence methods — •ALEKSANDR LUSHCHIK
KFM 11.5	Tue	11:10–11:40	EMH 225	Optical Formation and Manipulation of Topological Polar Superlattices — •JOHN FREELAND
KFM 17.1	Wed	15:00–15:30	EMH 225	Reversible and irreversible heat effects in batteries and battery materials — •ANDREAS JOSSEN
KFM 23.1	Thu	9:30–10:00	E 124	The Research Center FLAIR: Fermi Level Engineering of Oxide Electroceramics — •ANDREAS KLEIN
KFM 23.6	Thu	11:20–11:50	E 124	Designing Transition Metal Oxynitrides for Photoelectrochemical Applications — •VERENA STREIBEL, LAURA I. WAGNER, JOHANNA L. SCHÖNECKER, ELISE SIROTTI, JOHANNA EICHHORN, SASWATI SANTRA, IAN D. SHARP
KFM 24.1	Thu	9:30–10:00	EMH 225	Ion transport in battery electrolytes and related interphases — •JELENA POPOVIC-NEUBER
KFM 28.1	Thu	15:00–15:30	EMH 225	Every (ferroelectric) wall is a door - exploring the links between structure, dynamics, and emergent functionalities — •PATRYCJA PARUCH

Invited Talks of the joint Symposium Three-Dimensional Nanostructures: From Magnetism to Superconductivity (SYMS)

See SYMS for the full program of the symposium.

SYMS 1.1	Mon	9:30–10:00	H 0105	3D Racetrack Memory — •STUART PARKIN
SYMS 1.2	Mon	10:00–10:30	H 0105	Curved electronics: geometry-induced effects at the nanoscale — •PAOLA GENTILE
SYMS 1.3	Mon	10:30–11:00	H 0105	Curvilinear micromagnetism — •DENYS MAKAROV
SYMS 1.4	Mon	11:15–11:45	H 0105	Study of 3D superconducting nanoarchitectures — •ROSA CÓRDOBA
SYMS 1.5	Mon	11:45–12:15	H 0105	3D nanoarchitectures for superconductivity and magnonics — •OLEKSANDR DOBROVOLSKIY

Invited Talks of the joint Symposium SKM Dissertation Prize 2024 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H 1012	Nonequilibrium dynamics in constrained quantum many-body systems — •JOHANNES FELDMER
SYSD 1.2	Mon	10:00–10:30	H 1012	Controlled Manipulation of Magnetic Skyrmions: Generation, Motion and Dynamics — •LISA-MARIE KERN
SYSD 1.3	Mon	10:30–11:00	H 1012	Interactions within and between cytoskeletal filaments — •CHARLOTTA LORENZ

SYSD 1.4	Mon	11:00–11:30	H 1012	Field theories in nonequilibrium statistical mechanics: from molecules to galaxies — ●MICHAEL TE VRUGT
SYSD 1.5	Mon	11:30–12:00	H 1012	Lightwave control of electrons in graphene — ●TOBIAS WEITZ

Invited Talks of the joint Symposium Synergistic Imaging Techniques: From Spins and Atoms to Ferroic Domains (SYSA)

See SYSA for the full program of the symposium.

SYSA 1.1	Mon	15:00–15:30	H 0105	Imaging with coherent soft X-rays — ●BASTIAN PFAU
SYSA 1.2	Mon	15:30–16:00	H 0105	Exploring ferroelectric domains and domain wall dynamics with quantitative STEM — ●MARTA D. ROSSELL
SYSA 1.3	Mon	16:00–16:30	H 0105	Scanning Oscillator Piezoresponse Microscopy: new tools to explore domain wall dynamics — ●NEUS DOMINGO, SHIVA RAGHURAMAN, RALPH BULANADI, PATRYCJA PARUCH, STEPHEN JESSE
SYSA 1.4	Mon	16:45–17:15	H 0105	Imaging probe nuclei environments using perturbed angular correlation spectroscopy: Examples from multiferroic BiFeO₃ — ●DORU C. LUPASCU, THIEN THANH DANG, GEORG MARSCHICK, MARIANELA ESCOBAR, ASTITA DUBEY, IAN YAP CHANG JIE, JULIANA HEINIGER-SHELL
SYSA 1.5	Mon	17:15–17:45	H 0105	Exploring antiferromagnetic order at the nanoscale with a single spin microscope — ●VINCENT JACQUES, AUREORE FINCO

Invited Talks of the joint Symposium Advances in Ab-Initio Electronic Structure Theory of Time-Dependent and Non-Equilibrium Phenomena (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Tue	9:30–10:00	H 0105	Light control of charge transport and phase transitions — ●SHENG MENG
SYES 1.2	Tue	10:00–10:30	H 0105	Probing the transport of the interacting electron-phonon system self-consistently and <i>ab initio</i> — ●NAKIB PROTIK
SYES 1.3	Tue	10:30–11:00	H 0105	In- and out-of-equilibrium ab initio theory of electrons and phonons — ●GIANLUCA STEFANUCCI
SYES 1.4	Tue	11:15–11:45	H 0105	Phonon screening of excitons in semiconductors and insulators from first principles — ●MARINA RUCSANDRA FILIP
SYES 1.5	Tue	11:45–12:15	H 0105	Light-matter control of quantum materials: from Floquet to cavity engineering — ●MICHAEL SENTEF

Sessions

KFM 1.1–1.4	Sun	16:00–18:15	H 1028	Tutorial: Exploring Ferroic Materials: From Modelling to Imaging Techniques (joint session KFM/TUT)
KFM 2.1–2.3	Mon	9:30–10:30	EMH 025	High-resolution Lithography and 3D Patterning
KFM 3.1–3.6	Mon	9:30–11:30	EMH 225	Focus Session: (Multi-)Ferroic States I
KFM 4.1–4.12	Mon	9:30–13:00	EW 203	Perovskite and photovoltaics I (joint session HL/KFM)
KFM 5.1–5.8	Mon	9:30–11:45	A 053	Thin oxides and oxide layers (joint session DS/KFM)
KFM 6.1–6.4	Mon	10:40–12:00	EMH 025	Instrumentation and Methods for Micro- and Nanoanalysis
KFM 7.1–7.5	Mon	11:45–13:00	C 264	Materials for the Storage and Conversion of Energy (joint session MM/KFM)
KFM 8.1–8.3	Mon	12:10–13:10	EMH 025	Microscopy and Tomography with X-ray Photons, Electrons, Ions and Positrons
KFM 9.1–9.40	Mon	18:00–20:00	Poster E	KFM Poster Session
KFM 10.1–10.6	Tue	9:30–12:00	E 124	Diamond and Related Dielectric Materials I
KFM 11.1–11.7	Tue	9:30–12:20	EMH 225	Focus Session: (Multi-)Ferroic States II
KFM 12.1–12.6	Wed	9:30–11:50	EMH 025	Diamond and Related Dielectric Materials II
KFM 13.1–13.8	Wed	9:30–12:30	EMH 225	Focus Session: (Multi-)Ferroic States III
KFM 14.1–14.5	Wed	11:45–13:00	C 230	Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials (joint session MM/KFM)

KFM 15.1–15.11	Wed	15:00–18:00	EB 407	Multiferroics and Magnetoelectric Coupling (joint session MA/KFM)
KFM 16.1–16.6	Wed	15:00–17:10	E 124	Crystal Structure Defects / Real Structure / Microstructure I
KFM 17.1–17.11	Wed	15:00–19:05	EMH 225	Focus Session: Battery Materials – Experimental Characterisation and Safety Testing (joint session KFM/MM)
KFM 18.1–18.7	Wed	15:00–18:00	Poster E	SrTiO₃: A Versatile Material from Bulk Quantum Paraelectric to 2D Superconductor: Poster (joint session TT/KFM/MA/O)
KFM 19.1–19.8	Wed	15:30–18:00	C 130	Topical Session: In Situ and Multimodal Microscopy in Materials Physics (joint session MM/KFM)
KFM 20.1–20.3	Wed	17:15–18:00	C 230	Structurally and Chemically Complex Alloys (joint session MM/KFM)
KFM 21.1–21.7	Thu	9:30–12:45	H 0104	Focus Session: SrTiO₃: A Versatile Material from Bulk Quantum Paraelectric to 2D Superconductor (joint session TT/KFM/MA/O)
KFM 22.1–22.14	Thu	9:30–13:15	EW 203	Perovskite and Photovoltaics II (joint session HL/KFM)
KFM 23.1–23.6	Thu	9:30–11:50	E 124	Focus Session: Fermi level engineering of functional ceramics
KFM 24.1–24.11	Thu	9:30–13:35	EMH 225	Focus Session: Battery Materials – Ion Transport, Impurity Effects and Modelling (joint session KFM/MM)
KFM 25.1–25.5	Thu	11:45–13:00	C 264	Materials for Storage and Conversion of Energy (joint session MM/KFM)
KFM 26.1–26.11	Thu	15:00–18:00	H 0104	SrTiO₃: A Versatile Material from Bulk Quantum Paraelectric to 2D Superconductor II (joint session TT/KFM/MA/O)
KFM 27.1–27.4	Thu	15:00–16:20	EMH 025	Polar oxides: Lithium niobate and lithium tantalate
KFM 28.1–28.7	Thu	15:00–17:45	EMH 225	Focus Session: (Multi-)Ferroic States IV
KFM 29	Thu	18:10–19:00	EMH 225	Members' Assembly
KFM 30.1–30.11	Fri	9:30–12:30	H 0104	SrTiO₃: A Versatile Material from Bulk Quantum Paraelectric to 2D Superconductor III (joint session TT/KFM/MA/O)
KFM 31.1–31.13	Fri	9:30–13:00	EW 203	Perovskite and Photovoltaics III (joint session HL/KFM)
KFM 32.1–32.6	Fri	9:30–11:40	E 124	Crystal Structure Defects / Real Structure / Microstructure II
KFM 33.1–33.8	Fri	9:30–12:25	EMH 225	Focus Session: (Multi-)Ferroic States V

Members' Assembly of the Crystalline Solids and their Microstructure Division

Thursday 18:10–19:00 EMH 225

KFM 1: Tutorial: Exploring Ferroic Materials: From Modelling to Imaging Techniques (joint session KFM/TUT)

Recent developments in the study of ferroic materials have unveiled exciting features, encompassing phenomena such as skyrmions and multiferroic domain walls. This tutorial seeks to provide a comprehensive overview, spanning from fundamental theoretical concepts to advanced imaging techniques. We will learn how these cutting-edge developments now enable the bridging of length scales from the individual atom to the macroscopic understanding of the ferroic ordering.

Organizer: Felix Büttner (Univ. Augsburg), Jan Schultheiß (Univ. of Canterbury) Session Chairs: John Freeland (Argonne National Lab), Manuel Zahn (Univ. Augsburg)

Time: Sunday 16:00–18:15

Location: H 1028

Tutorial KFM 1.1 Sun 16:00 H 1028

Ferroelectric domains, domain walls, symmetry and thermodynamic models — ●JIRI HLINKA — Institute of Physics, Czech Acad. Sci., Prague, Czechia

Properties and applications of the materials with ferroelectric or other kind of ferroic domains separated by domain walls continue to stimulate our desire to image, model and understand these ultimate nanoscale interfaces in more and more details. We aim to present here only the most general theoretical concepts that can be useful in related physics and materials science activities. In this tutorial presentation, also aimed to facilitate the most recent achievements presented at the DPG meeting, we intend to cover the subject mostly from the phenomenological point of view, relying on the symmetry constraints and Ginzburg-Landau theory arguments.

Tutorial KFM 1.2 Sun 16:30 H 1028

Nanoscale ferroelectricity: insights from optical second harmonic generation — ●NIVES STRKALJ — Institute of Physics, Zagreb

Ferroelectric materials are a promising platform for energy-efficient electronic and optical devices. In thin films, relevant for applications, ferroelectricity is highly susceptible to the influence of interfaces through electrostatic and elastic boundary conditions. A large surface-to-volume ratio at the nanoscale thus leads to dramatic changes in polarization direction, magnitude, and domain configuration. However, evaluating ferroelectricity in thin films remains a challenge for conventional techniques because of significant non-ferroelectric contributions. A highly sensitive optical method, second harmonic generation (SHG), can be used to detect polarization in thin films. SHG has thus become an invaluable tool for studying size effects in nanoscale ferroelectrics.

In my talk, I will give an introduction to ferroelectricity, ferroelectric size effects, and approaches to tuning polarization in nanoscale films. I will present insights from SHG into the emergence and evolution of ferroelectricity in thin films. Finally, I will address the use of SHG for tracking polarization during the growth process - in situ - to access transient effects. I will conclude by showing examples of harnessing findings from SHG to engineer desired ferroelectric responses for specific applications.

15 min. break

Tutorial KFM 1.3 Sun 17:15 H 1028

Magnetic imaging with solid-state spin defects — ●VINCENT JACQUES — Laboratoire Charles Coulomb, CNRS and Uni. Montpellier, France

Experimental methods enabling the optical detection of single spins in the solid-state, which were initially developed for quantum information science, open new avenues for the development of highly sensitive quantum sensors. In this context, the electronic spin of a single nitrogen-vacancy (NV) defect in diamond can be used as an atomic-sized magnetometer, providing an unprecedented combination of spatial resolution and magnetic sensitivity, even under ambient conditions. In this talk, I will first introduce the principle of scanning-NV magnetometry and discuss how it can be used as a powerful tool for exploring the physics of ferroic materials. I will then discuss recent efforts in researching alternative material platforms that could expand the range of quantum sensing functionalities offered by diamond, with a focus on hexagonal boron nitride.

Tutorial KFM 1.4 Sun 17:45 H 1028

Exploring Ferroic Materials in 3D using Atom Probe Tomography — ●SHELLY CONROY — Department of Materials, London Centre for Nanotechnology, Imperial College London, London SW7 2AZ, UK

Ferroic materials can contain complex interfaces such as grain boundaries, dislocations, domain walls, and higher order topologies. Even slight changes in chemical composition can result in drastic changes in functionality such as conductivity and magnetism. As the regions of interest are often only a unit cell thick and can meander throughout the bulk material in 3D it is vital to have a characterisation method that can achieve the required spatial resolution in 3D. Atom probe tomography (APT) provides 3D compositional mapping of materials with sub-nanometre spatial resolution. In this tutorial the basics of APT characterisation will be discussed, including how to make samples, how to process APT data and specific examples of APT analysis of ferroic materials. Additionally correlative electron microscopy techniques will be detailed, and how to combine structural with chemical information from both techniques.

KFM 2: High-resolution Lithography and 3D Patterning

Chair: Theo Scherer (KIT Karlsruhe)

Time: Monday 9:30–10:30

Location: EMH 025

KFM 2.1 Mon 9:30 EMH 025

Diffractive Microoptics in Porous Silicon Oxide — ●LEANDER SIEGLE¹, DAJIE XIE², COREY A. RICHARD², PAUL V. BRAUN², and HARALD GIESSEN¹ — ¹4th Physics Institute, University of Stuttgart, Stuttgart, Germany — ²Beckman Institute for Advanced Science and Technology, University of Illinois Urbana-Champaign, Urbana, IL, USA

We demonstrate focusing as well as imaging using diffractive microoptics, manufactured by two-photon polymerization grayscale lithography (2GL) that has been written into porous silicon oxide. While typical doublet lens systems require support structures that hold the lenses in place, our optics are held by the porous media itself, decreasing both the fabrication time and design constraints. Compared to the typical two-photon polymerization fabrication process, 2GL offers better shape accuracy while simultaneously increasing throughput. To showcase 2GL fabricated optics in porous media, we fabricate singlet diffractive lenses with a diameter of 500 μm and numerical apertures of up to 0.6. We measure focusing efficiency and analyze the shape of the system with the 3D fluorescence signal of the photoresist. Furthermore, we design, print, and optimize a doublet lens system for imaging purposes with a thickness below 60 μm and examine the high-resolution imaging performance with a USAF 1951 resolution test chart.

KFM 2.2 Mon 9:50 EMH 025

3D-printed astigmatism-free microendoscope for in-vivo optical coherence tomography in coronary arteries — ●PAVEL RUCHKA¹, ALOK KUSHWAHA², ROUYAN CHEN², SIMON THIELE³, ALOIS HERKOMMER³, ROBERT MCLAUGHLIN², HARALD GIESSEN¹, and JIAWEN LI² — ¹4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — ²School of Electrical and Mechanical Engineering, Australian Research Council Centre of Excellence for Nanoscale BioPhotonics, Institute for Photonics and Advanced Sensing, University of Adelaide, Adelaide, SA 5005, Australia — ³Institute of Applied Optics (ITO) and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany

In the past few years, intravascular microendoscopy gained increasing significance in medical imaging and cardiovascular medicine, as such

diseases are among the biggest causes of death in the world. A fundamental challenge in microendoscopy is the fabrication of a small fiber-optic probe that can achieve similar functions as large complex optics, namely high resolution and extended depth of focus. Moreover, existing methods of fabrication cannot correct astigmatism/nonchromatic aberrations, which arise due to the use of catheter sheets and limit the resolution of at least one axis. Here, we introduce a two-photon 3D-printed lens on an optical fiber for cardiovascular in-vivo endoscopy, forming a Bessel beam with high resolution over a focal length of hundreds of micrometers, corrected for astigmatism arising due to catheter usage, and used for intracoronary imaging in a live pig.

KFM 2.3 Mon 10:10 EMH 025

3D beam-shaping by 3D printed holographic triplet on a fiber — ●ZIHAO ZHANG, LEANDER SIEGLE, PAVEL RUCHKA, and HARALD GIESSEN — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Non-Gaussian beams are crucial for many research areas such as imaging and material processing. To create arbitrary beams, beam-shaping with diffractive and holographic optical elements can be used. For example, beam-shaping for glass cutting provides a number of focus copies at tailored positions in a three-dimensional working space, resulting in precisely controlled energy deposition within a volume of transparent materials. Often these beam-shaping optics are quite complicated and bulky. However, in some specific scenarios there is a demand not only for the miniaturization and simplicity, but also for the ability to adapt and change the focal distribution rather rapidly. Here, we present a beam-shaper triplet, 3D printed on a single-mode fiber using the maskless rapid additive manufacturing technique of two-photon polymerization (2PP). The triplet comprises a collimating diffractive lens, a tailored phase mask, and a focusing lens. As a result, we demonstrate several 3-dimensionally distributed arrays of focal spots produced by such a triplet with tailored phase masks. The triplet which is 3D-printed on a single fiber can easily be adjusted for the desired foci distribution. Our technique can play a crucial role in the miniaturization of beam-shaping setups for laser cutting, imaging, and optical trapping.

KFM 3: Focus Session: (Multi-)Ferroic States I

The focus session is dedicated to (multi)ferroic states at interfaces and in heterostructures. The design of (emergent) properties at interfaces, modelling methods and advanced characterization tools will be of interest. Typical examples may include electrostatic and strain boundary conditions at interfaces, domains and domain walls in (multi)ferroics and applications in nano-electronic device

Chair: Johanna Nordlander (Paul Drude Institute)

Time: Monday 9:30–11:30

Location: EMH 225

KFM 3.1 Mon 9:30 EMH 225

Domain Size Engineering by Grain Scaling in Polycrystalline Hexagonal DyMnO₃ — ●RUBEN DRAGLAND, KATHARINA WOLK, ELVIA CHAVEZ PANDURO, KASPER AAS HUNNESTAD, JAN SCHULTHEISS, and DENNIS MEIER — Norwegian University of Science and Technology (NTNU), Trondheim, Norway

Controlling the density and distribution of ferroelectric domain walls is essential for the development of domain wall electronics, giving intriguing opportunities for continued downscaling of active electronic components. The microstructure is a vital parameter for domain engineering, and a proportional relation between grain and domain size is established. However, inversely proportional domain scaling has been observed in ErMnO₃, while domain-microstructure relations in other polycrystalline systems of the hexagonal manganite family remains to be explored.

Here, the domain structure in a hexagonal DyMnO₃ polycrystal is investigated, exhibiting a non-uniform grain size distribution which is attributed to the material's propensity to crystallize in the orthorhombic phase. By systematically quantifying the domain sizes during post-

processing, inverted scaling of domain size with grain size is observed, identifying the inverse scaling as an intrinsic phenomenon, effectively ruling out processing and heat treatment as the main origin. The observed impact of non-uniform grain sizes on the domain structure is of interest to understand the complex nanoscale domain physics in ferroelectric polycrystals, and reveals new opportunities for tuning their macroscopic response towards broader time scales.

KFM 3.2 Mon 9:50 EMH 225

The three-dimensional multiferroic domain structure of hexagonal manganites — LUKAS HECKENDORF, ●AARON MERLIN MÜLLER, MANFRED FIEBIG, and THOMAS LOTTERMOSER — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

We simulate and visualize the three-dimensional domain structure and associated topological features of multiferroic hexagonal manganites. Due to the improper nature of their ferroelectric order, hexagonal manganites exhibit unconventional six-fold vortices in their ferroelectric domain patterns. In 3D, these domain patterns are characterized by vortex lines, which are 1D topological defects that form loops in bulk

materials. Below the Néel temperature, an additional antiferromagnetic order rigidly coupled with the ferroelectric order emerges, forming vortex domain patterns of its own. In our simulations, we observe new types of antiferromagnetic three-fold, four-fold and six-fold vortex lines in addition to ferroelectric six-fold vortex lines. We relate the existence of these vortex lines to the rigid coupling between orders. Our numerical investigation is performed with a phase-field model to simulate the domain structure in three dimensions using a Landau-free-energy expansion.

KFM 3.3 Mon 10:10 EMH 225

Suppression of ferroelectric transition in hexagonal manganites — ●SOUJANYA MADASU and ARKADIY SIMONOV — Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Hexagonal manganites are an interesting class of multiferroics where the improper nature of ferroelectricity induces a structural crosstalk between high temperature polarization and low temperature frustrated antiferromagnetic.

In this talk, we will be addressing methods to suppress ferroelectric transition caused by the *up-up-down* cation displacement of hexagonal manganites through doping on the A site. This suppression of ferroelectric states destroys the template for low temperature antiferromagnetic ordering of Mn spins and thus frustrates the magnetic transition. We study this structural evolution by subjecting the doped manganites to various annealing conditions and then measure their low temperature magnetic behaviour. Finally, we compare experimental observations with theoretical considerations to analyze the magnetic properties and structure of these hexagonal manganites.

KFM 3.4 Mon 10:30 EMH 225

Reversible domain wall displacement in ferroelectric ErMnO_3 — ●MANUEL ZAHN^{1,2}, KYLE KELLEY³, AARON M. MÜLLER⁴, SABINE M. NEUMEYER³, THOMAS LOTTERMOSER⁴, SERGEI V. KALININ⁵, NEUS DOMINGO³, ISTVÁN KÉZSMÁRKI¹, DENNIS MEIER², and JAN SCHULTHEISS² — ¹University of Augsburg, Augsburg, Germany — ²Norwegian University of Science and Technology (NTNU), Trondheim, Norway — ³Oak Ridge National Laboratory, Oak Ridge, USA — ⁴ETH Zurich, Zurich, Switzerland — ⁵University of Tennessee, Knoxville, USA

Many of the intriguing characteristics of ferroelectric materials arise from the physical responses at the level of the domains. In conventional ferroelectric systems, such as like $\text{Pb}(\text{Zr,Ti})\text{O}_3$, BaTiO_3 , and LiNbO_3 , polarization reversal between monodomain states takes place through a nucleation and growth process. Different from these systems, hexagonal manganites (RMnO_3 , $R = \text{Sc, Y, In, and Dy-Lu}$) host topological meeting points of domain walls that cannot be erased, giving rise to a fundamentally different switching behavior. Here, we explore the confined switching dynamics of ferroelectric domains in ErMnO_3 , using band-excitation piezoresponse force microscopy (BE-PFM). Our measurements reveal reversible local displacement of ferroelectric walls induced by the electric field. Interestingly, we observe a continuous breathing-like mode of the domains when cycling the electric field. Our study provides new insights into the dynamics of the topologically protected domains and expands previous switching

studies towards the domain level.

KFM 3.5 Mon 10:50 EMH 225

Current distribution in simple ferroelectric domain-wall-based devices — ●LEONIE RICHARZ¹, JIALI HE¹, KONSTANTIN SHAPOVALOV², EDITH BOURRET³, ZEWU YAN^{3,4}, ANTONIUS T.J. VAN HELVOORT¹, and DENNIS MEIER¹ — ¹NTNU Norwegian University of Science and Technology, Trondheim, Norway — ²University of Liège, Liège, Belgium — ³Lawrence Berkeley National Laboratory, Berkeley, CA, USA — ⁴ETH Zurich, Zurich, Switzerland

Ferroelectric domain walls can exhibit fundamentally different electronic properties than the surrounding bulk material, making them interesting for the application in next-generation electronic devices. After comprehensive studies of the fundamental physics of domain walls, the community is now more and more shifting the focus towards their integration and performance in different device architectures.

Here, we investigate the distribution of electrical currents in domain wall networks in ErMnO_3 , considering basic two-terminal architectures. We deposit static metal electrodes on the domain walls and use a conductive atomic force microscopy tip as an additional movable monitoring contact. In this way, we can investigate the influence of the metal-semiconductor interface between the electrode and the sample, as well as the influence of the domain walls on the current distribution in the ferroelectric material.

Our results provide insight into the current evolution in ferroelectric domain wall systems, facilitating the design of ferroelectric domain wall-based devices.

KFM 3.6 Mon 11:10 EMH 225

Influence of ferroelectric domain structures on thermal conductivity in ErMnO_3 ceramics — RACHID BELRHITI NEJJAR¹, MANUEL ZAHN², FABIEN GIOVANNELLI¹, MAX HAAS², JAN SCHULTHEISS², DENNIS MEIER², and ●GUILLAUME F. NATAF¹ — ¹GREMAN UMR7347, CNRS, University of Tours, INSA Centre Val de Loire, 37000 Tours, France — ²NTNU Norwegian University of Science and Technology, Høgskoleringen 1, Trondheim 7034, Norway

Domain walls in ferroelectric and ferroelastic materials interact with phonons conducting heat and are thus interesting tools to tune thermal conductivity [1]. Recent results show that ferroelectric domain walls in single crystals of ErMnO_3 reduce thermal conductivity [2]. To reveal the full potential of domain walls for thermal applications, it is required to demonstrate their influence on thermal conductivity in ceramics, where grain sizes and grain boundaries can also play a role. Here, we investigated the thermal conductivity of several ceramics of ErMnO_3 with different grain sizes and different densities of domain walls. Different domain sizes were obtained by crossing the Curie temperature with different cooling rates. Different grain sizes result from different sintering temperatures [3]. Our measurements performed with a laser flash system between 160 K and 360 K demonstrate a correlation between the thermal conductivity and the domain structure in ceramics of ErMnO_3 , including at and above room temperature.

[1] Limelette et al. Phys. Rev. B 108, 144104 (2023) [2] Pang et al. Mater. Today Phys. 307, 100972 (2023) [3] Schultheiß et al. Adv. Mater. 34, 2203449 (2022)

KFM 4: Perovskite and photovoltaics I (joint session HL/KFM)

Time: Monday 9:30–13:00

Location: EW 203

KFM 4.1 Mon 9:30 EW 203

Improving Performance of Two-Step Processed Perovskite Top Cells for Tandem Photovoltaic Applications — ●RONJA PAPPENBERGER^{1,2}, ALEXANDER DIERCKS², JULIAN PETRY^{1,2}, PAUL FASSL^{1,2}, and ULRICH W. PAETZOLD^{1,2} — ¹Institute of Microstructure Technology, KIT, Germany — ²Light Technology Institute, KIT, Germany

For high-performance application of perovskite solar cells (PSCs) in monolithic perovskite/silicon tandem configuration, an optimal bandgap and process method of the perovskite top cell is required. While the two-step method leads to regular perovskite film crystallization, engineering wider bandgaps ($E_g > 1.65$ eV) for the solution-based two-step method remains a challenge. This work introduces an effective and facile strategy to increase the bandgap of two-step solution-processed perovskite films by incorporating bromide in both deposition steps, the inorganic (step 1, PbBr_2) and the organic (step 2, FABr) precursor deposition. This strategy yields improved charge carrier extraction and quasi-Fermi level splitting with PCEs up to 15.9%. Further improvements are achieved by introducing CsI in the bulk and utilizing LiF as surface passivation, resulting in a stable power output exceeding 18.9% for $E_g = 1.68$ eV. This additional performance boost arises from enhanced perovskite film crystallization, leading to improved charge carrier extraction. Laboratory scale planar monolithic perovskite/silicon tandem solar cells (TSCs) (1 cm^2 active area) achieve PCEs up to 25.7%. In addition, research is being conducted into implementation on textured monolithic perovskite/silicon TSCs.

KFM 4.2 Mon 9:45 EW 203

Optical In-Situ spectroscopy and reactive spin coating for improved control of perovskite thin film fabrication — ●SIMON BIBERGER, MAXIMILIAN SPIES, KONSTANTIN SCHÖTZ, FRANK-JULIAN KAHLE, NICO LEUPOLD, RALF MOOS, HELEN GRÜNINGER, ANNA KÖHLER, and FABIAN PANZER — University of Bayreuth, Bayreuth, Germany

Efficient solar cells require a high-quality halide perovskite (HP) film, which is typically achieved through a solution-based solvent engineering spin coating approach. Here, HP crystallization is induced by applying an antisolvent (AS) to the precursor solution film on the spinning substrate after a specific spinning time. The process involves various controllable and uncontrollable parameters that need to be considered. As a result, fabrication recipes (such as spin speed or timing of AS dispensing) are usually developed empirically and vary between labs. Additionally, factors like changes in the atmosphere that are hard to control can introduce substantial variations between and even within batches of devices. In this work we developed a closed-loop feedback system based on our multimodal optical In-Situ spin coater system in combination with a real-time analysis of the optical spectra during spin coating. We monitor the solvent layer thickness as the parameter of interest during the spin coating. When the target level is reached, the HP crystallization is induced by dispensing the AS via a syringe pump. This method compensates for the effects of uncontrolled parameters, like variation in solvent evaporation rate due to atmospheric changes, thus leading to reproducible film quality.

KFM 4.3 Mon 10:00 EW 203

Enhanced Circular Dichroism and Polarized Emission in an Achiral, Low Bandgap Bismuth Iodide Perovskite — ●PHILIP KLEMENT¹, JAKOB MÖBS², GINA STUHRMANN³, LUKAS GÜMBEL¹, MARIUS MÜLLER¹, JOHANNA HEINE², and SANGAM CHATTERJEE¹ — ¹Institute of Experimental Physics I, JLU Gießen, Germany — ²Department of Chemistry, PUM, Marburg, Germany — ³Institute of Nanotechnology (INT), KIT, Eggenstein-Leopoldshafen, Germany

Lead halide perovskites and related materials incorporating chiral organic cations exhibit intriguing properties such as chiroptical activity and chirality-induced spin selectivity enabling the generation and detection of circularly polarized light. However, understanding the structural origin of chiroptical activity presents a challenge due to macroscopic factors and experimental constraints. Here, we present the achiral perovskite derivative $[\text{Cu}_2(\text{pyz})_3(\text{MeCN})_2][\text{Bi}_3\text{I}_{11}]$ ($\text{pyz} = \text{pyrazine}$; $\text{MeCN} = \text{acetonitrile}$), which displays remarkable circular dichroism (CD) arising from the material's noncentrosymmetric structure. CuBiI exhibits a low, direct optical band gap of 1.70 eV and both linear

and circular optical activity with a substantial anisotropy factor of up to 0.16. Intriguingly, despite the absence of chiral building blocks, CuBiI exhibits a substantial degree of circularly polarized photoluminescence, reaching 4.9%. This value is comparable to the results achieved by incorporating chiral organic molecules into perovskites, typically ranging from 3 to 10% at zero magnetic field. Our findings shed light on the macroscopic origin of CD and provide valuable insights for the design of materials with high chiroptical activity.

KFM 4.4 Mon 10:15 EW 203

Explaining the tetragonal distortion of chalcopyrites and solving the puzzle of the peculiar bond length dependence in $(\text{Ag,Cu})(\text{In,Ga})\text{Se}_2$ — ●HANS H. FALK¹, STEFANIE ECKNER¹, KONRAD RITTER¹, SERGIU LEVCENKO¹, TIMO PFEIFFELMANN¹, EDMUND WELTER², JES LARSEN³, WILLIAM N. SHAFARMAN⁴, and CLAUDIA S. SCHNOHR¹ — ¹Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — ²Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ³Department of Materials Science and Engineering, Uppsala University, Sweden — ⁴Department of Materials Science and Engineering, University of Delaware, Newark, USA

$(\text{Ag,Cu})(\text{In,Ga})\text{Se}_2$ is a highly efficient thin film solar cell absorber. EXAFS studies of $(\text{Ag,Cu})\text{InSe}_2$ and $(\text{Ag,Cu})\text{GaSe}_2$ show that the element specific bond length of the common cation (In-Se or Ga-Se) decreases with increasing Ag content even though the lattice expands. This peculiar bond length dependence is not only counter-intuitive but also the opposite of what is commonly observed in other chalcopyrite alloys, like $\text{Cu}(\text{In,Ga})\text{Se}_2$ and $\text{Ag}(\text{In,Ga})\text{Se}_2$, where the bond length of the common cation (Cu-Se or Ag-Se) increases as the lattice expands. This puzzling difference in the behavior of the common cation bond lengths can be explained by minimizing the distortion energy (Keating potential) of bond angles and bond lengths. With simple calculations, focusing on the local tetrahedral neighborhood, we are able to reproduce both the tetragonal distortion and the bond length behavior of various chalcopyrite alloys, leading to a deepened understanding of these technologically relevant photovoltaic absorber materials.

KFM 4.5 Mon 10:30 EW 203

Nonlocal many-body dispersion for bulk properties: The particular case of cesium-based halide perovskites — LIN YANG¹, YA GAO¹, JINGRUI LI², ●GUO-XU ZHANG¹, and ZHENBO WANG¹ — ¹Harbin Institute of Technology, Harbin, P. R. China — ²Xi'an Jiaotong University, Xi'an, P. R. China

Cesium-based all-inorganic halide perovskites have shown excellent photovoltaic properties. However, phase stability and transformations in different polymorphs remain rather poorly understood. Here, we investigate the cohesive, electronic properties and structural instabilities of CsPbI_3 and CsSnI_3 based on first-principles density-functional theory (DFT) calculations. Care has been taken to choose exchange-correlation functionals and zero-point vibrational effects have been included by performing phonon calculations. In particular, we compare different van der Waals (vdW) corrections to the DFT approaches. Our results demonstrate that nonlocal many-body dispersion interactions play a vital role in predicting the cohesive properties and phonon spectra of halide perovskites studies here. In addition, we find the anharmonicity cannot be neglected in order to correctly predict the phase stability and transitions of polymorphs. The quasiharmonic approximation method that partially include the anharmonicity is able to improve the predictions, in particular for CsSnI_3 . We stress that both nonlocal many-body dispersion and full anharmonic terms should be considered for accurate studies of such type of materials.

KFM 4.6 Mon 10:45 EW 203

Changes in Polarization Mechanisms Following Dimensional Reduction of the Double Perovskite Octahedral Network in $\text{Cs}_2\text{AgBiBr}_6$ — ●TIM P. SCHNEIDER, JONAS GLASER, JONAS HORN, and DERCK SCHLETTWEIN — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen

Introduction of large organic cations into metal halide perovskites leads to dimensional reduction of the octahedral metal-halide network towards so-called 2D-perovskites with significant changes in the electronic system. Such 2D-perovskites are recently studied to enhance the performance of perovskite solar cells by reducing hysteretic behav-

ior and improving the contact formation of perovskite absorbing layers to transport layers. In this work, 2D $\text{PEA}_4\text{AgBiBr}_8$ is derived from its 3D counterpart $\text{Cs}_2\text{AgBiBr}_6$ by replacing Cs^+ by the large organic phenethylammonium (PEA^+) cation. Thin films of both materials, 3D $\text{Cs}_2\text{AgBiBr}_6$ or 2D $\text{PEA}_4\text{AgBiBr}_8$, were prepared onto microstructured metal electrode arrays to perform I - U measurements and spatially resolved Kelvin probe force microscopy. These experiments serve to characterize the contact formation of both materials and discuss hysteresis caused by ion migration in response to an applied electric field. It was revealed how the dimensional reduction of the octahedral network affects the polarization caused by ionic movements and the formation of contact resistances in the films and at the respective interface to the metal electrodes. Differences among the materials, implications for technical applications in devices and the respective origin of the different observed polarization phenomena will be discussed.

15 min. break

Invited Talk KFM 4.7 Mon 11:15 EW 203
Influence of the Organic Cation Orientation on the Absorption Spectra of 2D Hybrid Organic-Inorganic Perovskites — ●SVENJA JANKE — Department of Chemistry, University of Warwick, Coventry, UK

Hybrid organic-inorganic perovskites (HOIPs) allow combining organic and inorganic materials at the nanoscale and hence open up a wide area of tunability. In two-dimensional HOIPs, both organic and inorganic components can contribute to the electronic frontier levels. For the design of new devices like solar cells, a fundamental understanding of the electronic excitations, their photophysical signatures and the underlying atomic structure is essential. The 2D HOIP inorganic exciton binding energy depends approximately linearly on the inorganic band gap. To estimate the inorganic exciton contribution to the absorption spectrum, I benchmark the amount of Hartree Fock exchange in hybrid density functional theory calculations including spin-orbit coupling.

For the quaterthiophene-based 2D HOIP (AE4T) PbX_4 , variation of the halide anion leads to structural changes in the organic layer, causing changes in the absorption spectra. The bithiophene-based 2D HOIP (AE2T) PbI_4 shows disorder along the stacking direction in X-ray scattering experiments, resulting in several possible atomic structural models for the organic component.

Here, I demonstrate that we can use a Frenkel-Holstein-Hamiltonian-based model to investigate how different orientations of the organic cation alter the organic and inorganic exciton contribution to the absorption spectrum.

KFM 4.8 Mon 11:45 EW 203

Optical Simulations of Light Management in Ultrathin CIGSe Solar Cells with Nanophotonic Back Contacts — ●DANIEL JIMENEZ TEJERO, MERVE DEMIR, THOMAS SCHNEIDER, BODO FUHRMANN, ROLAND SCHEER, RALF WEHRSPHORN, and ALEXANDER SPRAFKE — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, 06120 Halle (Saale), Germany

Ultrathin $\text{Cu}(\text{In,Ga})\text{Se}_2$ (CIGSe) solar cells are in development to decrease material usage and broaden the range of applications. However, CIGSe absorber layers with thicknesses below $1\ \mu\text{m}$ suffer from reduced light absorption, especially for wavelengths near the bandgap, leading to decreased power conversion efficiency. To counteract this, we employ nanostructured functional back contacts to effectively increase the optical path length within the CIGSe absorber layer through nanophotonic mechanisms such as scattering and coupling into thin film modes. The focus lies on CIGSe absorber layers with a thickness of 300 nm to 500 nm deposited on SiO_2 nanostructures on a flat aluminium or gold back contact. Our approach employs nano-optical simulations using the finite element method and aims to identify designs with promising photocurrent enhancements feasible for fabrication and to clarify the underlying mechanisms.

KFM 4.9 Mon 12:00 EW 203

Multi-Phase Optical Exciton Dynamics in Mixed (2D/3D) Inorganic-Organic Hybrid Semiconductors — ●MOHAMMAD ADNAN^{1,2}, PAWAN KUMAR KANAUIYA², KSHETRA MOHAN DEHURY², and GADDAM VIJAYA PRAKASH² — ¹Institute of Physics, University of Münster, Wilhelm-Klemm-Straße 10 48149 Münster, Germany — ²Nanophotonics Lab, Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016 India

Inorganic-organic (IO) hybrid semiconductors are promising optoelec-

tronic materials due to their unique crystal packing, the wide variety of crystal phases, the wide bandgap tunability and the associated optical exciton characteristics. Here, we investigate the digitized intercalation process of various organic moieties, resulting in a mixed IO hybrid system of type $(\text{R-NH}_3)_2(\text{R}'\text{-NH}_3)_n\text{-1PbnI}_{3n+1}$. By employing continuous photoluminescence monitoring, we observe a progressive and dynamic structural evolution and elucidate the underlying mechanisms occurring during the intercalation process. The interplay of (i) cyclic (ii) long alkyl chain and (iii) small alkyl amine based organic moieties during the intercalation leads to the formation of either 2D $(\text{R-NH}_3)_2\text{PbI}_4$ or 3D $(\text{R}'\text{-NH}_3)_n\text{PbI}_3$ IO hybrid networks and causes significant structural phase variations within the 2D and 3D crystal packings.

KFM 4.10 Mon 12:15 EW 203

Exploring Mixed-Metal Chalcogenides $\text{M}(\text{II})_2\text{M}(\text{III})\text{Ch}_2\text{X}_3$ Compounds for Photovoltaic Applications — ●PASCAL HENKEL¹, JINGRUI LI², and PATRICK RINKE¹ — ¹Department of Applied Physics, Aalto University, P.O.Box 11100, FI-00076 AALTO, Finland — ²School of Electronic Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China

New photovoltaic materials are needed to increase power conversion efficiencies (PCEs), reduce costs, and improve device longevity to facilitate the renewable energy transformation. In this context, perovskite-inspired quaternary mixed-metal chalcogenides $\text{M}(\text{II})_2\text{M}(\text{III})\text{Ch}_2\text{X}_3$ have emerged as an interesting materials class, that has the potential to overcome the stability and toxicity problems of the currently favoured halid perovskites [1], and still deliver high PCEs [2].

In this study, we apply density functional theory to identify new $\text{M}(\text{II})_2\text{M}(\text{III})\text{Ch}_2\text{X}_3$ compounds. We considered a total of 54 materials each in three different space groups ($Cmcm$, $Cmc2_1$ and $P2_1/c$) for which we computed the energetic stability and the band gaps with the HSE06 hybrid functional. We identified a total of 22 $\text{M}(\text{II})_2\text{M}(\text{III})\text{Ch}_2\text{X}_3$ materials, which fulfill our stability requirements and have a direct band gap in the range 0.7 eV to 2 eV. Out of the 22, 8 lead-free and 9 lead-containing materials are new [3]. Overall for all 54 compounds, $P2_1/c$ is the thermodynamically preferred phase, whereas direct band gaps occur predominantly for $Cmcm$ and $Cmc2_1$.

[1] *Z. Anorg. Allg. Chem.* **468**, 91-98 (1980). [2] *Mater. Horiz.* **8**, 2709 (2021), [3] *Chem. Mater.* **35**, 7761-7769 (2023).

KFM 4.11 Mon 12:30 EW 203

Effective model for charge transport in hybrid organic-inorganic materials dominated by molecule-lattice interactions — ●FLORIAN KLUBENSCHIEDL, GEORGIOS KOUTENTAKIS, RAGHEED ALHYDER, and MIKHAIL LEMESHKO — Institute of Science and Technology Austria (ISTA), Am Campus 1, 3400 Klosterneuburg, Austria

The growing importance of crystalline hybrid materials with embedded molecular entities, such as hybrid organic-inorganic perovskites (HOIPs) or molecular organic frameworks, requires extensions of the conventional picture of charge transport based on electron-phonon interactions. Here we present a minimal, coarse-grained, two-dimensional model of charge transport based on the interactions of charge carriers with freely rotating molecules embedded in the inorganic lattice. Our phase diagram analysis reveals the presence of four phases, characterized by the distinct ordering of the molecular dipole moments, which strongly depends on the tunneling anisotropy of the carriers as well as on the strength of carrier-molecule interactions. The most striking outcome is the coexistence of degenerate ferroelectric phases of reduced symmetry beyond a certain threshold of interaction strength, even in the case of isotropic tunneling. The coexistence of these phases motivates a symmetry breaking mechanism similar to the Jahn-Teller effect, which introduces transport anisotropy into an otherwise symmetric system. We relate these results to the proposed formation of ferroelectric large polarons as an explanation of the remarkable optoelectronic properties of HOIPs.

KFM 4.12 Mon 12:45 EW 203

Cavity-enhanced absorption measurements of perovskite nanocrystals — ●INES AMERSDORFFER¹, ANDREAS SINGLDINGER¹, THOMAS HÜMMER^{1,2}, ALEXANDER URBAN¹, and DAVID HUNGER³ — ¹Faculty of physics, LMU Munich, Germany — ²Qlibri GmbH, Munich, Germany — ³Physikalisches Institut, KIT, Germany

The search for optimal materials for optoelectronic devices such as solar cells or quantum light emitters has piqued significant interest in perovskite nanocrystals. This is due to their outstanding proper-

ties, which range from easy, scalable synthesis at room temperature to ultra-wide colour tunability and high quantum efficiency.

Spectroscopy on single perovskite crystals helps to reveal their excitonic fine structure, which in thin films is concealed by inter-particle phenomena. However, measuring the marginal absorption of such nanocrystals is challenging. One way to overcome this issue is to use an optical resonator in which the light passes through the nanoscale sample multiple times and thereby enhances its absorption to a measurable amount.

To this end, we use a high-finesse microcavity to perform wavelength dependent absorption measurements on perovskite nanocubes. These are complemented by low-temperature photoluminescence and scanning electron microscopy images. The combination of these techniques will provide unprecedented insight into the size- and morphology dependence of the energetic structure of individual nanocrystals. The results show progress towards routine hyperspectral absorption measurements at the nanoscale.

KFM 5: Thin oxides and oxide layers (joint session DS/KFM)

Time: Monday 9:30–11:45

Location: A 053

KFM 5.1 Mon 9:30 A 053

Non-collinear spin texture in thin rare-earth ion doped nickel ferrite films — ●ANUPAM K. SINGH¹, KATAYOON MOHSENI¹, MALLESHWARA R. TANGI¹, VERENA NEY², ANDREAS NEY², ARTHUR ERNST², YICHENG GUAN¹, MANUEL VALVIDARES³, P. GARGIANI³, ILYA KOSTANVOSKIY¹, HOLGER L. MEYERHEIM¹, and STUART S. P. PARKIN¹ — ¹Max Planck Institute of Microstructure Physics, Weinberg 2, 06120, Halle (Saale), Germany — ²Johannes Kepler University Linz, Altenberger Straße 69, 4040 Linz, Austria — ³ALBA Synchrotron, E-08290 Cerdanyola del Vallès, Barcelona, Spain

Ferrites are abundantly used as magnetic materials, but thus far, the detailed magnetic structure in ultra-thin films has escaped clear-cut characterization. The recent observation of rare-earth-induced DMI in low-dissipation insulating oxides calls for a deeper insight into their spin texture [1]. We have studied the atomic and magnetic structure of 5 to 40 nm thick Dy-doped (5%) Zn/Al-substituted nickel ferrite (Ni_{0.65}Zn_{0.35}Al_{0.8}Fe_{1.2}O₄) films prepared by magnetron sputtering. Characterization by RBS, XRD, EXAFS and XMCD experiments at the Fe-K, L_{2,3} and the Dy-L_{2,3}, M_{4,5} edges establish the formation of a tetragonally distorted spinel structure where Dy³⁺ ions occupy octahedral sites with a redistribution of the Fe²⁺ and Fe³⁺ cations. Temperature-dependent SQUID, XMCD and MOKE experiments indicate a spin-reorientation transition from in-plane easy axis below 200 K, thereby showing a non-monotonic behavior of the M(T) curve which is interpreted as due to the formation of a non-collinear spin structure. [1] L. Caretta, et al., Nat. Comm. 11, 1090 (2020).

KFM 5.2 Mon 9:45 A 053

Defect and Strain Engineering in SrTiO₃ and CaTiO₃ Thin Films Epitaxially Grown by Metal Organic Vapor Phase Epitaxy (MOVPE) — ●MOHAMED ABDELDAYEM, CHANGMING LIU, IZAZ-ALI SHAH, ANDREAS FIEDLER, MARTIN ALBRECHT, and JUTTA SCHWARZKOPF — Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Neuromorphic devices attempt to imitate the human brain, and replace the conventional computer design to meet the demands of energy efficiency, and learning capacity. Memristive devices are a leading candidate to provide the physical properties needed for an artificial neural network. Here, we report a model in SrTiO₃ and CaTiO₃ thin films where resistive switching mechanism is based on polar nano-regions created by the formation of Ti anti-site defects in A-cation deficient growth regime. SrTiO₃ and CaTiO₃ thin films were grown epitaxially by metal-organic vapor phase epitaxy in which growth takes place near thermodynamic equilibrium and high oxygen partial pressure. This provides well-ordered epitaxial films with low defect density and negligible amount of oxygen vacancies. Moreover, chemical elements can be independently controlled by controlling the precursor fluxes in the gas phase, which enables the growth of stoichiometric and intentionally off-stoichiometric films. HRXRD, and AFM were used to verify epitaxial growth of high structural quality films with smooth surfaces. STEM-HAADF was utilized for detailed microscopic structural investigation, and showed the high homogeneity of stoichiometric films opposite to the intentionally defect ones with cloudy contrast and defect clustering.

KFM 5.3 Mon 10:00 A 053

Electronic Reconstruction and Anomalous Hall Effect in the LaAlO₃/SrRuO₃ Heterostructure — ●MERIT SPRING^{1,2,3}, JI SOO LIM^{1,2}, MARTIN KAMP^{1,4}, MATTHIAS SCHMITT^{1,2,3}, DEEP-NARAYAN BISWAS³, LOUIS VEYRAT⁵, PAVEL POTAPOV⁵, AXEL LUBK⁵, BERND BÜCHNER⁵, TIEN-LIN LEE³, MICHAEL SING^{1,2}, and RALPH CLAESSEN^{1,2} — ¹Physikalisches Institut, Würzburg, GER —

²Würzburg-Dresden Cluster of Excellence ct.qmat — ³Diamond Light-source Ltd., Didcot, UK — ⁴Wilhelm Conrad Röntgen-Center for Complex Material Systems, Universität Würzburg, GER — ⁵Leibniz Institute for Solid State and Materials Research, Dresden, GER

For the LaAlO₃/SrRuO₃ (LAO/SRO) system a similar electronic reconstruction to that of LaAlO₃/SrTiO₃ (LAO/STO) is expected, and charge is thought to be accumulated at the very interface giving rise to strong inversion-symmetry breaking and causing a topological transition of the electronic bands [1]. We show that the LAO capping drives the SRO, which turns insulating below 8 unit cells (uc) without capping, (deeper) into the metallic regime. Furthermore, we find not only signatures of an anomalous Hall effect (AHE) in 4 uc SRO films capped with LAO, but also an inversion of the sign of the AHE, when the 4uc SRO is replaced by metallic 10 uc of SRO indicating the topological phase transition. Moreover, we correlate these findings with hard and soft x-ray photoemission spectroscopy data, that show changes in the ruthenium electronic states, and discuss these changes in terms of correlated electrons. [1] Thiel, T. C. et al., Phys. Rev. Lett. 127, 127202 (2021)

KFM 5.4 Mon 10:15 A 053

Exploration of zirconium doping in pulsed laser deposited α -Ga₂O₃ for devices — ●SOFIE VOGT¹, THORSTEN SCHULTZ^{2,3}, CLEMENS PETERSEN¹, HOLGER VON WENCKSTERN¹, NORBERT KOCH^{2,3}, and MARIUS GRUNDMANN¹ — ¹Universität Leipzig, Felix-Bloch-Institut, Leipzig — ²Humboldt Universität zu Berlin, Institut für Physik, Berlin — ³Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Solar Energy, Berlin

Gallium oxide, known for its ultrawide bandgap, crystallizes in different polymorphs, of which the β -phase is the thermodynamically most stable and most investigated one. However, the metastable corundum structured α -phase exhibits a wider bandgap and therefore a potentially higher electrical breakdown field compared to β -Ga₂O₃[1]. Doping of α -Ga₂O₃ with tin, silicon and germanium has been demonstrated[2,3]. We present α -Ga₂O₃ thin films grown by pulsed laser deposition in a two-step process. Undoped α -Ga₂O₃ grown at high temperature is used as buffer layer. The zirconium doped α -Ga₂O₃ is deposited atop the buffer layer at a temperature < 600°C, to ensure the deposition of conductive thin films. The structural and electrical properties of Zr doped thin films are compared to Sn, Si and Ge doped thin films with regards to the crystal quality, conductivity, free carrier concentration and electron mobility. First Schottky barrier diodes based on the α -Ga₂O₃:Zr thin films are presented.

[1] Higashiwaki *et al.*, Appl. Phys. Lett., **100**, 013504 (2012)

[2] Akaiwa *et al.*, phys. status solidi (a), **217**, 3, 1900632 (2020)

[3] Vogt *et al.*, phys. status solidi (a), **220**, 3, 2200721 (2023)

15 min. break

KFM 5.5 Mon 10:45 A 053

Epitaxy and transfer of freestanding SrTiO₃ membranes — ●JEREMY MALTITZ, WEAAM AYAD, JENS MARTIN, and JUTTA SCHWARZKOPF — Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Layer transfer of thin films has established a new paradigm of material assembly and design in context of 2D-van-der-Waals crystals. Recently, freestanding oxide perovskite thin films have been achieved by introducing a perovskite-like, water-soluble sacrificial layer (Sr₃Al₂O₆) between substrate and functional film. In combination with layer transfer, this provides a playground for fundamental investigations and

technological applications of complex oxides beyond the limitations of classical heteroepitaxy. Requirements are the preparation of epitaxial oxide films with high structural quality of both sacrificial layer and functional oxide film and the controlled detachment from the growth substrate and transfer on another substrate. In this contribution, we will show the influence of the PLD parameters, film thicknesses and composition of the oxide films on the release process and crack formation in freestanding SrTiO₃ thin films by using the solid-solution family of (Ba,Ca,Sr)3Al₂O₆ as sacrificial layer. While cracking of the SrTiO₃ films during etching of the sacrificial layer can be largely avoided by the growth of an almost strain-free heterostructure, the transfer process remains challenging. One approach is the use of sub-mm small polymer stamps to transfer deliberately smaller pieces of the functional oxide film on the target substrate.

KFM 5.6 Mon 11:00 A 053

Investigation of electrical properties of metal oxide semiconductors thinfilms — ●PINAR ORUC¹, ALI ORKUN CAGIRTEKIN¹, SUKRU CAVDAR¹, NIHA TUGLUOGLU², and HALUK KORALAY¹ — ¹Gazi University, Faculty of Science Department of Physics, Ankara Turkiye. — ²Giresun University, Faculty of Engineering, Department of Energy Engineering, Giresun, Turkiye.

Metal oxide semiconductor materials such as TiO₂, ZnO, V₂O₅, and MoO₃ have very large technological area because of their useful properties [1]. Generally, these materials are interesting by scientific community because they have wide forbidden energy band gap, good electrical, and optical properties [2]. With the development of technology, the development of higher performance and cost-effective devices has become more important. For these reasons, the importance of these semiconductor metal oxide structures has gradually increased. In this study, electrical characterization of multilayer semiconductors device was investigated. Different metal oxide thin film layers were grown on the fluorine doped tin oxide (FTO) substrate by using different methods. It has been observed that both thin films obtained with different techniques have a homogeneous surface. Electrical measurements of the device were taken at different temperatures, widely frequency regions. As a result of electrical measurements, the device showed good diode behavior also electrical behavior of the fabricated device showed better electrical properties as the increasing temperature. According to the results, the fabricated device can be used many electronic areas.

KFM 5.7 Mon 11:15 A 053

Engineering electrochemical conversion in La₂NiMnO₆ using magnetic ground states — ●PIA HENNING and JASNAMOL PALAKKAL — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

For a more sustainable future, the identification of new electrocatalyst materials for the oxygen evolution reaction (OER) plays an important role. In the course of this, the oxide double perovskite La₂NiMnO₆ exhibits a promising role [1]. Especially interesting for this material is the interplay between magnetic ground state and OER activity. The catalytic activity of La₂NiMnO₆ powder samples is enhanced when a vibronic superexchange interaction is present, dominating over static exchange interactions [1]. However, the magnetic structure is closely linked to the oxygen content in the sample and a low Curie temperature can also be originating from oxygen vacancies in the lattice [2]. To resolve this, we prepared La₂NiMnO₆ thin films with our hybrid PLD set-up, combining standard PLD with MBE techniques. The samples were carefully modified by controlling the oxygen content. These modifications of the B-site electronic configuration were then related to the OER activities of the samples, using the magnetic properties as descriptor.

[1] Y. Tong, J. Wu, P. Chen, H. Liu, W. Chu, C. Wu, Y. Xie, *Journal of the American Chemical Society* 2018, 140(36), 11165.

[2] J. P. Palakkal, T. Schneider, L. Alff, *AIP Advances* 2022, 12(3), 035116.

KFM 5.8 Mon 11:30 A 053

Ferroelectric polarization rotation through He irradiation induced uniaxial strain — ●ANDREAS HERKLOTZ¹, ROBERT ROTH¹, KATHRIN DÖRR¹, ALESSANDRO MAZZA², and THOMAS ZAC WARD³ — ¹Institute for Physics, Martin-Luther-University Halle-Wittenberg, Halle, Germany — ²Los Alamos National Laboratory, Los Alamos, USA — ³Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, USA

The physical properties of ferroic thin films are typically dominated by their domain configurations and their responses to external fields. A central prerequisite to domain engineering and harnessing functionalities of ferroelectric thin films is thus the control of the polarization orientation. Historically, the symmetry of ferroelectric films has been mainly tailored by heteroepitaxial in-plane strain or a variation of growth conditions inducing defects.

Here, we deploy low-energy He implantation as an alternative approach. Ion implantation induces uniaxial out-of-plane strain, while the in-plane strain remains fixed due to epitaxial constraint. We show that this kind of uniaxial strain engineering effectively leads to polarization rotation from in-plane towards out-of-plane as the uniaxial strain is increasing. We find that this polarization rotation can be achieved via two different mechanisms: (i) via a sequence of phase transitions related to changes of crystal symmetries and (ii) via a continuous shift of the ferroelectric domain ratio towards out-of-plane oriented domains.

KFM 6: Instrumentation and Methods for Micro- and Nanoanalysis

Chair: Theo Scherer (KIT Karlsruhe)

Time: Monday 10:40–12:00

Location: EMH 025

KFM 6.1 Mon 10:40 EMH 025

Dynamical diffraction effects of inhomogeneous strain fields investigated by scanning convergent beam electron diffraction — ●LAURA NIERMANN, TORE NIERMANN, FREDERIK OTTO, and MICHAEL LEHMANN — Technische Universität Berlin, Berlin

Strain fields have a large influence on optical and electronic properties of semiconductors. Several transmission electron microscopy (TEM) techniques exist to measure the strain with high precision on a nanometer scale. The models behind these techniques make the assumption that the strain is constant along the electron beam direction. However, if the strain is inhomogeneous in beam direction, the strong diffraction conditions required for the strain mapping cause a non-linear influence on the resulting diffracted electron beam. This effect in turn can also be used to characterize the three dimensional strain field in the specimen. We report on systematic investigations of dynamical diffraction at inhomogeneous strain fields in electron beam direction by using an inclined layer structure producing a continuous change in the depth of the strain field. The strain mapping was performed by means of scanning convergent beam electron diffraction (SCBED) using a fast pixelated detector to record the whole diffraction pattern for each scan position. By comparing the experimental results to calculated diffraction patterns using multi-beam simulations and including effects like

surface relaxation and specimen bending, the observed intensity variations can directly be attributed to the dynamical diffraction behavior.

KFM 6.2 Mon 11:00 EMH 025

Planar Strain Tomography with X-ray Powder Diffraction — ●PETER MODREGGER — Department Physik, Universität Siegen — Center for X-ray and Nano Science, DESY, Hamburg

The measurement of local strain and residual stress fields in polycrystalline engineering materials constitutes an essential tool of materials science engineering. In general, there are two types of methods available: X-ray diffraction with conical slits and energy dispersive X-ray diffraction - both featuring anisotropic gauge volumes with aspect ratios of 1:20 or worse. Here, we introduce planar strain tomography based on X-ray powder diffraction that utilizes a high energy pencil beam and iterative reconstruction. The gauge volume is defined by the size of the pencil beam with typical aspect ratios close to 1:1. We will demonstrate the feasibility with data collected in a pilot experiment at P21.2 at PETRA III. The sample was shot peened martensite and the measured strain and residual stress field distributions meet expectations. The results will be compared to energy dispersive X-ray diffraction collected with the high energy wiggler beamline P61A at PETRA III as well as laboratory measurements. We will further

discuss limitations of the proposed approach in terms of stability of iterative tomographic reconstruction, suitable sample thicknesses (in the range of centimeters) and currently achieved strain sensitivity (in the order of $1e-4$).

KFM 6.3 Mon 11:20 EMH 025

MULTIPAC, a versatile TDPAC spectrometer — ●BJÖRN DÖRSCHHEL¹, IAN YAP¹, THIEN DANG¹, JULIANA SCHELL^{1,2}, NICOLE DE LIMA³, MAGNUS HÄGELUND⁴, BRUNO CORREA³, ARNALDO FILHO³, ALEXANDRE SOUZA⁵, and DORU LUPASCU¹ — ¹Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141 Essen, Germany — ²Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141 Essen, Germany — ³Universidade de São Paulo, 158 Av. Prof. Luciano Gualberto, Brazil — ⁴Institute of Material Science and Production, University of Aalborg, 9220 Aalborg, Denmark — ⁵Idaho National Laboratory, 1955 N Fremont Ave, Idaho Falls, ID 83415, USA

MULTIPAC is a spectrometer that can perform γ - γ time-differential perturbed angular correlation (γ - γ TDPAC) experiments under controlled conditions such as an applied external magnetic field up to 8.5 T and temperatures ranging between 3 to 375 K. MULTIPAC differs from conventional γ - γ TDPAC spectrometers in the use of modern multi-pixel photon counters (MPPC), which offers advantage over the standard photomultiplier tubes, due to its compact size, resistance to magnetic fields, ease of maintenance, and requiring only low voltage. Additionally, the MPPC maintains the same quantum efficiency ($< 25\%$) and the high gain ($\sim 10^5$) comparable to that of a photo multiplier tube. In addition, MULTIPAC also features a vibrating

sample magnetometer (VSM) to leverage upon the field provided by its inbuilt superconducting magnet.

KFM 6.4 Mon 11:40 EMH 025

Emission Mössbauer Spectrometer from Ilmenau (eMIL): An Update — ALICE KERN¹, JULIANA SCHELL^{2,3}, ●IAN CHANG JIE YAP³, THIEN THANH DANG³, MAGNUS HÄGELUND⁴, DMITRY ZYABKIN⁵, and PETER SCHAAP⁵ — ¹Fakultät für Festkörperelektronik, Technische Universität Wien, AT-1040, Wien — ²European Organization for Nuclear Research (CERN), CH-1211, Geneva — ³Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141 Essen, Germany — ⁴Institute of Material Science and Production, University of Aalborg, 9220 Aalborg, Denmark — ⁵Fakultät für Chemie, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The advanced emission Mössbauer spectrometer, eMIL (Emission Mössbauer from Ilmenau) was built for the emission Mössbauer (eMS) collaboration at ISOLDE/CERN. The set-up is based on the emission geometry and combines on-line and off-line isotope implantation used to measure hyper-fine interactions in condensed matter materials. Using radioactive Mössbauer probes that are ion-implanted into the sample, eMIL has multiple advantages over the more common transmission or electron conversion setups. The versatility of the set-up is epitomized through five different lids: rotation, magnetic, powder, hot and cold lid. These lids can be easily interchanged, without the need for re-alignment, which makes eMIL extremely flexible during beam time. eMIL had its first successful run this year, which marked the first beam time for the Mössbauer collaboration since 2018.

KFM 7: Materials for the Storage and Conversion of Energy (joint session MM/KFM)

Time: Monday 11:45–13:00

Location: C 264

KFM 7.1 Mon 11:45 C 264

Symmetry Matters: Machine Learning EFG Tensors for NMR Parameter Simulations — ●ANGELA F. HARPER¹, SIMONE KÖCHER^{1,2}, KARSTEN REUTER¹, and CHRISTOPH SCHEURER¹ — ¹Fritz-Haber-Institut der MPG, Berlin — ²IEK-9 Forschungszentrum Jülich

Electric field gradient (EFG) tensors are directly probed by experimental solid-state Nuclear Magnetic Resonance (NMR), and are crucial for deciphering the atomic-scale structure and dynamics of Li-ion battery materials. By employing a machine learning approach we devise a model capable of learning complete EFG tensors, using equivariant descriptors. We further show that it is not sufficient to simply learn scalar quantities derived from a tensor such as quadrupolar shift or asymmetry. To assess the model's performance, we curate an extensive dataset comprising over 60,000 EFG tensors calculated for a diverse set of equilibrium and non-equilibrium crystal structures of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ (LTO), a well-studied zero-strain insertion anode material in Li-ion batteries. We finally show that we predict the quadrupolar frequency to within a few kHz for the ^7Li nucleus, which is well within the level of error required to make meaningful predictions for ^7Li NMR. This work represents a significant step towards realizing *in silico* spectroscopy: the ability to calculate spectroscopic signals such as EFG tensors with the same accuracy as experimental spectroscopy, using machine learning.

KFM 7.2 Mon 12:00 C 264

Design criteria for zero-strain cathode materials of the tungsten bronze type compounds A_xFeF_3 (A=Li, Na, K) by first-principles — ●ALJOSCHA F. BAUMANN¹, DANIEL MUTTER², DANIEL F. URBAN^{1,2}, and CHRISTIAN ELSÄSSER^{1,2} — ¹Freiburg Materials Research Center, 79104 Freiburg, Germany — ²Fraunhofer IWM, 79108 Freiburg

Mechanical stresses in the microstructure of cathode materials during charge/discharge cycles can reduce the long-term stability of intercalation-type alkali-metal-ion batteries. In this context, crystalline compounds exhibiting *zero-strain* (ZS) behavior are of particular interest. For instance, near zero-strain sodiation was experimentally measured in the tetragonal tungsten-bronze (TTB) type compound Na_xFeF_3 . [Han, J. Mater. Chem. A, 4, 7382] By atomistic simulations, using a first-principles method based on density functional theory, we investigated the potential of iron-based fluoride compounds

with tungsten-bronze structures as ZS cathode materials. The simulations were conducted systematically to study the intercalation of the alkali metal ions Li^+ , Na^+ , and K^+ into the TTB and two related tungsten-bronze structures of the perovskite and hexagonal types. As the alkali-metal ions intercalate, the oxidation state of the Fe ions decreases, which leads to an enlargement of their surrounding Fluorine octahedra. We found that this effect can be partially compensated by the volume reduction of the F- polyhedra surrounding the alkali ions. We discuss the structural and chemical prerequisites of the host lattice for enabling a ZS insertion mechanism for ions in crystals.

KFM 7.3 Mon 12:15 C 264

Construction of cobalt oxyhydroxide nanosheets with rich oxygen vacancies as high-performance Lithium-ion Battery anodes — ●YONGHUAN FU^{1,2}, HUAPING ZHAO¹, JIANHONG LIU², and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²Graphene Composite Research Center, College of Chemistry and Environmental Engineering, Shenzhen University, Shenzhen, P. R. China

Cobalt oxyhydroxide (CoOOH) is a promising anode material for lithium-ion batteries (LIBs) due to its high electronic conductivity and theoretical specific capacity. Herein, CoOOH nanosheets are successfully obtained using a facile one-pot method, and a hierarchical nanoporous structure is formed by oxidizing cobalt hydroxide ($\text{Co}(\text{OH})_2$) in NaOH and $(\text{NH}_4)_2\text{S}_2\text{O}_8$ solution. The CoOOH anode shows better electrochemical performance compared to $\text{Co}(\text{OH})_2$ and Co_3O_4 electrodes when applied to LIBs. The hierarchical nanoporous structure and high electronic conductivity of the CoOOH anode contribute to its outstanding initial discharge capacity, high initial coulombic efficiency, and excellent cyclability. Experiments and density functional theory (DFT) calculations confirmed that the high ICE and prominent rate capability of the nanosheets could be ascribed to the rapid and complete conversion reaction of CoOOH upon lithiation/delithiation facilitated by hydroxyl groups and oxygen vacancies. This study provides new insights into the structure-property relationship of transition-metal oxyhydroxide anode materials for LIBs.

KFM 7.4 Mon 12:30 C 264

Preparation of Prussian blue analogue materials and their application to sodium ion storage — ●PING HONG, HUAPING ZHAO,

and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The development of a new generation of energy storage systems is necessary due to the limited availability of non-renewable energy resources and the substantial environmental impact associated with the utilization of renewable energy. Sodium ion batteries are likely to become the next generation of large-scale commercial energy storage systems because of their low cost and high energy density. Among various materials, Prussian blue analogs (PBAs) have received great attention for their open three-dimensional framework structure and rapid sodium ion insertion/de-insertion capability. And derivatives synthesized using PBAs as templates have been widely studied. Therefore, in this work, PBAs with a well-defined structure were prepared as cost-effective electrode materials by a simple co-precipitation method. The PBAs materials were applied to sodium ion batteries, showing excellent performance. To achieve outstanding performance, a series of adjustments were made to the binder, electrolyte, and voltage range used in the batteries. at a current density of 100 mA g⁻¹ within the voltage range of 2.0-4.2 V, the capacity remains around 120 mAh g⁻¹. Even at ultra-high loadings, the material demonstrates excellent capacity and cycling stability.

KFM 7.5 Mon 12:45 C 264

Multiscale defective FeCu interfaces for sodiophilic and catalytic-enhanced Na-CO₂ batteries — ●CHANGFAN XU, TZUCHIN HUANG, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Sodium-carbon dioxide (Na-CO₂) batteries are hindered by challenges such as unmanageable sodium deposition/ volume changes at anode and sluggish CO₂ reduction/ evolution reaction (CO₂RR/ CO₂ER) kinetics at CO₂ cathode upon cycling. Here, we propose a dual-functional electrode with multiscale defective FeCu interfaces (CP@FeCu) that acts as Na metal hosts and CO₂ cathode simultaneously. Microstructural, electrochemical reaction, and theoretical calculations investigations collectively reveal that multiscale defective FeCu interfaces are responsible for the enhancement of sodiophilicity for Na plating/stripping at anode and catalytic activity for CO₂RR/ CO₂ER at CO₂ cathode. Consequently, the CP@FeCu anode enables the uniform deposition of dendrite-free sodium, and the CP@FeCu cathode exhibited low overpotentials and exceptional long-term cycling stability. Significantly, implementation of a symmetrical Na-CO₂ battery with CP@FeCu@Na anode and CP@FeCu cathode demonstrates significantly improved electrochemical properties. The introduction of multiscale defective FeCu interfaces with sodiophilic and catalytic dual centers offers an effective method for the tailoring and optimization of sodium metal batteries with high energy density.

KFM 8: Microscopy and Tomography with X-ray Photons, Electrons, Ions and Positrons

Chair: Theo Scherer (KIT Karlsruhe)

Time: Monday 12:10–13:10

Location: EMH 025

KFM 8.1 Mon 12:10 EMH 025

High angular momentum vortex electron beams in crystals — ●CHRISTIAN BICK and DOROTHEE HÜSER — Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

Since the introduction of beams with an orbital angular momentum (OAM), commonly known as vortex electron beams, into scanning transmission electron microscopy (STEM), they have been used in electron magnetic circular dichroism (ECMD) and nanoparticle manipulation [1]. Understanding the behaviour of these beams in material can help to better interpret experimental results. Previous studies have shown that vortex electron beams change their angular momentum as they propagate through the crystal. This change can be modelled by a superposition of eigenstates of the OAM operator [2,3].

We present a simulation-based study on the behaviour of higher order angular momentum vortex electron beams in crystalline material. The study is based on multislice calculations, which are commonly used in simulating STEM measurements.

[1] S. M. Lloyd, M. Babiker, and J. Yuan, *Phys. Rev. A* 86, 023816 (2012).

[2] S. Löffler and P. Schattschneider, *Acta Crystallogr. A* 68, 443 (2012).

[3] A. Lubk et al., *Phys. Rev. A* 87, 033834 (2013).

KFM 8.2 Mon 12:30 EMH 025

Three dimensional classification of dislocations from single projections — ●TORE NIERMANN, LAURA NIERMANN, and MICHAEL LEHMANN — Technische Universität Berlin, Berlin

Many material properties are governed by dislocations and their interactions. Examples range from strengthening of metals and alloys to efficiency in semiconductor laser devices. Thus, knowledge of the three dimensional topology of dislocation networks is crucial for material engineering. A two-dimensional projection of dislocation networks can be readily obtained by conventional (scanning-) transmission electron microscopy (S/TEM) images. However, the reconstruction of the three-dimensional structure of the network so far is mainly achieved by tomographic tilt series with high angular ranges, which is experimentally challenging and additionally puts constraints on possible spec-

imen geometries. Here, we present a new way to reveal the three dimensional position of dislocations and simultaneously classify their type from single 4D-STEM measurements. The dislocation's strain field causes inter-band scattering between the electron's Bloch waves within the crystal. This scattering in turn causes characteristic interference patterns with sufficient information to uniquely identify the dislocations type and position in electron beam direction by comparison with multi-beam calculations. We expect this principle to lead to fully automated methods for reconstruction of the three dimensional strain fields from 4D-STEM measurements in future.

KFM 8.3 Mon 12:50 EMH 025

Lattice strain distribution within BCC polycrystals - How does the local grain neighbourhood influence strain localization — ●KONRAD PRIKOSZOVICH¹, JONATHAN WRIGHT², WOLFGANG LUDWIG^{2,3}, PATRIC GRUBER¹, and CHRISTOPH KIRCHLECHNER¹ — ¹Institute for Applied Materials IAM, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — ²ESRF- European Synchrotron Radiation Facility, Grenoble, France — ³MATEIS, INSA Lyon, Villeurbanne, France

Strain and stress heterogeneities determine the lifetime and failure of structural materials. The relationship between macroscopic and microscopic stresses is central for a quantitative understanding of the mechanical behaviour of polycrystalline materials. We performed Diffraction Contrast Tomography (DCT) measurements at ID11, ESRF, to determine the shape, arrangement, orientation and average elastic strain tensor of a representative ensemble of grains during mechanical loading. Here, we want to present our results from the latest beam time, where we managed to investigate up to 10000 grains during tensile deformation. Different annealing protocols have been utilized prior to the experiments to vary the eigenstrains of our samples in order to investigate how those eigenstrains affect the strain localization during loading. By analysing the different local microstructural aspects present in this unique dataset, we hope to identify parameters, which promote strain localization. This information can then be used to design microstructures with improved resilience against strain localization, leading to a higher lifetime of structural materials.

KFM 9: KFM Poster Session

Chair: Anna Grünebohm (RUB), Theo Scherer (KIT)

Time: Monday 18:00–20:00

Location: Poster E

KFM 9.1 Mon 18:00 Poster E

Modelling backscattered positron capture at the FRM II coincidence Doppler broadening spectrometer — ●DANNY R RUSSELL, FRANCESCO GUATIERI, LEON CHRYSOS, and CHRISTOPH P HUGENSCHMIDT — FRM II - Technische Universität München, München, DE

The coincidence Doppler broadening spectrometer (CDBS) at the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) provides state-of-the-art, depth dependent detection of defects and chemical composition at the annihilation site. A monoenergetic positron micro-beam (50 μm FWHM) is guided onto a sample where positrons annihilate with electrons. The Doppler broadening of the characteristic 511 keV annihilation peak is measured by observing both emitted photons simultaneously.

The measurement quality depends on the size and energy of the beam. However, up to $\sim 40\%$ of the incident positrons are backscattered at the sample surface. The annihilation events occurring when these backscattered positrons return to the sample or annihilate in experimental hardware contribute unwanted signal to the measured spectrum. We present simulations and hardware design for an upgrade to the CDBS which will allow backscattered positron capture. We use an in-house particle tracking code to design a positron dump that will capture backscattered positrons at a negatively biased electrode and will be shielded from detector lines of sight. This will remove the unwanted signal from the detected spectrum and improve the quality of CDBS data.

KFM 9.2 Mon 18:00 Poster E

High Active Labile Oxygen Due to Special Lattice Oxygen Structure — ●LINFENG SU¹, XU CHEN², HUAPING ZHAO¹, ZHIYI LU², and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²Key Laboratory of Advanced Fuel Cells and Electrolyzers Technology of Zhejiang Province, Ningbo Institute of Materials Technology and Engineering, CAS, Ningbo, Zhejiang, 315201, PR China

The difference between such active lattice oxygens and inactive lattice oxygens has not been thoroughly investigated. A unique oxygen structure was successfully synthesized at low temperatures, which is similar to the lattice oxygen structure but with higher activity. With the various characterize methods, the unique oxygen structure was determined as labile oxygen, which distinguishes it from ordinary lattice oxygen. As shown in the characterization of our research, the bridging oxygen between AlO_4 and other structures is identified as labile oxygen with relatively high activity. The activity of labile oxygen was proved by catalytic ozonation, which showed excellent performance with a high quasi-first order rate constant. Operando Raman and DFT simulations further proved that Olab acted as the catalytic active center, which activates ozone via an unusual surface peroxide pathway to generate surface high-oxidative Olab-O^* species. The research on the unique oxygen structure of silicate-aluminate provides theoretical guidance for the design and synthesis of catalysts with high catalytic activities for future industrial applications.

KFM 9.3 Mon 18:00 Poster E

High-performance rechargeable Na ion batteries based on berlin green cathode materials — ●PING HONG, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Prussian blue analogs (PBAs) are considered as promising carrier frameworks owing to their low cost and well-defined ion diffusion channels. And among them, Berlin Green (BG), distinguished by its ideal cathode plateau and unique framework structure has, has been extensively investigated. It can limit its cycle stability and rate performance in batteries. Thus, researchers solved this issue by adding various chelating agents to the synthesis process. Despite the successful synthesis of low-defect BG, the method's low yield and challenging washing conditions are not beneficial for practical applications. Therefore, in this work, a simple one-step precipitation method was used to syn-

thesize BG without the addition of any chelating agent. Synthesized cathode materials exhibit remarkable electrochemical properties. At a current density of 1 A/g, the capacity maintains at approximately 100 mAh/g in sodium-ion batteries. This research emphasizes that making simple adjustments to the synthesis process can significantly reduce the defects of cubic BG. This enables the preparation of cathode materials with excellent rate performance and cycle life, eliminating the necessity for any costly and complex treatment processes.

KFM 9.4 Mon 18:00 Poster E

Exploring the influence of pH and current density on zinc morphology via the electrodeposition method — ●DHARANI MADHAVI BUNDHOOA, JIAJIA QIU, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

This study investigates the impact of pH and current density on the morphology of zinc electrodeposits, intending to fabricate a dendrite-free anode. Characterization through SEM and XRD demonstrated that lower pH levels fostered more uniform growth, resulting in reduced dendritic formations. Moreover, tuning the current density for optimal values further enhanced homogenous growth, providing essential insights for the design of composite anode materials. The findings highlight the connection between zinc deposit morphology and superior electrochemical performance in relation to the applied electrodeposition current density and the pH of the electrolyte.

KFM 9.5 Mon 18:00 Poster E

Inspiring n-type redox reactions in carboxylated polyaniline for stable non-aqueous sodium/potassium-ion batteries — ●CHENGZHAN YAN, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany.

Polyaniline (PANI) plays a multifaceted role in energy storage because of its tunable composition, structure and morphology. In non-aqueous sodium/potassium-ion batteries, PANI is a prime organic cathode with p-type anion storage. However, its specific capacity is limited owing to the partial utilization of the chain and is of ease decay in changeable electrochemical environments. Moreover, n-type redox sites that co-exist with the p-type sites have not received much attention because they are difficult to introduce by in situ chemical oxidation. To this end, the elucidation of n-type reaction in PANI chain and its practice are urgently needed. Herein, a series of carboxylated polyaniline copolymers (named PA2A) are synthesized with a high proportion of quinoid nitrogen. PA2A delivers a high specific capacity of more than 300 mAh/g at a low current density. To further improve the rate performance, PA2A is post-treated by ammonia to achieve a self-doped chain structure (named PA2A-de). This structure greatly accelerates the n-type reaction kinetics and a low-carboxylated PA2A-de has a high capacity retention of over 70% as the current density increases 20 times from 0.1 A/g to 2 A/g. Besides, the long lifespan of PA2A-de is proven to be sustained in ether-based electrolytes.

KFM 9.6 Mon 18:00 Poster E

Building non-dendritic and activity-enhanced sodium CO₂ batteries via distorted FeCu interface — ●CHANGFAN XU, TZUCHIN HUANG, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Constructing suitable multifunctional electrodes for dendrite-free anodes and kinetics-enhanced CO₂ cathodes is considered one of the most important ways to further advance the practical application of Na-CO₂ batteries. Herein, FeCu nanoparticles grown on carbon paper (CP@FeCu) are rationally designed and employed as both Na anode and CO₂ cathode in Na-CO₂ batteries. The outstanding electrical conductivity, superior sodiophilicity, and high catalytic activity of CP@FeCu electrodes can simultaneously contribute to homogenous Na⁺ distribution and dendrite-free sodium structure, and strengthen discharge and charging kinetics. The morphological evolution confirms uniform deposition of Na on CP@FeCu anode with dense and flat interfaces, delivering enhanced Coulombic efficiency and cycling stabil-

ity. Meanwhile, Na-CO₂ batteries with CP@FeCu cathode demonstrates low overpotentials and excellent cycling stability. Significantly, excellent electrochemical properties are obtained in the full battery (CP@FeCu@Na || CP@FeCu), laying the foundation for practical applications of Na-CO₂ batteries.

KFM 9.7 Mon 18:00 Poster E

Sodiation-induced reactivation of micro-nano flower for long cycling life sodium-ion batteries — ●YUHUA CHEN, YULIAN DONG, HUAPING ZHAO, and YONG LEI — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

A rational micro-nano hierarchical structure is demonstrated to prolong the cycle life of sodium-ion batteries (SIBs) by relieving the volume expansion and preventing active material agglomeration. In this work, micro-nano flower 3D-VSx was fabricated as an anode electrode for SIBs. The advanced features of micro-nano flower and the unique crystal structures of NiAs-type vanadium sulfides synergistically contribute to enhancing the electrochemical kinetics of 3D-VSx, and finally achieved remarking electrochemical performances with an ultra-high capacity (961.4 mA h g⁻¹ at 2 A g⁻¹) and an ultra-long cyclability (more than 1500 cycles). Furthermore, ex situ X-ray diffraction and SEM bring to light a gradual reactivation process of 3D-VSx for sodium storage. Fortunately, upon reactivation, the electrochemical impedance of the 3D-VSx anode gradually weakens, and the diffusion-controlled charge storage mode further dominates compared to the capacitively-controlled mode, all of which facilitate the 3D-VSx to maintain a stable sodium storage capability. This work presents a general approach for preparing super-high specific capacity and rate capacity electrode materials for further improving the SIBs performance.

KFM 9.8 Mon 18:00 Poster E

Monte Carlo Simulation of Phase Transition from Crystalline to Amorphous Diamond — ●FLORIN HEMMANN, ULLRICH STEINER, and MATTHIAS SABA — Adolphe Merkle Institute, University of Fribourg, Switzerland

Continuous random networks model many amorphous materials, such as amorphous semiconductors [1] and disordered photonic structures found in animals and plants [2,3]. Such networks can be generated efficiently using a Monte Carlo bond-switch move proposed by Wooten, Winer, and Weaire [4]. As Vink observed, this algorithm breaks ergodicity. It is, therefore, only suited to model networks at zero temperature [5]. He overcame this limitation by including thermal fluctuations in the Monte Carlo move and simulated a structural phase transition in a 2D 3-coordinated network. We apply this finite-temperature Monte Carlo method to simulate the structural phase transitions in a 3D 4-coordinated network model, the transitions from a crystalline to an amorphous diamond. We characterize the phase transitions by means of the network's structure factor and local bond order parameters.

- [1] B. Haberl et al. (2009), Phys. Rev. B 79, 155209.
- [2] V. Bauerfeind et al. (2023), Adv. Funct. Mater. 2302720.
- [3] E. Moyroud et al. (2017), Nature 550, 469-474.
- [4] F. Wooten et al. (1985), Phys. Rev. Lett. 54, 1392.
- [5] R. L. C. Vink (2014), J. Chem. Phys. 140, 104509.

KFM 9.9 Mon 18:00 Poster E

Synthetic diamond for windows of the Heating & Current Drive System of ITER — ●SABINE SCHRECK¹, GAETANO AIELLO¹, PABLO ESTEBANEZ², ANDREAS MEIER¹, THEO SCHERER¹, DIRK STRAUSS¹, CHRISTOPH WILD³, and ECKHARD WÖRNER³ — ¹Karlsruhe Institute of Technology, Institute for Applied Materials, 76021 Karlsruhe, Germany — ²Fusion for Energy, 08019 Barcelona, Spain — ³Diamond Materials GmbH & Co. KG, 79108 Freiburg, Germany

With the aim to heat and stabilize the plasma of the ITER research reactor microwave radiation of around 1 MW power needs to be guided from gyrotrons into the plasma. This requires a number of windows that guarantee vacuum tightness, tritium confinement and high microwave transmission. The key component of such windows is a transparent disk made of synthetic polycrystalline diamond. Produced by an optimized microwave plasma assisted chemical vapor deposition (MPA-CVD) process, and after a specific post-processing the disks (D=70mm, d=1,11mm) typically exhibit a very low loss tangent (< 2*10⁻⁵). Because of the windows safety function each single disk, manufactured by Diamond Materials, needs to pass a qualification process, including the determination of the dielectric loss at disk center and its distribu-

tion over the disk area. At KIT dedicated Fabry-Perot resonators are used for the loss measurements. Further, optical inspections with a digital microscope and a determination of possible polarization effects are performed. Under a contract with F4E more than 25 disks (out of 60) have been already qualified and first conclusions can be made.

KFM 9.10 Mon 18:00 Poster E

Dynamics of the electrocaloric effect: High-resolution measurements on microsecond timescales — ●JAN FISCHER, DANIEL HAEGELE, and JOERG RUDOLPH — Ruhr University Bochum

The electrocaloric effect (ECE) in ferroelectrics is a promising candidate for improved cooling technologies and small cooling devices. While direct and reliable measurements of the reversible adiabatic temperature change ΔT as a caloric key parameter are already challenging, an access to the full dynamics $\Delta T(t)$ of the ECE and the correlation with the ferroelectric properties are highly desirable for a more fundamental understanding of the ECE.

Here, we present a direct and contactless method to investigate the temperature change $\Delta T(t)$ of the ECE with mK temperature resolution and μ s temporal resolution via the infrared emission of the sample. Ferroelectric properties are simultaneously recorded [1]. Measurements on material systems with a first order and a diffuse phase transition, respectively, show characteristic changes of the field dependence of the ECE as fingerprints of the order of the phase transition. Systematic studies of the frequency dependence of the ECE allow, e.g., to separate extrinsic effects like heat transport from the pure caloric temperature change. High-frequency measurements up to kHz further allow the direct measurement of ΔT even for μ m thin samples [2, 3].

- [1] J. Fischer, *et al.*, Review of Scientific Instruments 94, 4 (2023)
- [2] J. Döntgen, *et al.*, Energy Technology 6, 8 (2018)
- [3] J. Döntgen, *et al.*, Applied Physics Letters 106, 3 (2015)

KFM 9.11 Mon 18:00 Poster E

Ab initio determination of the Curie temperature of stoichiometric LiNbO₃ and LiTaO₃ crystals — ●FELIX BERNHARDT and SIMONE SANNA — Institut für theoretische Physik and Center for Materials Research, Justus-Liebig-Universität Gießen, Germany

Lithium niobate (LN) and lithium tantalate (LT) are ferroelectric crystals with a wide range of applications. As for some of them (i.e., in sensors) operation at high temperature is required, it is vital to understand their phase transition from the high-temperature, paraelectric phase to the low-temperature, ferroelectric phase. For low temperatures, LN and LT both exhibit a trigonal symmetry (R3c). The transition into a R $\bar{3}$ c symmetry at 1480K and 940K respectively is achieved mainly by a displacement of the central Li-ion in z-direction.

Here, the Curie-temperature of these two crystals is studied by employing the stochastic-self-consistent harmonic approximation (SSCHA). Within this method, the free energy of the crystal is minimized by optimizing the nuclear wave-function. Furthermore, the thermal expansion is taken into account by means of the quasi-harmonic approximation.

Inside these frameworks, phononic properties can be computed at a non perturbative level, including anharmonic effects. The comparison of phonon frequencies calculated within the common harmonic approximation implies non-negligible anharmonic contributions to both materials. By evaluating these refined phononic dispersions, we can determine the Curie-temperature by calculating and comparing the corresponding free energies of both phases.

KFM 9.12 Mon 18:00 Poster E

Investigation of intrinsic defect formation energies in lithium niobate-tantalate solid solutions. — ●NILS ANDRE SCHÄFER and SIMONE SANNA — Institute for Theoretical Physics, Justus Liebig University Giessen, Germany

The optical response of LiNbO₃ (LN) and LiTaO₃ (LT) is influenced, among other properties, by intrinsic defects. In particular, spectroscopic signatures of quasiparticles known as polarons are a hallmark of LN and LT, respectively. Unfortunately, very little is known about the intrinsic defects in LiNb_{1-x}Ta_xO₃ solid solutions (LNT), which are employed to tune the materials properties by composition. In order to improve our understanding of the defect structure in LNT, we model different microscopic realizations of small bound polarons, bipolarons as well as lithium vacancies.

We systematically explore changes in the formation energy of microscopic polaronic structures across varying concentrations of LNT. Additionally, we investigate the existence of a preferred positions of these defects within LNT. Our atomistic calculations were carried out

using the DFT+U method as implemented in VASP.

KFM 9.13 Mon 18:00 Poster E

Investigation of hydrogen diffusion in LiNbO₃ from density-functional theory — ●CHRISTA FINK and SIMONE SANNA — Institute for Theoretical Physics, Justus Liebig University Giessen, Germany

Hydrogen is always present in LiNbO₃ crystals. Therefore, the lattice location of hydrogen within the crystal as well as its diffusion and mobility have been a matter of research for many years. While the energetically most favorable positions of hydrogen within the atomic lattice have been investigated intensely and suggest mostly comparable results [1, 2, 3], there exist less investigations of diffusion path and energy barriers [3]. To fully understand the hydrogen diffusion in LiNbO₃ and to complete the current knowledge on this topic, we calculate energy barriers and three-dimensional minimum energy paths for hydrogen diffusion using the nudged elastic band method based on density-functional theory as implemented in VASP [4, 5]. Starting from the energetically most favorable position, we calculate the minimum energy path through the crystal towards the next equivalent position. [1] H. H. Nahm, C. H. Park, Appl. Phys. Lett. 78, 3812-3814 (2001). [2] K. Lengyel et al., IOP Conf. Ser.: Mater. Sci. Eng. 15, 012015 (2010). [3] T. Köhler et al., J. Mater. Chem. C 11, 520-538 (2023). [4] G. Kresse, J. Furthmüller, Computational Materials Science 6, 15 (1996). [5] G. Kresse, J. Furthmüller, Phys. Rev. B 54, 11169 (1996).

KFM 9.14 Mon 18:00 Poster E

Stability of Mixed Cation Hybrid Perovskites Using DFT -1/2 — MWANAI NAMISI¹, ●MOHAMMAD MOADDELI², MANSOUR KANANI², and ANNA GRÜNEBOHM¹ — ¹Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany — ²Department of Materials Science and Engineering, School of Engineering, Shiraz University, Shiraz, Iran

Hybrid perovskites APbX₃(A=MA, FA ; X=Br, I) have emerged as prominent materials owing to their diverse applications in photovoltaics [1] and potential for caloric cooling [2]. Their structural stability, polarizability, field-induced changes of entropy as well as their electronic structure depend on the choice of the A and X cations [3]. However, the impact of the choice and combination of these ions is not fully understood. Here, we investigate the structural and electronic properties of hybrid and mixed cation APbX₃ using the DFT-1/2 approach. We show that structural stability is enhanced in mixed cation systems and explore the materials* potential for caloric cooling.

References

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KFM 9.15 Mon 18:00 Poster E

Synthesis of Aero-ZnS micro-nanoarchitectures on 3D networks of sacrificial ZnO microtetrapods — ●TUDOR BRANISTE¹, VLADIMIR CIOBANU¹, IRINA JIN¹, VEACESLAV URSAKI^{1,2}, VICTOR ZALAMAI¹, EMIL RUSU³, VADIM MORARI³, RAINER ADELUNG⁴, and ION TIGINYANU^{1,2} — ¹National Center for Materials Study and Testing, Technical University of Moldova, Stefan cel Mare Ave. 168, MD-2004 Chisinau, Republic of Moldova — ²Academy of Sciences of Moldova, Stefan cel Mare Ave. 1, MD-2001 Chisinau, Republic of Moldova — ³Institute of Electronic Engineering and Nanotechnology, Technical University of Moldova — ⁴Institute for Materials Science, Kiel University, Kaiserstrasse 2, D-24143 Kiel, Germany

Aeromaterials are a new class of highly porous materials that attract increasing interest due to their potential applications in electronics, sensorics, microfluidics, etc. In this work, we report on fabrication of aero-ZnS by using two technological approaches: hydride vapor phase epitaxy (HVPE) and physical vapor transport (PVT) on sacrificial templates consisting of networks of ZnO interconnected microtetrapods. The aero-ZnS fabrication based on HVPE resides in growth of CdS on sacrificial micro-tetrapods of ZnO with subsequent transformation of CdS into ZnS and removal of the sacrificial ZnO core. For the aero-ZnS fabrication by PVT, the Sn₂S₃ crystals and networks of ZnO microtetrapods were used as precursors. The morphology of the produced material was investigated by SEM, while its crystalline and optical quality is assessed by X-ray diffraction analysis and PL spectroscopy, respectively.

KFM 9.16 Mon 18:00 Poster E

An X-ray diffraction studie on AlCrVY(O)N thin films — ●ERIC SCHNEIDER¹, MICHAEL PAULUS¹, FINN ONTRUP², NELSON FILIPE LOPES DIAS², and WOLFGANG TILLMANN² — ¹Fakultät Physik/DELTA TU Dortmund University, 44221 Dortmund, Germany — ²Institute 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 different AlCrN, AlCrVYN, AlCrVYON coatings. For this purpose, the coating systems were deposited on a WC-Co composite substrate by direct-current magnetron sputtering (dcMS), high power impulse magnetron sputtering (HiPIMS) and a hybrid dcMS/HiPIMS process. For the investigation of the samples we used synchrotron radiation at beamline BL9 of the synchrotron radiation source DELTA (Dortmund, Germany). 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 by X-ray diffraction. We thank DELTA for providing synchrotron radiation. This work was supported by the DFG via TO 169/21-1.

KFM 9.17 Mon 18:00 Poster E

ASCII: The Ultra-Low Energy Ion Implantation of Radioisotopes for Surface Characterization at ISOLDE-CERN — ●NICOLE PEREIRA DE LIMA^{1,2}, HANNES GÜRLICH^{2,3}, JULIANA SCHELL^{2,4}, KOEN VAN STIPHOUT^{5,6}, LUKAS M. ENG³, MAGNUS HEGELUND^{2,7}, DORU LUPASCU⁴, BRUNO CORREA¹, LEVY SCALISE¹, BORIS KOPITZ³, SAMUEL SEDDON³, and HANS HOFSSÄSS^{2,6} — ¹University of Sao Paulo, Sao Paulo, Brazil — ²European Organization for Nuclear Research (CERN) — ³Technische Universität Dresden (TUD) — ⁴University Duisburg-Essen — ⁵KU Leuven — ⁶University of Göttingen — ⁷Aalborg University

In solid-state physics, radioactive isotopes have been used for a long time to study the crystallographic, electric, and magnetic characteristics of nanostructures. The favored technique for introducing radioactive nuclei into the crystal structure is ion implantation at energies between 1 and 100 keV. However, the increased scientific interest in 2D materials, multiferroics, and especially their interfaces demands different approaches to isotope implantation.

Thus, the ASCII chamber's purpose is to decelerate and then implant radioactive ions (usually PAC-isotopes) at various energies, including ultra-low energies (> 20 eV). When implanting with these low energies, as in the initial ASPIC chamber, an extremely high vacuum of up to $p < 10^{-9}$ mbar is required. All these improvements will allow us to study hyperfine techniques on multiple systems. ASCII is therefore an innovative instrument system that promises to contribute to surface and interface research in solid-state physics.

KFM 9.18 Mon 18:00 Poster E

Defects, Fine and Hyperfine Interactions of the Historical Prussian Blue Compound Giese-Salt: Ammonium-Ferric-Hexacyano-Ferrate — ●SASCHA ALBERT BRÄUNINGER¹, DAMIAN ALEXANDER MOTZ¹, FELIX SEEWALD², SEBASTIAN PRAETZ³, CARLA VOGT⁴, BIRGIT KANNENGIESSER³, HANS-HENNING KLAUSS², and HERMANN SEIFERT¹ — ¹Institute for General Radiology and Medical Physics, University of Veterinary Medicine Hannover Foundation, Bischofsholer Damm 15, Hanover, 30173, Lower Saxony, Germany — ²Institute of Solid State and Materials Physics, TU Dresden, Haackelstraße 3, Dresden, 01069, Saxony, Germany — ³Institute of Optics and Atomic Physics, TU Berlin, Hardenbergstraße 36, Berlin, 10623, Berlin, Germany — ⁴Institute of Analytical Chemistry, TU Bergakademie Freiberg, Leipziger Straße 29, Freiberg, 09599, Saxony, Germany

Prussian Blue compounds (PBC) have shown a huge potential of applications in physics, chemistry, medicine and radioecology, e.g., selected PBC are acting as efficient ion exchanger extracting the radioisotope ¹³⁷Cs in solutions. In this study, the focus is the PBC ammonium iron(III) hexacyanoferrate(II) (NH₄{Fe(III)[Fe(II)(CN)₆}]₂), also known as *Giese-salt*, which is the ammonium derivative of the classic ("soluble") Prussian Blue as applied in veterinary medicine. Here, we investigate the Giese salt by a variety of techniques (XRD, ATR-IR, REM,...) highlighting the results of our Raman, XAFS and ⁵⁷Fe-Mössbauer study confirming a local distribution of hyperfine parameters as expected for a disordered system.

KFM 9.19 Mon 18:00 Poster E

Leveraging Automatic Differentiation in Complex Model Fitting — ●ERIK THIESSENHUSEN¹, RITZ AGUILAR¹, MICHAL

SMID¹, THOMAS KLUGE¹, MICHAEL BUSSMANN^{1,2}, THOMAS COWAN¹, NICO HOFFMANN¹, LINGEN HUANG¹, and JEFFREY KELLING¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf — ²Center for Advanced System Understanding

Understanding laser-solid interactions is important for the development of laser-driven particle and photon sources, e.g., tumor therapy, astrophysics, and fusion. Currently, these interactions can only be modeled by simulations that need to be verified experimentally. Consequently, pump-probe experiments were conducted to examine the laser-plasma interaction that occurs when a high intensity laser hits a solid target. Since we aim for a femtosecond temporal and nanometer spatial resolution at European XFEL, we employ Small-Angle X-ray Scattering (SAXS) and Phase Contrast Imaging (PCI) that can each be approximated by an analytical propagator. In our reconstruction of the target, we employ a gradient descent algorithm that iteratively minimizes the error between experimental and synthetic patterns propagated from proposed target structures. By implementing the propagator in PyTorch we leverage the automatic differentiation capabilities, as well as the speed-up by computing the process on a GPU. We perform a scan of different initial parameters to find the global minimum, which is accelerated by batching multiple parallel reconstructions.

KFM 9.20 Mon 18:00 Poster E

Raman spectroscopy on KNbO₃ single crystal: investigation of phase transitions, ferroelastic domains and dislocations — ●FELIX DRECHSLER¹, CAMELIU HIMCINSCHI¹, OLIVER PREUSS², XUFEI FANG², and JENS KORTUS¹ — ¹TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg, Germany — ²TU Darmstadt, Department of Materials and Earth Sciences, Division Nonmetallic-Inorganic Materials, D-64287 Darmstadt, Germany

We investigated a KNbO₃ single crystal with Raman spectroscopy regarding phase transitions, ferroelastic domains and mechanically imprinted dislocations. In a temperature range between 150 K and 550 K the material passes two phase transitions from the rhombohedral crystal structure (C_{3v}) at low temperatures to orthorhombic (C_{2v}) at room temperature and to tetragonal (C_{4v}) at high temperatures. A thermal hysteresis could be observed. Due to the changes in crystal structure, Raman spectroscopy is a suitable method to investigate phase transitions. With the help of 1D and 2D Raman mappings it was possible to determine the size of strip-like ferroelastic domains. We carried out extensive Raman investigations on mechanically imprinted dislocations in the ceramic KNbO₃. There were clear differences in the Raman spectra between the dislocation areas and the pristine material. These were also observed in the temperature-dependent Raman measurements during the transition from rhombohedral to orthorhombic phase, which remained until the second phase transition. A correlation between dislocation density and peak position was also found.

KFM 9.21 Mon 18:00 Poster E

Helium Interaction with Atomic Level Defects in Tungsten Studied by Positron Annihilation Spectroscopy — ●VASSILY VADIMOVITCH BURWITZ^{2,1}, ANNEMARIE KÄRCHER^{2,3}, THOMAS SCHWARZ-SELINGER³, MAIK BUTTERLING⁵, ERIC HIRSCHMANN⁵, EMMA HUNTLEY¹, ADRIAN LANGREHR¹, MACIEJ OSKAR LIEDEKE⁵, LUCIAN MATHES^{2,1}, CHRISTOPH SPRINGL¹, MONIA VADRUCCHI⁴, ANDREAS WAGNER⁵, and CHRISTOPH HUGENSCHMIDT¹ — ¹Heinz Maier-Leibnitz Zentrum, TU München — ²TU München, School of Natural Sciences, Physics Department — ³MPI für Plasmaphysik, Garching bei München — ⁴ENEA Frascati, Development of Particle Accelerators and Medical Applications — ⁵Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics

Understanding the type and evolution of lattice defects in tungsten (W) is of interest in nuclear fusion materials research. We therefore investigated W(111) mono-crystals by positron annihilation Doppler-broadening spectroscopy (DBS) and positron annihilation lifetime spectroscopy (PALS). Both complementary methods are sensitive tools for the examination of the defect type and concentration. The literature currently lacks conclusive experimental work regarding the influence of He decoration of vacancies on PAS. We therefore irradiated samples by 4.5 MeV electrons to different damage levels in order to specifically produce mono-vacancies in W. We will present DBS and PALS measurements, both performed with a slow positron beam, before and after plasma loading with 50 eV He ions. The implantation energy is chosen low enough to prevent displacement damage.

KFM 9.22 Mon 18:00 Poster E

Using convolutional networks to predict the long term evolu-

tion of a multiphasic material — ●SHING WAN and NIGEL CLARKE — Department of Physics and Astronomy, University of Sheffield, Sheffield, UK

Understanding the solidification and morphology of alloys has gathered resurgent interest with the recent advancements in metallic based additive manufacturing and low dimensional materials such as graphenes. The physical property of a material such as flexibility, tensile strength among others depends on the morphology of the material. The morphology can be inferred using the distribution of interfaces, regions between grains/phases, throughout the material.

Morphological properties of a material acquired via experiments can be represented as an image. This transforms the task of morphological evolution prediction to a frame prediction /generation task similar to those used in video games.

We are developing a machine learning approach to predicting microstructure evolution. Our methodology is based on a convolutional autoencoder in combination with a convolutional Long Short Term Memory. To investigate the effectiveness of the machine learning model, we used grain growth evolution of a multiphase alloy system, simulated using multiphase field theory.

KFM 9.23 Mon 18:00 Poster E

Nanoscale 3D chemical mapping of functional oxides using atom probe tomography — ●KATHARINA WOLK, KASPER A. HUNNESTAD, CONSTANTINOS HATZOGLOU, JULIA GLAUM, and DENNIS MEIER — Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), 7491 Trondheim, Norway

The functional properties of oxide materials are closely linked to their chemical composition and their three dimensional atomic-scale structure. To better understand the local defect-property relations in complex oxides and obtain quantitative information at the unit cell length scale, we apply atom probe tomography (APT). APT is an advanced analytical method that enables 3D compositional mapping with chemical sensitivity better than 100 ppm and sub-nanometer spatial resolution.

Here, I give a basic introduction to APT and present how to use focused ion beam (FIB) nanostructuring to prepare needle-shaped specimens for the analysis by APT. As an instructive example for information that can be extracted via APT analysis, I show a 3D needle reconstruction, which exhibits pronounced chemical variations at the nanoscale. Our research is applicable to a wide range of oxide systems, giving new opportunities for their characterization and defect-driven property engineering.

KFM 9.24 Mon 18:00 Poster E

Interplay between Defects and Ferroelectric Domain Wall Properties — ●EGIL Y. TOKLE¹, LEONIE RICHARZ¹, EDITH BOURRET², ZEWU YAN^{2,3}, and DENNIS MEIER¹ — ¹NTNU Norwegian University of Science and Technology, Trondheim, Norway — ²Lawrence Berkeley National Laboratory, Berkeley, CA, USA — ³ETH Zurich, Switzerland

Ferroelectric domain walls are natural interfaces separating volumes with different orientation of the spontaneous polarization. These walls can display fundamentally different conduction properties than the surrounding material. For instance, the conductance at domain walls in hexagonal manganites can range from insulating to highly conducting relative to the ferroelectric domains. Interestingly, the transport behavior correlates with the oxygen off-stoichiometry of the system. In previous studies, we observed that annealing in reducing atmosphere can significantly increase the relative domain wall conductance.

In this work, we systematically study the influence of different annealing parameters - such as annealing temperature and dwell time - and monitor the impact on the electronic transport behavior of domain walls Er(Mn,Ti)O₃, using conducting atomic force microscopy. Our results provide new insights into the underlying microscopic mechanisms and give detailed guidelines for property engineering at the level of the domain walls.

KFM 9.25 Mon 18:00 Poster E

KPFM imaging and magnetic resonance detection of single nitrogen-vacancy centers in diamond — ●SERGEI TROFIMOV, KLAUS LIPS, and BORIS NAYDENOV — Berlin Joint EPR Laboratory and Department Spins in Energy Conversion and Quantum Information Science (ASPIN), Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Nitrogen-vacancy (NV) centers are color defects in diamond that are used for quantum sensing with high sensitivity and nano-scale spatial resolution. The spin-dependent luminescence allows optical readout of the NV spin state. Furthermore, electrical detection of NV centers, based on spin-dependent photocurrent, has been recently reported [1]. It opens a route to manufacturing compact sensors utilizing NV centers.

Here we present an alternative detection scheme – photovoltage imaging of single shallow NV centers using Kelvin probe force microscopy (KPFM) under laser excitation with moderate power (less than 1 mW). To conduct these experiments, a confocal microscope was combined with an AFM system, where scanning probe and optical imaging could be performed simultaneously. Moreover, we demonstrate that the electron spin state of single NV centers can also be detected with KPFM. We refer to this technique as VDMR (voltage-detected magnetic resonance). The results suggest that photovoltage detection of NV centers could be another solution on the way to compact quantum sensing devices.

[1] P. Siyushev *et al.*, *Science* 363, 728 (2019).

KFM 9.26 Mon 18:00 Poster E

Laser-induced crystallization of Sb₂S₃ and GeSe at different excitation wavelengths — ●RAMON PFEIFFER, MAXIMILIAN MÜLLER, and MATTHIAS WUTTIG — Institute of Physics (IA), RWTH Aachen University, 52074 Aachen, Germany

The laser-induced crystallization of materials such as Sb₂S₃ and GeSe at a wavelength of 658 nm requires high laser powers to recrystallize an amorphous region. Even higher powers are needed to induce vitrification back into the glassy phase. Since these materials possess a much higher absorption coefficient at shorter wavelength, more efficient switching is expected employing a blue laser diode. A shorter wavelength, and hence a reduced spot size, also results in a smaller possible device structure. For this reason, we have implemented a laser with a wavelength of 405 nm into the 658 nm setup of our optical phase change tester. This enables a straightforward comparison of the switching properties of different compounds.

KFM 9.27 Mon 18:00 Poster E

High pressure hydrostatic cells for X-ray scattering applications — ●KEVIN LEHNINGER¹, MICHAEL PAULUS¹, CHRISTIAN STERNEMANN¹, and PATRICK DEGEN² — ¹Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — ²Carl Bechem GmbH, 58089 Hagen, Germany

Small-angle and wide-angle X-ray scattering (SAXS/WAXS) at moderate pressures are of increasing importance for the investigation of e.g. protein denaturation or stimulus-responsive materials. One of the experimental challenges are the precise pressure control in the pressure range up to 10 kbar with simultaneous separation of the sample volume from the pressure-transmitting medium at the largest possible opening angle. We present a pressure- and temperature dependent SAXS/WAXS study of greases and motivate two hydrostatic high-pressure cells dedicated for use at beamlines BL2 and BL9 of the DELTA synchrotron radiation source (Dortmund, Germany). The WAXS cell with an opening angle of 60 degrees enables a sample volume with a cross-sectional area of one square millimetre to be exposed to a maximum pressure of 5 kbar, while the SAXS cell can be operated up to a pressure of 10 kbar, providing an opening angle of 20 degrees.

KFM 9.28 Mon 18:00 Poster E

Exploring the bonding in quasicrystals — ●FELIX MEESSEN¹, JAN KÖTTGEN¹, MICHAEL FEUERBACHER³, CHRISTIAN STENZ¹, THOMAS SCHMIDT¹, JONATHAN FRANK¹, YUAN YU¹, and WUTTIG MATTHIAS^{1,2,4} — ¹Institute of Physics (IA), RWTH Aachen University, 52074 Aachen, Germany — ²JARA Institute "Energy-efficient information technology (PGI-10)", RWTH Aachen University, Germany — ³Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen (ER-C), Forschungszentrum Jülich GMBH, 52428 Jülich, Germany — ⁴JARA-FIT, RWTH Aachen University, Germany

Quasicrystals are a fascinating class of materials. The characteristics and properties are neither typical for covalent compounds nor metals. Instead, the electrons in these solids are in the critical state between delocalization as in metals and localization as in covalent solid. Hence, we have employed Atom Probe Tomography (APT) to investigate the bonding characteristics of quasicrystals, specifically AlPdMn, ZnMgDy, and an AlPdMn approximant. Our focus has been to establish a correlation between the bond-breaking behavior observed in APT and its effects on electrical conductivity, particularly at the crit-

ical juncture of electron localization and delocalization. Additionally, we have explored the impact of these atomic-scale interactions on optical properties using Fourier Transform Infrared Spectroscopy (FTIR). The central theme of our study is to understand how these phenomena relate to multivalent bonding. Our findings provide significant insights into the electrical, optical and bonding behavior of these complex materials, offering a deeper understanding of their unique properties.

KFM 9.29 Mon 18:00 Poster E

QuaCCAToo - Quantum Colour Centres Analysis Toolbox — ●ANMOL SINGH, LUCAS TSUNAKI, SERGEI TROFIMOV, and BORIS NAYDENOV — Department Spins in Energy Conversion and Quantum Information Science (ASPIN), Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Colour centres are prominent in different fields of quantum technologies: sensing, computing, communication, and cryptography due to their relative stability, and manoeuvrability. This attracts the attention of an increasing number of academic researchers, students and industry members. A free and open platform allowing one to quickly visualise and simulate the behaviour of these systems would help in further advancement of the field not just in a research setting but also as a pedagogical tool. We present here, an alpha version of QuaCCAToo, a set of Python modules for performing simulations and analysis of NV centres in diamond. We focus initially on NV centres in diamond, but it can be easily extended for other colour centres, too. Python was chosen for its relative ease of use in numerics and the rich ecosystem of scientific libraries. The calculations are done on top of optimised pathways provided by QuTip and NumPy.

KFM 9.30 Mon 18:00 Poster E

Investigation of the feasibility of the re-convolution approach in positron annihilation lifetime spectroscopy using a Geant4 simulation — ●DOMINIK BORAS, DANNY PETSCHKE, and TORSTEN STAAB — Julius-Maximilians University, Würzburg, Germany

Positron lifetime spectroscopy (PALS) is a powerful technique for studying material properties at the atomic level. The iterative least-squares re-convolution approach determines the best fit of the recorded lifetime spectrum by re-convoluting a sum of N expected exponential decays with the numerical data of the experimentally obtained instrument response function. For a PALS using a sample-source-sandwich, two possible radioactive isotopes ⁶⁰Co and ²⁰⁷Pb are existing to obtain the instrument resolution function. In this study, we systematically investigated the potential of re-convolution with these isotopes using Geant4, a versatile simulation toolkit for particle interactions. Our research focused on the interaction of the gammas with different energies in the scintillator material and the resulting photomultiplier-pulses. The results shed light on the feasibility and possible benefits of employing re-convolution techniques in enhancing the precision of positron lifetime spectroscopy, offering valuable insights for future advancements in materials characterization and analysis. Here we present a detailed study on the basis of plastic scintillators regarding the spectra decomposability by using the re-convolution technique with simulated spectra by Geant4.

KFM 9.31 Mon 18:00 Poster E

Defect analysis of beta to gamma phase transition in Gallium Oxide — ●UMUTCAN BEKTAS, MACIEJ OSKAR LIEDKE, FABIAN GANSS, and GREGOR HLAWACEK — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Gallium oxide (Ga₂O₃) is a unique material for power electronics, optoelectronics, and batteries. However, controlling the metastable polymorph phases of Ga₂O₃ is challenging, and the fabrication technology at the nanoscale is immature. We aim to understand and control the polymorph conversion to establish new fabrication methods of single-phase polymorph coatings, buried layers, multilayers, and different nanostructures in Ga₂O₃.

Under ion beam irradiation, most semiconductors show the transformation from crystalline to amorphous structure due to ion beam-induced damage. However, we showed that this transformation is suppressed in Ga₂O₃, and a polymorph conversion is observed instead. Here, we analyzed the defect formation during the beta-Ga₂O₃ to gamma-Ga₂O₃ phase transition, induced by ion implantation with different ions and fluences. Characterization of the samples was conducted by Positron annihilation lifetime spectroscopy (PALS), Doppler broadening variable energy positron annihilation spectroscopy (DB-VEPAS), and X-ray Diffraction (XRD). The first results indicate that

the defect size and concentration depend on the implanted ion type, fluence, and annealing temperature. This work is supported by the state of Saxony.

KFM 9.32 Mon 18:00 Poster E

NV center creation by CW laser irradiation of nitrogen implanted diamond — ●ALEXIOUS ENKE — Universität Leipzig, Leipzig, Deutschland

Diamond as a host of color centers has been extensively studied due to its wide range of centers connected to various defects and elements. Among these defects, the nitrogen vacancy (NV) center in diamond is one of the most researched. Its high photo stability and ability for spin manipulation with long spin coherence time make it highly suitable for applications in quantum sensing and quantum information technology.

Ion implantation methods have been successful in the controlled fabrication of NV centers. However, these methods require subsequent thermal annealing to heal implantation damage and induce defect diffusion, which promotes NV center generation. The drawback is that the heating process affects the entire diamond, limiting its localized application.

Femto-second laser irradiation has been proven effective in creating vacancies and initializing color center creation in diamond in a highly localized manner. In this study, the focus is on investigating the potential of continuous wave (CW) laser irradiation as a tool for local NV center creation.

We show that this technique is suitable for the creation of NV center ensembles as well as the monitored generation of single centers. Furthermore, we try to gain insights into the dynamics and correlations of this technique and deepen the understanding of the underlying physical processes involved in the creation of NV centers.

KFM 9.33 Mon 18:00 Poster E

Lithium depth profiling with proton beam NRA — ●PATRICK KIRSCHT, FELIX JUNGE, and HANS HÖFSÄSS — Georg August Universität - II Physikalisches Institut, Göttingen

Lithium is one of the most important elements for energy storage. There are several methods available for detection - one of which is nuclear reaction analysis (NRA). The nuclear reaction $7\text{-Li}(p,\alpha)4\text{-He}$ with a Q value of 17 MeV is suitable for lithium detection [1]. Two alpha particles with 7.5 MeV each are generated, which are detected using PIN diodes. We use our Pelletron accelerator to generate a proton beam with an energy of 2.5 MeV. The aim of the investigations is to make a statement about the depth profile of the lithium which is not dominated by the statistical energy distribution of the alpha particles. For this purpose, ta-C coated silicon wafers are implanted with 30 keV lithium, measured, covered with an additional carbon layer using sputter deposition and measured again. This leads to a shift in the alpha spectrum to lower energies due to the additional energy loss in the deposited carbon. Furthermore, the experiments are simulated using the binary collision approximation (BCA) Monte Carlo program IMINTDYN [2,3]. Additionally to the aspects of ion-solid interactions, IMINTDYN offers the option of generating the NRA for a specific isotope and projectile after simulating an implantation, taking into account energy loss and deflection of the projectiles and the generated alpha particles.

KFM 9.34 Mon 18:00 Poster E

Antiferrodistortive rotations at grain boundaries in SrTiO₃ — ●PAVLÍNA KRUŽÍKOVÁ^{1,3} and DAVID R. BOWLER^{2,3} — ¹Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany — ²London Centre for Nanotechnology, London, UK — ³Department of Physics and Astronomy, UCL, London, UK

A typical property of SrTiO₃ perovskite oxide, namely the antiferrodistortive (AFD) rotations, is not yet being taken advantage of in applications. This is because it is usually only present at temperatures lower than 105 K, i.e., below the phase transition temperature. This situation could change after an experiment detected AFD rotations at a $\Sigma 13$ (510) grain boundary in SrTiO₃ at room temperature. Such temperature would allow for practical optical or electrical applications, together with the potential to use grain boundary defects for tuning the materials properties. The open source DFT code CONQUEST was used to perform cell and ionic relaxations as well as post processing, with the goal of obtaining the atomic and electronic structure of this SrTiO₃ grain boundary and further insights about the AFD mechanism. Several related systems were also studied to compare the findings, e.g., the $\Sigma 13$ (210) grain boundary, SrTiO₃ bulk with AFD rotations and SrTiO₃ bulk with O vacancies. The obtained

atomic structure matches the AFD rotations detected in experiment. Additionally, an in-plane ferroelectric displacement was identified. In the electronic structure, localised states were found at the bottom of the conduction band in the grain boundary core. Out of all studied systems, these findings were specific to this grain boundary type.

KFM 9.35 Mon 18:00 Poster E

DFT study of local ferroic properties at twin walls in ferroelastic CaMnO₃ — ●IDA CATHRINE SKOGVOLL and SVERRE MAGNUS SELBACH — Department of Materials Science and Engineering, NTNU - Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

Ferroic domain walls display compelling properties for nanoscale device applications, where suppression of the primary order parameter and local symmetry-breaking can give rise to phenomena absent in the bulk. In ferroelastic materials, twin walls exhibit breaking of inversion symmetry which can activate polar instabilities, yielding a local polarization. CaMnO₃ with space group $Pnma$, is a nonpolar antiferromagnetic material with strong spin-phonon coupling. This implies that antiferrodistortive distortions couple strongly to the magnetic structure, and that the strain field across a ferroelastic twin wall can modify local magnetic properties. It is thus a candidate material for realizing multiferroicity in a single-phase material. In this work, DFT + U calculations were carried out on ferroelastic domain walls in CaMnO₃, implementing different patterns of intra-plane and inter-plane magnetic orders, to conduct an investigation of the local magnetic properties along with the induced ion displacements. We find that the polarization profile at the wall is dependent on the type of magnetic order, as well as the local environment of octahedral distortions. Furthermore, the magnetic wall preferentially resides at the twin wall as opposed to the bulk. Finally, we discuss the emerging prospects of realizing room-temperature multiferroicity in ferroelastic domain walls.

KFM 9.36 Mon 18:00 Poster E

Coherent properties of ensembles of shallow NV centers with surface modifications on diamonds — ●CHENG-I HO¹, ROUVEN MAIER², VADIM VOROBYOV², ANDREJ DENISENKO², ANKE KRUEGER¹, and JÖRG WRACHTRUP² — ¹Institute of Organic Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart — ²3rd Physics Institut, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

The negatively-charged nitrogen-vacancy center (NV⁻) is a defect in diamonds for quantum applications. The coherent properties of NVs and the functional groups on the surface of diamonds critically affect the applicability for quantum sensing. In this research, we attempt different preparation process to create ensembles of shallow (less than 50-nm depth) NV centers, namely ion implantation and delta doping in CVD growth. T2 relaxation time differ from one to hundreds of microseconds with different preparing strategies. We also study properties of NVs with different functional groups on the surface of diamonds. We attempt to find the optimal condition to create ensembles for NV-NMR measurements.

KFM 9.37 Mon 18:00 Poster E

Ultrafast small-polaron dynamics in lithium niobate tantalate solid solutions studied by fs-pump, supercontinuum-probe spectroscopy — ●NIKLAS DÖMER¹, JULIAN KOELMANN¹, ANTON PEANNSTIL¹, MIRCO IMLAU¹, and STEFFEN GANSCHOW² — ¹Inst. Physics, Barbarastr. 7, Osnabrück Univ., Germany — ²Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, Berlin, Germany

The investigation of photo-excitation, transport and recombination dynamics of optically generated small polarons with strong coupling in the model system lithium niobate tantalate (LNT, LiNb_xTa_{1-x}O₃ with 0 ≤ x ≤ 1) enables insight into the electronic and microscopic (defect) structure of the polar oxide mixed crystal. Recently, fs-pulse induced transient absorption in LNT was studied to explore the influence of a tunable (by the composition x) intrinsic defect structure on small polaron densities, revealing new 3D hopping transport phenomena. We extended our studies using a supercontinuum light source as a probe, offering nearly gap-free spectral access for observing UV-VIS-NIR induced absorption features. We thus are able to detect broad absorption bands being associated with optically-induced small polaron hopping and analyze our findings in conjuncture with transient absorption data on long time scales (up to seconds). A microscopic model based on the simultaneous presence of two types of intrinsic antisite defect centers, Nb_{Li} and Ta_{Li}, is deduced to explain the observation of two different polaron decay channels. Financial support

by the DFG (project IM 37/12-1 within the research unit FOR 5044).

KFM 9.38 Mon 18:00 Poster E

Small polaron dynamics in lithium niobate tantalate in presence of optical damage — ●JULIAN KOELMANN¹, SÖREN DOMKE¹, ANTON PFANNSTIEL¹, STEFFEN GANSCHOW², and MIRCO IMLAU¹ — ¹School of Mathematics/Informatics/Physics, Barbarastr. 7, Osnabrück University, Osnabrück, Germany — ²Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, Berlin, Germany

Optical damage is reported for the mixed crystal system $\text{LiNb}_{1-x}\text{Ta}_x$ ($0 \leq x \leq 1$) in accordance with the findings of its edge compositions lithium niobate (LN, $x = 0$) and lithium tantalate (LT, $x = 1$). Remarkably, the recording of e.g. holographic phase grating does not require doping with extrinsic deep centers such as $\text{Fe}_{\text{Li}}^{3+/4+}$, that may be interpreted by a more pronounced landscape of intrinsic defects in LNT including the photo-excitation of small bound $\text{Nb}_{\text{Li}}^{4+}$ and Ta_{Li} antisites. Simultaneously, the undisturbed optical characterisation of LNT, in particular the application of time-resolved fs-/ns-pump-probe spectroscopy to elucidate the dynamics of the electron-phonon interaction, is severely hampered. Here, we present our efforts to access small polaron dynamics despite the appearance of light-incurred, long-lived changes of the index of refraction and suppress its appearance by applying an appropriate pre-treatment protocol. As a result, the intensity dependence is accessed and a pronounced increase of the small polaron number density in comparison with LN and LT is clearly validated. Financial support by the DFG (project IM 37/12-1 of the research unit FOR 5044).

KFM 9.39 Mon 18:00 Poster E

Polarized absorption spectroscopy of optically gated small polarons in thermally reduced lithium tantalate — ●ANTON PFANNSTIEL¹, TOBIAS HEHEMANN¹, SIMONE SANNA², NILS SCHÄFER², YURIY SUHAK³, HOLGER FRITZE³, and MIRCO IMLAU¹ — ¹Inst. Physics, Barbarastr. 7, Osnabrück Univ., Osnabrück — ²Dept. of Physics, Heinrich-Buff-Ring 16, Justus Liebig University, Giessen — ³Inst. of Energy Research and Physical Technology, Am Stollen 19 B, Clausthal University of Technology, Goslar

The optical absorption features of small bound polarons in lithium tantalate are characterized by a broad ($\sim 1.0\text{eV}$) band at $\sim 2.1\text{eV}$ and are likely assigned to $\text{Ta}_{\text{Li}}^{4+/5+}$ antisites. Also, the presence of inter-

stitial Ta_i^{3+} defect centers is discussed in literature, but experimental evidence for respective small polaron formation is missing in literature, so far. We have addressed this question by polarized absorption spectroscopy of optically gated small polarons in thermally reduced LiTaO_3 (congruently melting composition). Upon exposure to gating light ($\lambda = 488\text{nm}$) and polarized detection of the absorption change at $T=80\text{K}$, we discovered that the NIR absorption feature is due to a superposition of two individual bands peaking at 1.6eV and 2.1eV , respectively. These findings are found in agreement with the energies estimated for $\text{Ta}_{\text{Li}}^{4+}$ and Ta_i^{4+} sites by density functional calculations. An alternative interpretation that is based on the particular structural distortion of the defect environment in the polaron state is discussed. Financial support by the DFG is acknowledged (project IM 37/12-1; SU1261/1-1; FR1301/42-1; SA 1948/3-1; research unit FOR 5044).

KFM 9.40 Mon 18:00 Poster E

Probing energetics of defects with experimental thermodynamics to unravel hydrogen adsorption sites — ●ANNA SHELYUG¹, CHUKWUDALU OKAFOR², OLIVER PREUSS², JUDITH JUNG¹, CHRISTOPH GEBERT¹, CHRISTOPH KIRCHLECHNER¹, HANS-JÜRGEN SEIFERT¹, and XUFEI FANG^{1,2} — ¹Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — ²Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany

Defects can significantly impact materials ability to adsorb hydrogen. Understanding of defects energetics is essential for designing materials with optimal hydrogen storage and utilization properties while mitigating issues related to embrittlement and other undesired effects.

To quantitatively probe the amount of energy stored in materials in the form of various defects utilizing experimental thermodynamics, this study aims to provide a proof of concept using single-crystal oxides with introduced dislocations, which are further subjected to experimental thermodynamics testing using two major techniques: high-temperature oxide-melt solution calorimetry and differential scanning calorimetry. The first one allows for the evaluation of the overall energy that is associated with any material property and the other one aims to distinguish between various processes that might take place in a structure when it is heated.

Obtained thermodynamic data would provide means for the further investigations on stability of defect structures in the further study of hydrogen-defects interaction.

KFM 10: Diamond and Related Dielectric Materials I

Chair: Theo Scherer (KIT Karlsruhe)

Time: Tuesday 9:30–12:00

Location: E 124

Invited Talk

KFM 10.1 Tue 9:30 E 124

Exploring of the accumulation and thermal annealing of radiation defects in metal oxides via optical absorption, EPR and luminescence methods — ●ALEKSANDR LUSHCHIK — Institute of Physics, University of Tartu, W.Ostwald str. 1, 50411, Tartu, Estonia

High tolerance to intense radiation encourages the use of metal oxides in fission-reactor technologies and allows considering them as promising window materials for the projected fusion facilities. The functionality of optical materials is determined by the creation and accumulation of interstitial-vacancy Frenkel pairs, which are predominantly created via the elastic collisions of fast neutrons/ions with material nuclei.

The radiation damage caused by fast neutrons or $\sim\text{GeV}$ heavy ions was studied in Al_2O_3 , MgO , MgAl_2O_4 crystals via optical and EPR methods. The correlations between the EPR and optical characteristics (emission/absorption bands) allowed the tracking of the creation and thermal annealing of F-type defects (an oxygen vacancy with one/two trapped electrons) in MgO , corundum and mineral spinel. The measured annealing kinetics of the F and F+ centers were modelled in terms of diffusion-controlled reactions. A number of novel EPR-active radiation defects was revealed in spinel (set of hole-type V centers) and corundum (a single oxygen interstitial; a double charged F2 dimer). The ability and limitations of the use of cathodoluminescence as a control tool of radiation damage recovery in corundum was considered.

KFM 10.2 Tue 10:00 E 124

Glovebox with a controlled atmosphere for nano-scale nu-

clear magnetic resonance spectroscopy — ●KSENIYA VOLKOVA¹, ABHIJEET KUMAR², KAROLINA SCHÜLE³, JENS FUHRMANN³, KIRILL BOLOTIN², and BORIS NAYDENOV¹ — ¹Department Spins in Energy Conversion and Quantum Information Science (ASPIN), Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — ²Department of Physics, Freie Universität Berlin, Berlin, Germany — ³Institut für Quantenoptik, Universität Ulm, Ulm, Germany

The unique properties of nitrogen-vacancy (NV) centers in diamond allow to use them as efficient quantum sensors even at room temperature. An example application is NMR spectroscopy on nuclear spin ensembles transferred on the diamond surface using single NV centers few nanometers below the surface. The measurement sensitivity is fundamentally dependent on the spin's lifetime, which is mainly limited by NV centers' environment. In addition, diamond surface properties influence stability of shallow NV centers. We investigate few layered phosphorene flakes deposited on diamond for their possible application as a quantum simulator, but this material degrades under ambient conditions. We present a confocal microscope with a glovebox enclosure for performing NV-based NMR spectroscopy on multi-layered phosphorene.

KFM 10.3 Tue 10:20 E 124

Ambiguous Resonances in Quantum Sensing of Single Nuclear Spins — ●LUCAS TSUNAKI, KSENIYA VOLKOVA, ANMOL SINGH, and BORIS NAYDENOV — Department Spins in Energy Conversion and Quantum Information Science (ASPIN), Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin,

Germany

Quantum sensing is driving technology to ever increasing levels of precision and accuracy of measurements, all based on the fact that quantum states are extremely sensitive to their environment. However, this core element is also a major source of vulnerability, as quantum sensors are subject to complex interactions leading to responses that can be confused with the actual signal to be measured. In this talk, we discuss multipulse decoupling sequences in the context of NV centers in diamond, which are used to measure single nuclear spins at room temperature. Different factors that give rise to these ambiguous resonances are considered, where we compare experimental data and simulations. We also provide a graphical user interface database tool to distinguish these ambiguous resonances from actual single nuclear spins, where over 100,000 simulations can be compared with the user's experiments.

20 min. break

KFM 10.4 Tue 11:00 E 124

Fabrication steps for realization of quantum tokens — ●MIRIAM MENDOZA DELGADO¹, JAN THIEME², JOHANN PETER REITHMAIER¹, KILIAN SINGER², and CYRIL POPOV¹ — ¹Institute of Nanostructure Technologies and Analytics (INA), University of Kassel, Germany — ²Institute of Physics, University of Kassel, Germany

Nitrogen-vacancy (NV) color centers in diamond have acquired great relevance in quantum technology, since they represent an “atom-like” solid state system with optically accessible spin properties. NVs can be implemented as single photon sources with high optical stability and quantum yield, even at room temperature. Furthermore, the coherent electron spin of NV can be used as a long lived qubit which can be applied in quantum information technology, e.g. in quantum repeaters or tokens. In order to enhance the photon collection efficiency from NVs, they should be incorporated in photonic structures, like nanopillars. The aim of the current work is the fabrication of diamond nanopillars incorporated with NVs and integrated with microwave antennas and electrodes for the realization of quantum tokens. Arrays of monocrystalline diamond nanopillars with diameters between 150 nm and 250 nm, 1 μ m height and center-to-center distance of 10 μ m were defined by electron beam lithography and structured subsequently by inductively coupled plasma reactive ion etching with oxygen. Different techniques

are studied for the creation of NVs, which affect both their density and properties.

KFM 10.5 Tue 11:20 E 124

Optical and dielectric properties of artificial diamond — ●THEO ANDREAS SCHERER — Karlsruhe Institute of Technology (KIT-IAM-AWP), Germany

Optical and dielectric properties are key features for the application of artificial diamond as windows for nuclear fusion reactor devices in heating and current drive of the plasma and diagnostics as well. The properties of diamond are unique in the sense of extraordinary values in comparison to other dielectric crystalline materials, like sapphire, spinel, garnet or other oxide materials. The influence of defects and microstructural effects will be discussed based on vibrational bands and RAMAN experiments. Doped diamond is also considered, especially related to electric conductivity experiments. Doped diamond can be used for detector applications.

KFM 10.6 Tue 11:40 E 124

Examining atomic-scale material properties with an SnV electrometer in diamond — ●GREGOR PIEPLOW¹, CEM G. TORUN¹, JOSEPH H. D. MUNNS², FRANZISKA M. HERRMANN¹, ANDREAS THIES³, TOMMASO PREGNOLATO³, and TIM SCHRÖDER¹ — ¹Department of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — ²PsiQuantum, 94304 California Palo Alto, USA — ³Ferdinand-Braun-Institut, Gustav-Kirchhoff-Straße 4, 12489 Berlin, Germany

The transport of free charge carriers in solid-state materials, particularly in the presence of crystal defects, is an active area of research. Currently, existing in-situ sensing methods struggle to precisely localize single charges at the lattice scale. Our work introduces a sensor that is highly sensitive to single charges even amidst high-density background noise, common in wide-bandgap materials. We demonstrate the sensor principle using the tin-vacancy center in diamond, placed in a perturbed crystal lattice. The sensor allows us to pinpoint defect positions with high resolution, understand charge dynamics, and assess defect densities and formation yields. Importantly, this sensor aids in predicting optical performance in quantum technologies based on defect concentration, offering insights into achieving optimal optical coherence.

KFM 11: Focus Session: (Multi-)Ferroic States II

The focus session is dedicated to (multi)ferroic states at interfaces and in heterostructures. The design of (emergent) properties at interfaces, modelling methods and advanced characterization tools will be of interest. Typical examples may include electrostatic and strain boundary conditions at interfaces, domains and domain walls in (multi)ferroics and applications in nano-electronic device

Chair: Nives Strkalj (Institute of Physics, Zagreb)

Time: Tuesday 9:30–12:20

Location: EMH 225

KFM 11.1 Tue 9:30 EMH 225

Polar textures on silicon — ●CATHERINE DUBOURDIEU — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — Freie Universität Berlin, Berlin, Germany

In nanoscale ferroelectrics, the polarization pattern depends on the chemical, mechanical and electrical boundary conditions and is the result of a delicate balance to minimize electrostatic energy costs associated with the depolarization field. In recent years, new exotic polar textures featuring curled polarization patterns (vortices, skyrmions, merons, etc...) have been unraveled in ultrathin films, superlattices or nanostructures. The development of topological nanoelectronics on chips that would take advantage of such polar nanodomains requires their integration on silicon. I will present in this talk the growth and the resulting polarization patterns of (BaTiO₃/SrTiO₃)_n superlattices and of BaTiO₃ nanoislands on silicon substrates. The epitaxy on Si of both types of heterostructures is realized by molecular beam epitaxy, which will be detailed. Based on X-ray diffraction, scanning transmission electron microscopy and piezoresponse force microscopy characterizations, I will discuss the strain state, the peculiar polar textures that develop in these systems and their response under electric field. The evidence of curled polarization nanodomains in the different BaTiO₃-based heterostructures is a first step towards the integration

of topological defects into nanoscale devices.

KFM 11.2 Tue 10:00 EMH 225

In-situ monitoring of polarization dynamics during the epitaxial integration of BaTiO₃ thin films on silicon templates — ●BIXIN YAN, IPEK EFE, MANFRED FIEBIG, and MORGAN TRASSIN — Department of Materials, ETH Zurich, Switzerland

Ferroelectric oxides host technologically-relevant properties, and their integration onto the CMOS-compatible silicon platform is key for the next generation of oxide electronics. However, the interplay of thermal coefficient mismatch and strain relaxation during the growth of ferroelectric epitaxial thin films on silicon results in a multi-domain configuration in the films, deviating from the application-relevant single-domain state. Here, taking BaTiO₃ as our ferroelectric model system, we directly investigate the polarization state of our films during the pulsed laser deposition growth on SrTiO₃ (STO)-buffered silicon using in-situ optical second harmonic generation (ISHG). We monitor the emergence of out-of-plane polarization in the early stage of the growth and track in real-time the thickness-dependent in-plane polarized domain formation induced by interfacial strain relaxation. We shed light on the role of growth conditions on the final polarization state of our films and compare the observed behavior with the case of coherently

strained thin films grown on conventional single crystalline STO substrates. Finally, ISHG measurements during post-growth cooldown isolate the impact of thermal expansion coefficient mismatch in the final domain architecture in the films. Hence, our work provides new insights into the integration of ferroelectric oxides on silicon templates, a necessary step for the realization of energy-efficient technologies.

KFM 11.3 Tue 10:20 EMH 225

Epitaxial Strain in Arbitrary Orientation in BaTiO₃ films and BaTiO₃/SrTiO₃ superlattices — •LAN-TIEN HSU¹, ANNA GRÜNEBOHM¹, and FRANK WENDLER² — ¹Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Universitätsstr. 150, 44801 Bochum, Germany — ²Institute of Materials Simulation, Department of Materials Science, Friedrich-Alexander University of Erlangen-Nürnberg, Dr.-Mack-Strasse 77, 90762 Fürth, Germany

Interface strain plays a crucial role in ferroelectric thin films and multilayer systems, which have potential in e.g. high-frequency capacitors and random-access memories[1]. Epitaxial (001), (110), and (111) strains can alter phase stability and enhance ferroelectric properties in BaTiO₃ films[2]. However, it is still unclear how the epitaxial strain in low symmetric orientation influences films and multilayer systems.

In this work, we study the epitaxial strain in low symmetric orientations in bulk-like BaTiO₃ (without a depolarization field) and in BaTiO₃/SrTiO₃ superlattices, using ab initio based coarse-grained molecular dynamics[3]. Complex multidomain structures appear, particularly in superlattices due to the presence of depolarization fields. Furthermore, we compare these strain-induced phases with those induced by electric fields along arbitrary directions.

[1] A. Grünebohm et al., J. Phys. 34, 2021

[2] H. Wu et al., AIP Advances 6, 2016

[3] T. Nishimatsu et al., Phys. Rev. B 78, 2008

KFM 11.4 Tue 10:40 EMH 225

Interplay of layer and spontaneous polarization in superlattices of metallic SmNiO₃ and ferroelectric BaTiO₃ — •EDITH SIMMEN and NICOLA A. SPALDIN — Materials Theory, ETH Zurich, Switzerland

We present a density functional theory (DFT) study of superlattices containing metallic SmNiO₃ (SNO) and ferroelectric BaTiO₃ (BTO). The interface of SNO with BTO hosts numerous interesting functionalities which can compete or cooperate: Since BTO and SNO are II-IV and III-III perovskites, respectively, the different layer charges lead to a built-in polar discontinuity in addition to the spontaneous polarization of BTO. These two sources of polarization can both interact with each other and with the SNO via its metallic screening. We find that despite the metallicity of SNO, the polar electrostatics strongly affect the ground state. The system avoids a polar discontinuity by aligning the spontaneous polarization of the BTO parallel to the layer polarization of the SNO in the so-called ‘happy’ orientation. We find that this happy polarization is stable down to a single unit cell of BTO, in contrast to the 6-unit-cell critical thickness previously found for BTO with II-IV metallic electrodes [1]. The opposite ‘unhappy’ polarization orientation is however highly unfavoured, with the stability depending strongly on the thickness of the BTO layer and the tilts within the SNO layer.

[1] J. Junquera et al., Nature 422, 506 (2003)

10 min. break

Invited Talk

KFM 11.5 Tue 11:10 EMH 225

Optical Formation and Manipulation of Topological Polar Supertextures — •JOHN FREELAND — X-ray Science Division, Argonne National Laboratory, Lemont, IL USA

Ultrafast stimuli can stabilize and control metastable states of matter inaccessible by equilibrium means. Establishing the spatiotemporal link between ultrafast excitation and metastability is crucial to un-

derstanding these phenomena. This talk will focus on superlattices of PbTiO₃ (PTO) and SrTiO₃ (STO) that host a variety of extended polar textures such as supercrystals, vortices, skyrmions, collectively dubbed polar supertextures. In particular we will explore the formation of polar supercrystals[1], which is a highly order phase created via optical excitation of these PTO/STO heterostructures. Since the transition is irreversible, an understanding of the formation pathway, we needed to use the high intensity ultrafast X-ray pulses from a free electron laser to track the single-shot dynamics of polar supercrystal creation from ps to us timescales. Together with dynamical phase field modeling, these results enabled tracking of the irreversible formation of this metastable polar supertexture and understanding of the creation process.

The work at Argonne is supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357. The development of the materials and ultrafast experiments is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC-0012375.

[1] Stoica, V. A. et al. Nat. Mater. 18, 377 (2019).

KFM 11.6 Tue 11:40 EMH 225

Investigation of local structure in polar skyrmions using three-dimensional diffuse X-ray scattering — •JOOHEE BANG¹, NIVES STRKALJ², MARTIN SAROTT¹, MORGAN TRASSIN¹, and THOMAS WEBER¹ — ¹Department of Materials Science, ETH Zurich — ²Institute of Physics, Zagreb

The discovery of nontrivial polar topologies have attracted great attention as it holds promise for alternative device configurations for microelectronics. Specifically, superlattices consisting of ferroelectric lead titanate and dielectric strontium titanate have shown a number of nontrivial topologies such as polar vortex-antivortex pairs [1] and polar skyrmions [2]. In fact, short-period (of only a few unit cells) superlattices were previously reported to exhibit improper ferroelectricity associated with octahedral tilts [3]. However, the phase and magnitude of octahedral tilts in the system are yet to be fully investigated. Detailed investigation of the local atomic structure and the interlayer correlation of the polarization domains in these nontrivial topological systems also remains elusive. Here, we perform an in-depth analysis of octahedral tilts as well as that of cation displacements in polar skyrmion structures via a comprehensive reciprocal space investigation. The observation of A-cation displacements associated with octahedral tilts as a function of temperature and the investigation of their correlation strength is the primary focus of our work.

[1]Yadav et al., Nature 530, 2016

[2]Das et al., Nature 568, 2019

[3]Bousquet et al., Nature 452, 2008

KFM 11.7 Tue 12:00 EMH 225

Brownian Electric Bubbles — •HUGO ARAMBERRI¹ and JORGE ÍÑIGUEZ-GONZÁLEZ^{1,2} — ¹Luxembourg Institute of Science and Technology (LIST), Esch/Alzette, Luxembourg — ²University of Luxembourg, Belvaux, Luxembourg

Magnetic skyrmions are point-like topological defects with a magnetization opposite to its embedding matrix. They have been studied for over a decade. Some of their most promising applications are in the field of unconventional computing, in which the stochastic motion of these nanometric objects plays a pivotal role. At the same time, electric skyrmion bubbles were recently predicted (and soon after experimentally confirmed) in electrostatically frustrated ferroelectrics. However, the field of electric bubbles is still at a nascent stage, and a fundamental characterization of these objects is still lacking. Importantly, the dynamics of electric bubbles still remain largely unexplored.

In this talk I will present second-principles atomistic molecular dynamics simulations of electric bubbles in ferroelectric/paraelectric superlattices (PbTiO₃/SrTiO₃), showing that they can present Brownian motion at room temperature. This work establishes the quasiparticle nature of electric bubbles, and sets the stage for their use as purely electric alternatives to magnetic skyrmions.

Aramberri and Íñiguez, arXiv:2308.01716 (2023).

KFM 12: Diamond and Related Dielectric Materials II

Chair: Theo Scherer (KIT Karlsruhe)

Time: Wednesday 9:30–11:50

Location: EMH 025

KFM 12.1 Wed 9:30 EMH 025

Diamond-based platforms for biochemical measurements of time-resolved clock cell signaling in response to external zeitgebers and coupling factors — ●REZVANEH GHASEMITABESH¹, DANIEL MERKER¹, DANIELA BERTINETTI², FRIEDRICH W. HERBERG², and CYRIL POPOV¹ — ¹Institute of Nanostructure Technologies and Analytics, Center for Interdisciplinary Nanostructure Science and Technology (CINSA^T), University of Kassel, Germany — ²Department of Biochemistry, CINSA^T, University of Kassel, Germany

Nowadays, techniques for immobilization of biomolecules for biosensor fabrication have been investigated on various diamond substrates due to their exceptional properties. This study focuses on the potential application of ultrananocrystalline diamond (UNCD) films as biosensor platforms for detection of biomolecules, such as neuropeptides (e.g. pigment dispersing factor (PDF)), secreted by clock neurons. To achieve an effective biosensor, calibration tests are initially conducted. These tests involve non-covalent and covalent immobilizations of green fluorescence protein (GFP) on nanostructured UNCD films. The results of non-specific binding of GFP to O-, H- and F-terminated UNCDs demonstrate that with decreasing GFP concentration, the fluorescence intensity is decreasing. Also, the immobilizations of various nanobodies against GFP show promising initial results. The long-term goal is to immobilize PDF-binding proteins for capturing PDF released from clock neurons and detecting it using a reporter complex composed of a binding protein and a fluorescent molecule.

KFM 12.2 Wed 9:50 EMH 025

Application and design evolution of CVD diamond windows in fusion experiment devices — ●PETER SPAEH — KIT, Institute for applied materials, Karlsruhe

For experimental fusion devices and also for future fusion power plants, efficient plasma heating concepts based on high frequency electromagnetic waves are essential. Electron Cyclotron Resonance Heating (ECRH) is one of these heating systems. An ECRH system generates very high power radiation at millimetre wavelength in Gyrotrons, which are basically evacuated masers. From there the millimetre waves are coupled out and guided through transmission lines into the torus chamber of the fusion reactor aiming for plasma heating or plasma stabilisation. To separate these sections from each other, radiation transparent windows are required, which enable millimetre wave passage at very low dielectrical losses, while at the same time acting as mechanical barriers to cope with pressure gradients and contamination issues. Beside window materials like sapphire, boron nitride or beryllium oxide, the most promising material for low-loss transmission and high mechanical strength under vacuum safe long pulse operation is synthetic diamond. With the continuous progress on growing diamond by CVD (chemical vapour deposition), also the applicability and the performance of CVD diamond windows in experimental fusion devices has evolved substantially. This talk gives an overview on various configurations and design evolutions of CVD diamond windows for nuclear fusion applications. Also respective design requirements, relevant design parameters and associated material properties are presented.

KFM 12.3 Wed 10:10 EMH 025

Initial characterization of MPA CVD diamond to be investigated by fracture toughness measurements — ●GAETANO AIELLO, CARSTEN BONNEKOH, ANDREAS MEIER, THEO SCHERER, SABINE SCHRECK, KLAUS SEEMANN, and DIRK STRAUSS — Karlsruhe Institute of Technology, Institute for Applied Materials, 76021 Karlsruhe, Germany

Microwave Plasma Assisted (MPA) Chemical Vapour Deposition (CVD) optical quality polycrystalline diamond is used in shape of disks with thickness of 1 to 2 mm in window units for plasma heating and stabilization in nuclear fusion devices. Due to limited body of work in literature and the important safety role of the disks, fracture toughness measurements on this type of diamond are planned to check its resistance against crack propagation. In this work, the activities aiming to characterize the diamond samples prior to the experiments are discussed mainly with reference to X-ray diffraction, electron backscatter

diffraction and loss tangent measurements. For in-depth understanding, thermal grade diamond has been also considered. It grows much faster than the optical grade and it has a greater density of microfeatures. In addition, the design and thermo-mechanical performance of a typical diamond window unit in nuclear fusion devices are presented.

20 min. break

KFM 12.4 Wed 10:50 EMH 025

Diamond dielectric characterization with superconducting LC micro-resonators — ●FRANCESCO MAZZOCCHI, DIRK STRAUSS, and THEO SCHERER — Karlsruhe Institute of Technology, IAM-AWP, Hermann Von Helmholtz Platz 1, 76344, Eggenstein Leopoldshafen

The development of high optical quality, ultra-low losses single crystal diamond windows is paramount for the realization of future nuclear fusion facilities like DEMO, given the foresaw increase in power of microwave ECRH systems. Precise determination of the dielectric characteristics (ϵ_r and $\tan\delta$) of these innovative materials have so far relied on techniques involving Fabry-Perot microwave open resonators in various configurations. High Q, superconducting thin film resonators can be effectively used to determine dielectric characteristics of extremely low losses materials like single- and poly-crystalline diamond. Their extremely high-quality factors allow for a substantial increase in resolution in the determination of these parameters when compared to state-of-the-art Fabry Perot open resonators. We hereby report the simulation study that lead to the final design of the devices and the first characterization measurements performed on a prototype resonator patterned on a single crystalline diamond substrate.

KFM 12.5 Wed 11:10 EMH 025

Optimizations of Single-Crystal Diamond Surfaces for Implantation, Membranes and Nanophotonic Structures — ●LUKAS WOLFRAM, JULIA HEUPEL, JOHANN PETER REITHMAIER, and CYRIL POPOV — Institute of Nanostructure Technologies and Analytics (INA), University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Due to its exceptional physical and chemical characteristics, single-crystal diamond (SCD) is a promising material for the fabrication of high-quality photonic devices and for envisioned applications in quantum information technologies (QIT). The preparation of smooth and defect-free surfaces is important to yield optimal optical properties and reduce losses by e.g. scattering. Here, a solution to remove defects originating from polishing or etching procedures (e.g. grooves and pits) is presented, while avoiding the micro masking effect during the inductive coupled plasma reactive ion etching (ICP-RIE) process. Thereby, we achieved surface roughness down to 0.2 nm using optimized Ar/Cl₂ etching recipes. The planarized diamonds are then used, as it will be shown in the talk, for structuring membranes (thickness between 500-500 nm), nanophotonic devices or preparing implantation masks with hole sizes down to 40 nm.

KFM 12.6 Wed 11:30 EMH 025

Energy dissipation on magic angle twisted bilayer graphene — ●MARCIN KISIEL¹, ALEXINA OLLIER¹, URS GYSIN¹, MARTINO POGGIO¹, XIAOBO LU², DMITRI EFETOV³, and ERNST MEYER¹ — ¹Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — ²International Center for Quantum Materials, Collaborative Innovation Center of Quantum Matter, Peking University, 100871, Beijing, China — ³Department of Physics, Ludwig-Maximilians-University München, Geschwister-Scholl-Platz 1, 80539 München, Germany

While traditional Joule dissipation omnipresent in today's electronic devices is well understood, the energy loss of the strongly interacting electron systems remains largely unexplored. Twisted bilayer graphene (tBLG) is a host of interaction-driven correlated insulating phases, when the relative rotation is close to the magic angle (1.08deg). Here, we report on low temperature (5K) nanomechanical energy dissipation of tBLG measured by sharp tip of the pendulum atomic force microscope (pAFM). Ultrasensitive cantilever tip acting as an oscillating gate over the quantum device shows dissipation peaks attributed to

different fractional filling of the flat energy bands. pAFM provides exquisite spatial resolution and thus allows to determine the twist angle distribution of tBLG. Application of magnetic fields provoked

strong oscillations of the dissipation signal at 3/4 band filling, which we identified as familiar to Aharonov-Bohm oscillations arising from wavefunction interference present between domains of different doping.

KFM 13: Focus Session: (Multi-)Ferroic States III

The focus session is dedicated to (multi)ferroic states at interfaces and in heterostructures. The design of (emergent) properties at interfaces, modelling methods and advanced characterization tools will be of interest. Typical examples may include electrostatic and strain boundary conditions at interfaces, domains and domain walls in (multi)ferroics and applications in nano-electronic device.

Chair: Morgan Trassin (ETH Zürich)

Time: Wednesday 9:30–12:30

Location: EMH 225

KFM 13.1 Wed 9:30 EMH 225

What can we expect from multiferroic antiskyrmions? — ●JIRI HLINKA — Institute of Physics, Czech Acad. Sci., Prague, Czechia

The prediction and experimental confirmation of magnetic skyrmions - the objects with nontrivial swirling spins patterns - revolutionized the physics of nanoscale magnetism and opened new horizons for spintronics. In spite of the inherently shorter and faster correlations of the electric polarization, the recent developments in electric skyrmionics follow these innovations. Our recent work with M. Goncalves and M. Pasiać[arXiv:2303.07389] reveals that classical ferroelectric perovskite - barium titanate - can host 2-3 nm wide polar columns spontaneously surrounded by a unique noncollinear polarization pattern that has never been described before. Based on the reference-frame-invariant topological charge of this topological defect, we name it *ferroelectric antiskyrmion*. In this contribution we shall address the question about the existence and properties of whether similar topological defects can exist in multiferroic materials like bismuth ferrite.

KFM 13.2 Wed 10:00 EMH 225

Topological aspects of switching in ferroic materials — FRANCESCO FOGGETTI^{2,1}, MARGHERITA PARODI^{1,3}, NAOTO NAGAOSA⁴, and ●SERGEY ARTYUKHIN¹ — ¹Italian Institute of Technology, Genova, Italy — ²Dept. of Physics and Astronomy, Uppsala University, Sweden — ³Department of Physics, University of Genova, Italy — ⁴CEMS RIKEN, Tokyo, Japan

Topology has played a prominent role in condensed matter physics in the recent years. In magnetism, topological properties of domain walls and vortices were known for a long time, and more recently topological magnon band structures and other aspects were discussed. However, switching, one of the most important processes from the viewpoint of applications, has not been discussed in the context of topology until recently, when magnetoelectric switching in GdMn₂O₅ [1], the first known topologically protected ferroic switching phenomenon, was discovered. Here we discuss electric field induced switching in spiral multiferroics, where topology plays an important role.

[1] Louis Ponet, SA, Th. Kuhn et al., Nature 607, 81 (2022).

KFM 13.3 Wed 10:20 EMH 225

Atomic-scale control of exchange bias at ferroelectric BaTiO₃ and ferromagnetic La_{0.67}Sr_{0.33}MnO₃ interface — ●MANISHA BANSAL¹, TUHIN MAITY^{1,2}, and JUDITH L. MACMANUS-DRISCOLL² — ¹School of Physics, Indian Institute of Science Education and Research Thiruvananthapuram, Thiruvananthapuram, Kerala 695551, India — ²Department of Materials Science and Metallurgy, University of Cambridge, CB3 0FS, UK

The atomic-scale interfaces in 3D transition-metal oxides give rise to intriguing phenomena, including magnetoelectric coupling and unconventional exchange bias (EB) coupling. They hold promises for the next-generation nanoscale spintronics applications such as high-density memory and sensor technologies. We demonstrate EB coupling (~ 40 Oe at 2 K) at the interface of epitaxially grown ferromagnetic (FM) La_{0.67}Sr_{0.33}MnO₃ (LSMO)-ferroelectric (FE) BaTiO₃ (BTO) bilayer thin films on TiO₂ terminated SrTiO₃ (STO) substrates in the absence of any conventional antiferromagnetic (AFM) material due to strain induced FE screening effect by BTO. Such EB is only observed when the thickness (t) of BTO is $5 < t < 10$ unit cells (uc) and LSMO is only a few unit cells (≤ 14 uc). The out-of-plane (OOP) polarization is lost in thicker BTO followed by the negligible EB due to multi domains formation. STEM and DFT confirms the OOP polarized Ti atoms

which further displaces the interfacial Mn sites from their centrosymmetric positions in LSMO. This modifies the d-orbital occupancy of interfacial Mn, favoring an interface induced EB in LSMO-BTO bilayer films without any AFM material.

KFM 13.4 Wed 10:40 EMH 225

Unraveling Coupled Martensitic and Magnetic Microstructure of Freestanding Multiferroic Ni-Mn-based Heusler Films — ●SATYAKAM KAR^{1,2,3}, YUKI IKEDA⁴, KORNELIUS NIELSCH^{1,2}, HEIKO REITH¹, ROBERT MAASS^{4,5}, and SEBASTIAN FÄHLER³ — ¹Leibniz IFW Dresden, Dresden, Germany — ²TU Dresden, Dresden, Germany — ³Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — ⁴Federal Institute of Materials Research and Testing, Berlin, Germany — ⁵University of Illinois Urbana-Champaign, Illinois, USA

Ni-Mn-based Heusler alloys combine ferroelasticity and ferromagnetism to achieve multifunctional applications like high stroke actuation, multicaloric effects, and thermomagnetic energy harvesting. The underlying principle in these applications is a reversible martensitic phase transformation. In bulk, this first-order transformation is governed by an invariant plane, connecting both phases: austenite and martensite. Theory predicts that this plane should converge to a line for ultrathin films, but experimental evidence is missing. Here, we examine 500 nm thick freestanding epitaxial Ni-Mn-Ga films using electron microscopy and magnetic force microscopy techniques and demonstrate that a line constraint controls the martensitic microstructure. This line constraint results in a complex martensitic and magnetic microstructure, differing from the bulk and the constrained film microstructures. Using a simple phenomenological model, the martensite microstructure can be deduced from a line constraint. Our findings show that finite size effects on martensitic transformation are accessible at a film thickness suitable for microsystem technologies.

10 min. break

KFM 13.5 Wed 11:10 EMH 225

Experimental evidence for the PJTE in alkali niobates — ●LEIF CARSTENSEN and WOLFGANG DONNER — Technical University of Darmstadt, Germany

The electronic origin of antiferroelectricity is considered not fully understood by most of the scientific community. Sodium niobate evolves from a paraelectric cubic to an antiferroelectric orthorhombic structure via a series of phonon instabilities. A combination of Rietveld refinement and Maximum Entropy Method is performed to gain insight into the differences between ferroelectrics and antiferroelectrics with respect to their electron density. Using this technique, the electron density distributions of room temperature sodium niobate and potassium niobate have been calculated from powder diffraction experiments to study the extent to which the Pseudo-Jahn-Teller effect changes the electron distribution from the originally fully ionic bonding proposed for the cubic structures of these perovskites. This study delivers experimental results to back up the PJTE theory and proves that the Rietveld-MEM approach is not limited to large radiation facility data, making it much more commonly available.

KFM 13.6 Wed 11:30 EMH 225

Charged twin domain walls in antiferroelectric-like K₃[Nb₃O₆(BO₃)₂] — ●IVAN N. USHAKOV¹, KASPER A. HUNNESTAD¹, CHRISTOPH GRAMS², JOACHIM HEMBERGER², PETRA BECKER², LADISLAV BOHATÝ², THOMAS M. TYBELL¹, and DENNIS

MEIER¹ — ¹Norwegian University of Science and Technology (NTNU), Trondheim, Norway — ²University of Cologne, Cologne, Germany

Antiferroelectric materials exhibit an anti-polar alignment of electric dipoles, giving rise to intriguing physical properties and functional behaviors. In this work, we apply different scanning probe microscopy techniques to image and investigate the domains and domain walls in $K_3[Nb_3O_6(BO_3)_2]$, a ferroelectric with antiferroelectric-like structure and properties. Using piezoresponse force microscopy, we show that the domains exhibit a pronounced piezoresponse, consistent with the non-centrosymmetric crystal structure. At the nanoscale, a chevron-like pattern of twin domains develops, where the crystallographic structure changes by 120° across the domain walls. Interestingly, we observe the formation of charged twin walls with distinctly different piezoelectric and electrostatic responses, arising from a small canted electric moment of the otherwise anti-polar arrangement of electric dipoles. Furthermore, the charged domain walls can be controlled by local electric fields. Our findings provide insight into novel types of ferroic domain walls with unusual mechanical and electronic properties.

KFM 13.7 Wed 11:50 EMH 225

Origin of antiferroelectric-like behaviour in a quaternary compound: Multiscale insights from first principles and phase-field simulations — •MUHAMMAD ZEESHAN KHALID¹, IVAN USHAKOV¹, BAI-XIANG XU², DENNIS MEIER¹, and SVERRE MAGNUS SELBACH¹ — ¹Department of Materials Science and Engineering, Norwegian University of Science and Technology, Trondheim, NO-7491, Norway. — ²Mechanics of Functional Materials, Department of Materials and Geoscience, Technical University of Darmstadt, Darmstadt, 64287, Hessen, Germany

Understanding domain switching behavior in ferroelectric and antiferroelectric materials is pivotal for optimizing their utility in diverse applications. Here, we investigate the domain characteristics of $K_3Nb_3B_2O_{12}$, which was recently reported to exhibit antiferroelectric-like switching behavior. Employing the ab-initio calculation and the Landau theory, we parameterize the Landau potential, ex-

ploring the mechanisms governing the domain switching from the non-centrosymmetric high-temperature P-62m phase to the room-temperature phase Pma21. Following the calculations of phase-field coefficients and potentials, we conduct multiscale simulations to analyze the domain formation and evolution. External electric fields are applied to reproduce the antiferroelectric-like hysteretic switching, providing new insight into the switching dynamics of $K_3Nb_3B_2O_{12}$ at the level of the domains.

KFM 13.8 Wed 12:10 EMH 225

Structural and electrical properties of $Bi_0.5Na_0.5TiO_3$ -based ceramics synthesized by optimized sol-gel method — •THOMAS FOURGASSIE^{1,2}, CÉCILE AUTRET-LAMBERT^{1,2}, PIERRE-EYMERIC JANOLIN², and BRAHIM DKHIL² — ¹Laboratoire GREMAN, UMR 7347 Université de Tours, CNRS, INSA CVL, 37200 Tours, France — ²Laboratoire SPMS, UMR 8580 Université Paris-Saclay, CNRS, CentraleSupélec, 91190 Gif-sur-Yvette, France

The energetic needs of our society seems to grow endlessly, that is why we need to increase our energy storage capacity for a sustainable future. Novel lead-free solid solutions are promising candidates to replace lead-based piezoelectric ceramics such as $Pb(Zr,Ti)O_3$. Among the lead-free material, $Bi_0.5Na_0.5TiO_3$ (BNT) ceramics have attracted a large attention for their excellent and competitive dielectric properties. Our goal is to synthesize a new lead-free material based on BNT presenting high energy storage properties in a wide range of temperature. BNT was chosen as a base material for his high maximum polarization (P_{max}) and his relaxor properties making his phase transition more diffuse, resulting in broad peaks of dielectric permittivity. In order to improve the electrical properties for our final material, we decided to work on the optimization of the base material BNT by sol-gel method. We therefore report the impact of different synthesis processes, with different temperature of calcination or different time of calcination on the structural and dielectric properties of BNT, as well as the impact of the addition of dopants or excess of already present cations on the high leakage current usually seen in pure BNT.

KFM 14: Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials (joint session MM/KFM)

Time: Wednesday 11:45–13:00

Location: C 230

KFM 14.1 Wed 11:45 C 230

Atomic cluster expansion for binary Ag-Pd alloys — YANYAN LIANG, •MATOUS MROVEC, YURY LYSOGORSKIY, and RALF DRAUTZ — ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany

Binary alloys of silver and palladium have recently attracted increased attention due to their applications in catalysis and nanotechnology. However, the binary Ag-Pd system lacks reliable and efficient interatomic potentials that provide an accurate description of structural and thermodynamic properties, in particular for atomistic simulations of nanoparticles as well as large scale simulations of mechanical properties. In this work, we present an atomic cluster expansion (ACE) parameterized for Ag-Pd with ab-initio accuracy. We show that the ACE parametrization provides an accurate description of the elastic, structural and thermodynamic properties of both elements as well as their compounds. We demonstrate the computational efficiency and the applicability of the developed potential for atomistic simulations of complex phenomena in elemental as well as Ag-Pd systems.

KFM 14.2 Wed 12:00 C 230

Training strategies for machine-learning potentials suitable to simulate mechanical response of ceramics — •SHUYAO LIN^{1,2}, ZHUO CHEN³, LUIS CASILLAS-TRUJILLO², FERENC TASNADI², ZHAOLI ZHANG³, LARS HULTMAN², PAUL H. MAYRHOFER¹, DAVIDE G. SANGIOVANNI², and NIKOLA KOUTNA^{1,2} — ¹Institute of Materials Science and Technology, TU Wien, A-1060, Vienna, Austria — ²Department of Physics, Chemistry, and Biology (IFM), Linköping University, SE-58183, Linköping, Sweden — ³Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, A-8700, Leoben, Austria

Machine-learning interatomic potentials (MLIPs) offer a powerful avenue for simulations beyond length and timescales of *ab initio* methods. In particular, MLIPs enable investigations of mechanical properties and fracture behaviour of materials with supercell sizes, loading

geometries and temperatures relevant for real operation conditions. Using the example of hard TiB_2 ceramic, in this talk we propose a strategy for fitting MLIPs suitable to simulate mechanical response of monocrystals from atomic to nanoscale, including strains until fracture and deformation-induced phase transformations. After validation, the best-performing MLIP is employed to carry out molecular dynamics simulations of various loading conditions, with main focus on tensile and shear deformation. Consequently, we derive size-dependent trends in theoretical strength, toughness, and crack initiation patterns of TiB_2 . To approach experimental observations, we additionally apply our MLIP to models containing a pre-crack and/or grain boundaries.

KFM 14.3 Wed 12:15 C 230

Investigating the yield stress anomaly of Ni_3Al with physically informed machine-learning potential — •XIANG XU, XI ZHANG, SIEGFRIED SCHMAUDER, and BLAZEJ GRABOWSKI — University of Stuttgart, Stuttgart, Germany

The anomalously increasing yield stress with temperature of some intermetallics is predominately controlled by the Kear-Wilsdorf lock (KWL), of which the formation and unlocking are closely related to a cross-slip process. Yet so far, knowledge of this cross-slip process is limited, leading to significant approximations in existing models for predicting the mechanical behavior of those materials. In this study, molecular dynamics simulations were conducted by using a physically informed machine-learning potential to replicate dislocation activities of Ni_3Al . For the first time, it is observed that the formation and unlocking of KWL occurs with a step-by-step cross-slip process, of which the distance varies between one or two atomic planes inside each step. Moreover, a strong temperature dependence of the necessary stress to unlock a KWL was discovered, differing from previous approximations. This study not only advances the understanding on the yield stress anomaly in Ni_3Al , and also establishes a systematic workflow for yielding multiscale atomistic simulations using machine-learning

potentials.

KFM 14.4 Wed 12:30 C 230

The Effect of Al Sublattice in Tuning Elastic Anisotropy in Fe-Ta-Al Laves Phases — ●NISA ULUMUDDIN, CHRISTINA GASPER, ZHUOCHENG XIE, and SANDRA KORTE-KERZEL — RWTH Aachen Institut für Metallkunde und Materialphysik

As Laves phases found in alloys are often undesirable due to its brittleness, fundamental knowledge on tuning its mechanical properties can pave the pathway for the enhanced design of engineering alloys. The structural motifs arising from the substitutional mixing of Al into the Fe_2Ta Laves phase at varying Al:Fe ratios were studied by first-principles. The presence of an Al sublattice was found to reduce elastic anisotropy, owing to changes within the bonding nature of the crystal. They induce a higher degree of metallic bonding within the crystal as Al is relatively less electronegative than Fe. The increased degree of non-directional bonding decreases the directional preference for elastic deformation. These results signify the possibility of adjusting the mechanical properties of intermetallics by considering the electronic properties of their individual components.

KFM 14.5 Wed 12:45 C 230

Effect of the V-VIB groups ternary elements on the prop-

erties of Ti2AlM-type O-phases: A first-principles study — ●ZEINAB HEIDARI PEBDANI^{1,2}, FLORIAN PYCZAK^{1,2}, and REBECCA JANISCH³ — ¹Helmholtz-Zentrum Hereon, Geesthacht, Germany — ²BTU Cottbus-Senftenberg, Cottbus, Germany — ³ICAMS, Ruhr-Universität Bochum, Germany

Despite the recent introduction of γ -TiAl-based alloys into service, the assessment of TiAl-alloys based on the ternary Ti2AlM orthorhombic O-phase, which are promising high-temperature structural materials, has not yet been completed. The focus of this contribution is on the impact of ternary alloying elements of the V-VIB groups of the periodic table on phase stability, structural, mechanical, thermal properties, and lattice dynamics of Ti2AlM (M= V, Nb, Ta, Mo, W) type O-phases. All Ti2AlM compounds satisfy the Born stability criteria, but their properties are largely affected by the ternary element M. According to the energy of formation, Ti2AlMo is the most stable type of O-phase. The bonding behavior of all compounds is investigated by analyzing the electronic density of state plots. It was found that stronger Ti-M bonding enhances while stronger Ti-Al bonding decreases the ductility in the Ti2AlM compounds. The thermodynamic stability of the intermetallic phases is key information to further develop these materials. To consider this we have used a set of comprehensive ab initio methods, in order to determine the temperature dependence of the properties of those intermetallic phases.

KFM 15: Multiferroics and Magnetoelectric Coupling (joint session MA/KFM)

Time: Wednesday 15:00–18:00

Location: EB 407

KFM 15.1 Wed 15:00 EB 407

Real-time imaging of nonequilibrium domain evolution into a multiferroic phase — ●JAN GERRIT HORSTMANN¹, YANNIK ZEMP¹, EHSAN HASSANPOUR YESAGHI¹, THOMAS LOTTERMOSER¹, MADS C. WEBER², and MANFRED FIEBIG¹ — ¹Dept. of Materials, ETH Zurich, Switzerland — ²Institut des Molécules et Matériaux du Mans, Le Mans Université, France

We investigate the dynamics of magnetic domain formation across spin-reorientation transitions in multiferroic $\text{Dy}_{0.7}\text{Tb}_{0.3}\text{FeO}_3$. Combining Faraday imaging at kHz frame rates with fast optical excitation we find that thermal quenches of the system can be harnessed to imprint the characteristic bubble domain pattern of the weak ferromagnetic order at elevated temperatures onto the low-temperature multiferroic phase. We identify the quenching rate across the different spin reorientation transitions as the decisive parameter governing the domain memory and the formation of metastable domain states forbidden in thermal equilibrium. Our results highlight the potential of optical stimuli for the switching and control of multiferroic domain structures, enabling the creation of new functional states via nonequilibrium pathways.

KFM 15.2 Wed 15:15 EB 407

Asymmetry of the magnetic-field-driven phase transition in h-ErMnO₃ — ●LEA FORSTER¹, IPEK EFE¹, MORGAN TRASSIN¹, MANFRED FIEBIG¹, THOMAS LOTTERMOSER¹, and MADS C. WEBER² — ¹Department of Materials, ETH Zurich, Switzerland — ²IMMM UMR 6283, University Le Mans, France

We report on the asymmetry of the magnetic-field-induced phase transition of the Mn^{3+} order in hexagonal ErMnO_3 under magnetic field application along the six-fold axis. Below the Néel temperature, we observe that with increasing magnetic field the Mn^{3+} and Er^{3+} appear to reorder simultaneously. However, with decreasing magnetic field, the reverse phase transition of the Mn^{3+} shows an intermediate stage where the spins are partially in the zero-field and partially in the applied-field state, while the Er^{3+} reverses almost instantaneously to its zero-field state. This asymmetry of the forward and reverse transition in the Mn^{3+} order becomes more and more pronounced at lower temperatures. We gain access to both the Mn^{3+} and Er^{3+} sublattices using optical second-harmonic generation and SQUID magnetometry. Our investigation of this asymmetric magnetic field-induced phase transition further underlines the complex coupling mechanisms of the Mn^{3+} order to the rare-earth orders in hexagonal manganites.

KFM 15.3 Wed 15:30 EB 407

Magnetoelectric Effects in 2D Magnets: A Multiscale Approach Applied to Topological Solitons in CrI_3 — ●ALEXANDER

EDSTRÖM¹, PAOLO BARONE², SILVIA PICOZZI³, and MASSIMILIANO STENDEL^{4,5} — ¹Department of Applied Physics, KTH Royal Institute of Technology, 10691 Stockholm, Sweden — ²CNR-SPIN, Area della Ricerca di Tor Vergata, Via del Fosso del Cavaliere 100, I-00133 Rome, Italy — ³CNR-SPIN, c/o Università degli Studi 'G. D'Annunzio', 66100, Chieti, Italy — ⁴ICMAB-CSIC, Campus UAB, 08193 Bellaterra, Spain — ⁵ICREA, 08010 Barcelona, Spain

Topological defects, such as domain walls or Skyrmions, are expected to carry an electrical polarization, opening for the possibility to stabilize, control and detect them with electric fields, even in collinear ferromagnets like CrI_3 . Here, we present a multiscale approach, combining atomistic and continuum magnetoelectric models, to accurately describe magnetoelectric coupling at different length scales, with all parameters extracted from first principles. The models are validated for spin spirals, revealing a sizeable magnetoelectric polarization. We describe the relation of the magnetoelectric parameters to electric field-induced Dzyaloshinskii-Moriya interactions. The models are then used to calculate the electric polarization and net dipole moments of magnetic domain walls (DWs) and Skyrmions, revealing e.g. that Skyrmions carry an out-of-plane electric dipole moment, while that of anti-Skyrmions lies in the plane. Finally, we discuss the possibility to stabilize these magnetic textures, none of which are otherwise energetically stable in the monolayer limit of CrI_3 , using electric fields.

KFM 15.4 Wed 15:45 EB 407

Electric field-driven dynamics of meron domain walls in spin spiral multiferroics — ●LUCA MARANZANA^{1,2} and SERGEY ARTYUKHIN¹ — ¹Italian Institute of Technology, Genoa, Italy — ²University of Genoa, Genoa, Italy

Spin spiral multiferroics exhibit strong coupling between magnetic and ferroelectric orders, allowing cross-control. Since their discovery by Kimura et al. in 2003, these materials have attracted great interest galvanized by the prospect of new high-efficiency information storage devices, where the magnetic bits are switched through an external electric field. Nevertheless, the electric field-driven dynamics of domain walls in spin spiral multiferroics (i.e. the mechanism underlying this switching) is still poorly understood. Here, we address this problem for meron domain walls, which arise at low anisotropy and consist of a periodic chain of merons (half-skyrmions). The topological charge lies at the heart of the dynamics and can be controlled by modifying the meron configuration or applying an external magnetic field. Domain walls with zero total topological charge present a low-field dynamics reminiscent of a massive particle in one dimension. In contrast, those with non-zero total topological charge evince a peculiar nonlocal dynamics where all the spins in the system rotate and the mobility is drastically reduced.

KFM 15.5 Wed 16:00 EB 407

Antimagnetolectricity in multiferroic BiCoO₃ from first-principles — ●BOGDAN GUSTER¹, MAXIME BRAUN^{1,2}, HOURIA KABBOUR², and ERIC BOUSQUET¹ — ¹Physique Théorique des Matériaux, QMAT, CESAM, Université de Liège, B-4000 Sart-Tilman, Belgium — ²Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181-UCCS-Unité de Catalyse et Chimie du Solide, F-59000 Lille, France

The lack of magnetolectric response in a multiferroics is prompted by the magnetic space group symmetry. This is the case of BiCoO₃ where the C-AFM ground state prohibits the promotion of a magnetolectric coupling. However, at the microscopic level, the local magnetolectric coupling could exhibit non-zero responses for both spin and orbital components. Here we show from first-principles calculations that the amplitude of dynamical magnetic charges arising from both spin- and orbital-lattice coupling in the C-AFM phase of BiCoO₃ are large when compared to the paradigmatic Cr₂O₃. While globally the response is zero, we resolve that the pseudo-tensorial character of the dynamical magnetic charges manifests an alternating sign for atoms yet on the same Wyckoff position. Consequently, unlocking the C-AFM phase, one could potentially allow for a large magnetolectric response. To prove this, we calculate the full magnetolectric response in the ferromagnetic phase of BiCoO₃ and we find a colossal response of 1000 ps/m, among the largest responses found so far in a single-crystal. We will discuss several strategies on how this large response could be released in some specific conditions and why the response is large.

KFM 15.6 Wed 16:15 EB 407

Electric field induced reversal of spin alignment in graphone/hexagonal boron nitride on Ni(111) — JAIME OLIVEIRA DA SILVA and ●FERNANDO NOGUEIRA — CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal

Spintronic applications require a precise and efficient way of manipulating the material's magnetisation. This work demonstrates that it is possible to revert the surface magnetisation of a graphene sheet covered in half by hydrogen by applying an external electric field. To demonstrate this possibility, we study a prototypical material where this effect occurs: a 2D layer material formed by a Ni(111) substrate, an hBN monolayer and a graphone sheet. Screening of the Coulomb interactions between the ferromagnetic surface and the graphone layer plays a key role in the magnetisation reversal, enabling graphone to partially recover its isolated magnetisation value. The screening is due to the forming of an ionic bond between the N and B atoms in the hBN sheet. As the proposed material has a flat band at the Fermi level, our work also provides prospects for investigating flat-band instabilities.

15 min. break

KFM 15.7 Wed 16:45 EB 407

Thermal conductivity in multiferroic CaBaCo₄O₇ — ●REZA FIROUZMANDI¹, MATTHIAS GILIG¹, YUSUKE TOKUNAGA², YASUJIRO TAGUCHI², YOSHINORI TOKURA², CHRISTIAN HESS³, VILMOS KOCSIS¹, and BERND BÜCHNER¹ — ¹IFW-Dresden, Dresden, Germany — ²RIKEN-CEMS, Wako, Japan — ³University of Wuppertal, Wuppertal, Germany

The coupling between the electronic and magnetic degrees of freedoms can lead to exotic transport phenomena in multiferroic materials. Particularly the propagation of charge neutral heat carriers can reveal interesting features in the thermal transport properties. Here, we report the thermal conductivity measurements in multiferroic CaBaCo₄O₇ which is built up by alternating Kagome and triangular layers of edge sharing CoO₄ tetrahedra in mixed valence state. We find anomalies related to the magnetic ordering as well as huge anisotropy in thermal conductivity. Field dependence of the thermal conductivity resembles to that of the ferroelectric polarization. We attribute the anisotropy to the strong phonon scattering on the orthorhombic twinning.

KFM 15.8 Wed 17:00 EB 407

Non-trivial Spin Structures And Multiferroic Properties Of The DMI-Compound Ba₂CuGe₂O₇ — ●KORBINIAN FELLNER¹, SEBASTIAN MÜHLBAUER¹, PETER WILD¹, MICHAL DEMBSKI-VILLALTA¹, TOMMY KOTTE², MARKUS GARST³, ALEXANDRA TURRINI⁴, and BERTRAND ROESSLI⁴ — ¹Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — ²Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Ger-

many — ³Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — ⁴Paul Scherrer Institut (PSI), Villigen, Switzerland

Incommensurate spiral magnets have raised tremendous interest in recent years, mainly motivated by their wealth of spin structures, such as skyrmions. A second field of interest is multiferroicity: Helical spin structures are in general ferroelectric, enabling the coupling of the electric and magnetic properties. Ba₂CuGe₂O₇, featuring a quasi-2D structure with Dzyaloshinskii-Moriya interactions (DMI), is a material that is interesting in both of these regards and combines them with a third one: a variety of unconventional magnetic phase transitions. Neutron diffraction is used for an examination of the distribution of critical fluctuations in reciprocal space, associated with the paramagnetic to helimagnetic transition of Ba₂CuGe₂O₇. Its reduced dimensionality prompts a transition from incommensurate antiferromagnetic fluctuations to 2D antiferromagnetic Heisenberg fluctuations, showcasing a varied array of magnetic phase transitions in spiral textures. Recently, a new phase with a vortex-antivortex magnetic structure has been theoretically described and experimentally confirmed.

KFM 15.9 Wed 17:15 EB 407

Atomic-scale visualization of multiferroicity in monolayer NiI₂ — MOHAMMAD AMINI¹, ●ADOLFO FUMEGA¹, HECTOR GONZALEZ-HERRERO^{1,2,3}, VILIAM VANO^{1,4}, SHAWULIENU KEZILEBIEKE⁵, JOSE LADO¹, and PETER LILJEROTH¹ — ¹Department of Applied Physics, Aalto University, FI-00076 Aalto, Finland — ²Departamento de Física de la Materia Condensada, Universidad Autonoma de Madrid, E-28049 Madrid, Spain — ³Condensed Matter Physics Center (IFIMAC), Universidad Autonoma de Madrid, E-28049 Madrid, Spain — ⁴Joseph Henry Laboratories and Department of Physics, Princeton University, Princeton, NJ 08544, USA — ⁵Department of Physics, Department of Chemistry and Nanoscience Center, University of Jyväskylä, FI-40014 University of Jyväskylä, Finland

Multiferroics have been seen as a disruptive building block for technological applications. Recently, evidence of multiferroicity has been provided in monolayer NiI₂. However, the multiferroic order in monolayer NiI₂ has not been characterized yet. In order to address this issue, here we perform an atomic-scale visualization of monolayer NiI₂. This is achieved by exploiting the atomic-scale magnetolectric coupling in NiI₂ to image spin-spiral multiferroics via scanning tunneling microscope (STM) experiments. Moreover, we directly show external electric field control of the multiferroic domains. Our result demonstrates a novel methodology to analyze and characterize the magnetic and electric orders in this type of multiferroics materials.

KFM 15.10 Wed 17:30 EB 407

Ptychographic imaging of multiferroic domains in freestanding BiFeO₃ films — ●TIM A. BUTCHER¹, NICHOLAS W. PHILLIPS¹, CHIA-CHUN WEI², CARLOS A. F. VAZ¹, ARMIN KLEIBERT¹, SIMONE FINIZIO¹, JAN-CHI YANG^{2,3}, SHIH-WEN HUANG¹, and JÖRG RAABE¹ — ¹Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — ²Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — ³Center for Quantum Frontiers of Research & Technology (QFort), National Cheng Kung University, Tainan 70101, Taiwan

The multiferroic domains in freestanding bismuth ferrite films were imaged with the synchrotron technique of soft X-ray ptychography, which can achieve a high spatial resolution in the order of 5 nm. The ferroelectric domains show a linear dichroic contrast at the Fe L₃ edge, while the antiferromagnetic spin cycloid was reconstructed from its diffraction peak under resonant scattering conditions. The results directly visualise the strong magnetolectric coupling and the changes in the multiferroic domain patterns with varying film thickness.

KFM 15.11 Wed 17:45 EB 407

Imaging the antiferromagnetic domains in LiCoPO₄ via the optical magnetolectric effect — ●BOGLÁRKA TÓTH¹, VILMOS KOCSIS^{2,3}, and SÁNDOR BORDÁCS^{1,4} — ¹Department of Physics, Institute of Physics, Budapest University of Technology and Economics, Hungary — ²RIKEN Center for Emergent Matter Science (CEMS), Japan — ³Institut für Festkörperforschung, Leibniz IFW-Dresden, Germany — ⁴ELKH-BME Condensed Matter Research Group, Budapest University of Technology and Economics, Hungary

LiCoPO₄ is a widely researched compound. Not only it is a very promising candidate as a cathode material for lithium-ion batteries, but also shows strong linear magnetolectric (ME) effect. Its two sub-

lattice antiferromagnetic (AFM) order emerging below $T_N = 21.7$ K breaks spatial inversion and time-reversal symmetries, and correspondingly gives rise to the ME effect. We investigated the optical ME effect of LiCoPO_4 , which manifests in the so-called directional dichroism; the light absorption difference for counter propagating beams. The absorption of polarized light in the sample was measured after poling, i.e.,

field-cooling the sample across T_N in external E and B fields simultaneously, to stabilize one or the other AFM domain. There is a finite absorption difference for the two AFM domains, which, considering they are time-reversal pairs of each other, we interpret as directional dichroism. A simple transmission microscope setup was constructed to image the AFM domains based on their absorption difference.

KFM 16: Crystal Structure Defects / Real Structure / Microstructure I

Chair: Theo Scherer (KIT Karlsruhe)

Time: Wednesday 15:00–17:10

Location: E 124

KFM 16.1 Wed 15:00 E 124

Ultrafast laser induced structural motion in crystalline and amorphous gold — ●OTHMANE BENHAYOUN¹, EMILIANO PRINCIPPI², BERND BAUERHENNE³, DMITRY IVANOV⁴, and MARTIN GARCIA¹ — ¹University of Kassel, Theoretical physics II, Kassel, Germany — ²Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy — ³University of Kassel, Theoretical physics I, Kassel, Germany — ⁴Moscow, Russia

An Ultrafast Electron Diffraction (UED) experiment showed a time-dependent nonuniform compression and expansion of a monocrystalline gold foil. This led to the time modulation of the Au Bragg peaks in both height and width that was measured by the experiment. The same effect is however not observed in polycrystalline gold. We thus perform Molecular Dynamics - Two Temperature Model (MD-TTM) simulations aiming to understand the results of the experiment. In our simulations, we obtain similar peak oscillations and determine the major mechanisms that lead to such lattice dynamics in the monocrystalline case and compare them with the polycrystalline case.

KFM 16.2 Wed 15:20 E 124

Laser-assisted formation of local defined absorbers for Cu(In,Ga)Se₂-micro-concentrator solar cells — ●SETAREH ZAHEDI AZAD¹, OWEN.C. ERNST¹, TORSTEN BOECK¹, HEIKE VOSS², SONJA CINQUE², JÖRN BONSE², JÖRG KRÜGER², JAN LUCASSEN³, MARTINA SCHMID³, and JENS MARTIN¹ — ¹Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, 12489, Germany — ²Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, 12205 Berlin, Germany — ³Universität Duisburg-Essen, Forsthausweg 2, 47057 Duisburg, Germany

The micro-concentrator design for high-performance Cu(In,Ga)Se₂ (CIGSe) solar cells is a promising approach to reduce the consumption of Indium and Gallium [1]. To save these rare materials, the local nucleation of (In,Ga)-islands at a micrometre scale is investigated. Our results show that the selective formation of an array of indium and gallium islands on Mo-coated soda-lime glass substrates is possible using localized laser-heating by a cw-laser, a diffractive optical element (DOE), and the use of trimethylindium and triethylgallium as precursors. The results indicate that nucleation is dependent on the laser power and the roughness of Molybdenum. By evaporation of Copper in a PVD chamber followed by selenization, the (In,Ga)-islands turn to CIGSe-islands serving as absorbers for micro-concentrator solar cells. Since the size and pattern of the CIGSe-islands can be easily controlled using the laser-heating/DOE-setup, this novel method can also be applied to large-scale production. [1] Sadewasser, S., Solar Energy 158 (2017): 186-191.

KFM 16.3 Wed 15:40 E 124

Influence of Ga concentration on crystal structure of CoCrFeNiGa_x (x = 0.5, 1) high-entropy alloys — ●TATIANA SMOLIAROVA¹, IVAN TARASOV¹, MARINA SPASOVA¹, ANDRÁS KOVÁCS², RAFAEL E. DUNIN-BORKOWSKI², MICHAEL FARLE¹, and NATALIA SHKODICH¹ — ¹Faculty of Physics and Center for Nanointegration, Universität Duisburg-Essen, Duisburg, Germany — ²Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, Germany

High-entropy alloys (HEAs) offer a novel approach to explore multi-component phase diagrams, leading to the discovery of new materials. Here, we report a transmission electron microscopy (TEM) study of the structural changes observed in micro-sized CoCrFeNiGa_x (x = 0.5, 1.0) powders, prepared by high-energy ball milling (HEBM) in planetary ball mills at room temperature. The process results in the

formation of an FCC crystal structure and compositional homogeneity. Additionally, we find in bulk samples obtained by consolidating the prepared micropowder using the spark plasma sintering (SPS) process (1073 K) preferential fcc structure for the CoCrFeNiGa_{0.5} powder, and a partial transformation of the FCC into a BCC structure for the equiatomic CoCrFeNiGa powder. Financial support by DFG, CRC/TRR 270 (project ID 405553726) is acknowledged.

10 min. break

KFM 16.4 Wed 16:10 E 124

Temperature-dependent Peierls Distortion in the Phase Change Material In₃SbTe₂ — ●MARIA HÄSER¹, MARTIN ETTER², HENRIK JEPPESEN², SEBASTIAN GEISLER³, OLIVER OECKLER³, and MATTHIAS WUTTIG¹ — ¹I. Institute of Physics (IA), RWTH Aachen University, Germany — ²Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — ³Faculty of Chemistry and Mineralogy, Institute of Mineralogy, Crystallography and Materials Science, Leipzig University, Germany

In recent years, interest in chalcogenide-based phase change materials (PCMs) has increased in photonic applications due to their significant difference in optical properties between the amorphous and crystalline phases. A promising candidate for photonic devices is In₃SbTe₂ (IST), which is a plasmonic PCM with metallic properties in the crystalline phase and semiconducting properties in the amorphous state. Using synchrotron radiation, the temperature-dependent atomic arrangement of crystalline IST has been investigated. The simulation of measured Powder X-Ray Diffraction (P-XRD) and Pair Distribution Function (PDF) data allows a direct comparison of the average and the local atomic arrangement: Although IST crystallizes in NaCl structure type (space group Fm-3m (225)) on average, we report local deviations from this structure. These Peierls-like deviations increase with increasing temperature. This finding can explain the temperature dependent behavior of IST and similar materials.

KFM 16.5 Wed 16:30 E 124

Where is the hydrogen going? – An investigation of lithium metal oxides — ●THOMAS KÖHLER¹, MATTHIAS ZSCHORNAK¹, PATRICK REICHART², ERICA BRENDLER¹, CHRISTIAN RÖDER¹, GÜNTHER DOLLINGER², HARTMUT STÖCKER¹, and DIRK C. MEYER¹ — ¹TU Bergakademie Freiberg, 09599 Freiberg, Germany — ²Universität der Bundeswehr München, 85579 Neubiberg, Germany

The incorporation of hydrogen into LiNbO₃ and LiTaO₃ during crystal growth has attracted the interest of researchers for more than 50 years. Our studies address the following open points: (i) the model description of the occupation sites, (ii) the diffusion kinetics, and (iii) the hydrogen concentration determination. Hydrogen bonds to oxygen and forms hydroxyl (OH⁻) defects. Since the shape of the vibrational modes strongly depends on the crystal stoichiometry, we can use them to elucidate the presence of different hydrogen occupation sites and the associated chemical environment.

Experimental and theoretical studies indicate that the intrinsic and extrinsic defects of the crystals are crucial, as hydrogen only decorates these defects. The diffusion of hydrogen was studied using elevated temperatures and different atmospheric conditions. Differences in diffusion rate and activation energy are dependent on the dominating defect type. Finally, the question arises: What is the natural hydrogen concentration in these materials? Hydrogen microscopy using proton-proton scattering is found to be the only reliable tool for absolute quantification and can be applied to obtain a calibration factor for infrared spectroscopy.

KFM 16.6 Wed 16:50 E 124

Evaluation of structural phase transition in spin-1/2 frustrated Dirac-magnon antiferromagnet: Cu_3TeO_6 — ●ISHA ISHA¹, M. ISOBE², N. P. LALLA¹, and ARVIND KUMAR YOGI¹ — ¹UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India — ²Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

We report the structural and physical properties of spin-1/2 ($3d^9$ as Cu^{2+}) ultra-high quality single-crystals of Cu_3TeO_6 . The susceptibility measured over single-crystal is showing quasi-1D behavior as confirmed by using Bonner-Fisher spin-1/2 1D chain model in the tem-

perature range from 20 K to 200 K. From magnetic susceptibility we deduce the nearest neighbor (NN) antiferromagnetic coupling constant $J \sim 113.2$ K. We show that this compound made of weakly coupled infinite chains of CuO_6 octahedral. Moreover, we have performed detailed x-ray diffraction technique to elucidate a structural-phase transition and our detailed analysis suggests an isostructural transition, resulting in an unusually temperature dependence of cubic cell parameter and atomic displacement below the second-order phase transition ($T_N \sim 61$ K) which indicates strong magneto-elastic coupling. Our results reveal yet another interesting facet of the magneto-elastic coupling in the Cu_3TeO_6 spin-web lattice.

KFM 17: Focus Session: Battery Materials – Experimental Characterisation and Safety Testing (joint session KFM/MM)

The focus session is dedicated to the characterization of microstructure, electrochemical, thermal and safety properties of Lithium-ion and Post-Lithium cells and their individual active and passive materials. This is required to obtain quantitative and reliable data, which are necessary to improve the current understanding in order to design and develop better and safer materials and cells. Potential topics include, but are not limited to electrochemical characterization techniques, thermal characterisation techniques, safety testing, development of safer materials and cell designs, thermodynamic modelling of materials, modelling of thermal runaway and propagation.

Chair: Carlos Ziebert (KIT Karlsruhe)

Time: Wednesday 15:00–19:05

Location: EMH 225

Invited Talk

KFM 17.1 Wed 15:00 EMH 225

Reversible and irreversible heat effects in batteries and battery materials — ●ANDREAS JOSSEN — Technical University of Munich, School of Engineering and Design, Department of Energy and Process Engineering, Chair for Electrical Energy Storage Technology, Arcisstrasse 21, 80333 Munich, Germany

Heat generation within batteries is caused by different effects, as entropy, over-potentials and voltage hysteresis. These effects depend on the state of charge and the state of health of the battery and the resulting temperature strongly influences the performance of the system. Therefore measuring of these heat effects is of high interest to support the material and cell design development. Especially of large format cells, as used in electric vehicles, the heat balance strongly influences the fast charge capability on system level. The presentation introduces the different effects and describes measurement methods (calorimetric and electrical based) and discusses the challenges for the different methods. Improved measurement methods are presented and measurement examples for some high-energy materials are discussed. An example where upscaling from a material level to large format cell is shown

KFM 17.2 Wed 15:30 EMH 225

Temperature dependency of the heat capacity of Lithium-ion batteries during Heat-Wait-Seek Tests in Accelerating Rate Calorimetry — ●PHILIPP FINSTER, HANS J. SEIFERT, and CARLOS ZIEBERT — Karlsruhe Institute of Technology (KIT), Institute of Applied Materials - Applied Materials Physics (IAM-AWP), Eggenstein-Leopoldshafen, Germany)

The Heat-Wait-Seek test in Accelerating Rate Calorimeter (ARC) can be used to estimate the safety performance of Lithium-ion cells by extracting parameters such as critical temperatures or generated heat. To calculate the generated heat, it is essential to know the heat capacity of the cell as a function of temperature.

In this study we show an accurate way to calculate the heat capacity of the cell, based on its individual components with respect to temperature. Additionally, we will discuss time dependency of the heat capacity, for instance while melting of the separator or venting. Using this dependence of temperature results in a significant difference in the calculated heat capacity of about 15 % in the temperature range from 298 K to 498 K. In this work the approach is applied to commercial type 21700 cells. The cells were measured in an ES-ARC from Thermal Hazard Technology, UK. The generated heat was compared for either fresh cells or cells after cyclic aging.

With this approach the generated heat in abuse tests can be predicted more accurately to simulate the propagation of heat during a single cell failure in a pack or to calculate the appropriate thickness of

a heat barrier for safer battery packs.

KFM 17.3 Wed 15:50 EMH 225

Thermal Runaway analysis of lithium-ion batteries with different electrolyte compositions — ●KARSTEN GEUDER, HANS JÜRGEN SEIFERT, and CARLOS ZIEBERT — Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Investigation of the safety of lithium-ion batteries, particularly with respect to thermal runaway, is critical because of the wide application of these batteries. This study specifically examines the influence of electrolyte and additives on battery safety and aims to improve our understanding of thermal runaway in full cells through comparative analysis.

Unlike commercial lithium-ion batteries, the electrolyte composition is well known. The control electrolyte of the 1Ah pouch cells is a 3:7 mixture of ethylene carbonate (EC) and ethyl methyl carbonate (EMC). In addition, we used the control electrolyte with either 5% vinylene carbonate (VC) or 5% fluoroethylene carbonate (FEC). To assign the different thermal processes and reactions in the full cells, the dry cells were disassembled and the components were analyzed by differential scanning calorimetry. The full cells were characterized for their thermal runaway behavior using both Heat-Wait-Seek and over-charge tests in accelerating rate calorimeters. We were able to correlate the endothermic behavior of the full cell at about 115 °C with the onset of separator melting. A comprehensive understanding of thermal runaway is critical to ensuring the safety of lithium-ion batteries. An accurate understanding of the electrolyte composition provides deeper insight into its safety implications.

KFM 17.4 Wed 16:10 EMH 225

Comparison of thermal safety of new and aged commercial 21700 lithium-ion batteries with different cathode materials by Accelerating Rate Calorimetry (ARC) — ●SEBASTIAN OHNESEIT, NILS UHLMANN, HANS JÜRGEN SEIFERT, and CARLOS ZIEBERT — Karlsruhe Institute of Technology (KIT), Institute for Applied Materials - Applied Materials Physics (IAM-AWP), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Cylindrical lithium-ion batteries (LIB) of type 21700 have multifaceted usage applications, such as consumer goods, battery electric and hybrid electric vehicles. In consequence, their safety in new and aged state is of particular interest. In this experimental study, the different cathode materials NMC, NCA and LFP were compared, as well as high power and high energy cells. Calendar and cyclic aging with different test conditions (temperature, discharge rate) was performed on the listed cell types and subsequently safety tests were performed on the aged cells, in comparison to results of new cells of the same type.

Thermal abuse was done by the heat-wait-see test in an Accelerating Rate Calorimeter (ARC). Several critical temperatures and temperature rates, as well as exothermal data, were determined. Furthermore, the grade of destruction and mass loss was determined, and all data was compared for aged and unaged cells. It was found that, for aged NMC and NCA cells, the aging parameter modified the exothermal reaction onset and overall, a lower maximum temperature was found for the aged cell state. LFP cells reacted, as expected, at significantly higher temperatures, making the cell chemistry considerably safer.

KFM 17.5 Wed 16:30 EMH 225

Are Li-ion cells safe for 2nd-Life Applications - The Case of Lithium Plating — •THOMAS WALDMANN^{1,2}, GABRIELA G. GEROSA¹, MAX FEINAUER¹, MARKUS HÖLZLE¹, and MARGRET WOHLFAHRT-MEHRENS^{1,2} — ¹Zentrum für Sonnenenergie- und Wasserstoff-Forschung (ZSW), Helmholtzstrasse 8, D-89081 Ulm — ²Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU), Helmholtzstrasse 11, D-89081 Ulm

Increased sustainability and reduced dependence on foreign critical resources (e.g. Co, Ni, Li) go hand in hand with increased cycle life and re-use of aged Li-ion batteries in 2nd-life applications before recycling. However, there is a lack of knowledge on the safety of aged cells with the mechanism of lithium plating. Lithium plating leads to fast aging of Li-ion cells due to reaction of the deposited lithium with electrolyte and formation of "dead lithium". We show results on the influence of lithium plating in commercial Li-ion cells in the 1st-life on safety in 2nd-life. Possibilities to detect and avoid lithium plating which we investigated recently are discussed. Arrhenius plots of the aging rate in the 1st-life show the typical V-shape and the transition to lithium plating as main aging mechanism below 25°C. Our safety tests show higher hazard levels for cells with lithium plating after the 1st-life. Therefore, lithium plating is an aging mechanism which is to be avoided. Possibilities are shown to avoid Li plating and for early detection of unsafe behavior.

15 min. break

KFM 17.6 Wed 17:05 EMH 225

Microstructural Impact on Filament Growth in All Solid-state Sodium Batteries — •ZIMING DING¹, YUSH TANG¹, TILL ORTMANN², JANIS KEVIN ECKHARDT², MARCUS ROHNKE², GEORGIAN MELINTE¹, CHRISTIAN HEILIGER², JÜRGEN JANEK^{1,2}, and CHRISTIAN KÜBEL^{1,3} — ¹Institute of Nanotechnology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — ²Institute for Physical Chemistry and Center for Materials Research, Justus Liebig University Giessen, Giessen, Germany — ³Karlsruhe Nano Micro Facility, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Although the intergranular growth mechanism in inorganic solid electrolytes (SEs) based lithium-based all solid-state batteries (ASSBs) is well studied, there is still much to be learned for sodium-based ASSBs. The polycrystalline Na-β'-alumina is selected as a model material to investigate its microstructural impact on Na-filament growth. Using in situ biasing transmission electron microscopy, the Na-filament growth at the interface between the SE and electrode and grain boundaries (GBs) within the SE, were observed during Na deposition. The relationship between the microstructure of SE and filaments is further studied through the orientation analysis and correlative imaging. It is found that anisotropic ion transport due to layered crystal structure can contribute to distinctive Na-ion transport behaviors at different GBs during operation and influence the Na-filament growth. This work helps to understand Na-filament formation and how a critical filament network might form leading to failure of the battery.

KFM 17.7 Wed 17:25 EMH 225

Computational and experimental investigation of Na and Y co-doping on electrochemical performance of LiNi_{0.8}Co_{0.15}Al_{0.05}O₂ cathode material for Li-ion batteries — SAHAR ZIRAKI¹, •MANSOUR KANANI¹, BABAK HASHEMI¹, and MOHAMMAD MOHSEN LOGHAVI² — ¹Department of Materials Science and Engineering, School of Engineering, Shiraz University, Shiraz, Iran — ²Department of Energy Storage, Institute of Mechanics, Shiraz, Iran
LiNi_{0.8}Co_{0.15}Al_{0.05}O₂ (NCA) has attracted a lot of attention owing to its high voltage, specific energy density, and specific capacity. However, the cycle durability of the NCA material is still a challenge. In this study, the addition of sodium (Na) on Li-site and yttrium (Y)

on metal-site, and their co-doping into NCA material, were investigated experimentally and theoretically. For the first time, we proposed a framework for parameterization of the structural and thermal stability of NCA during the lithiation/delithiation process in terms of first-principle density functional theory (DFT) calculations. The computational results confirmed the positive effect of Na⁺ and Y³⁺ on the structural and thermal stability of the NCA cathode systematically. Following those outcomes, different percentages of the dopants were added to the cathode material experimentally, and electrochemical tests were performed. The underlying mechanisms of observed experimental improvements were interpreted and discussed according to the computational outcomes.

KFM 17.8 Wed 17:45 EMH 225

Pits and Traps in the Impedance Analysis of Ionic Conductors — •JANIS K. ECKHARDT^{1,2,3}, SASCHA KREMER^{2,3}, MATTHIAS T. ELM^{2,3,4}, PETER J. KLAR^{3,4}, JÜRGEN JANEK^{2,3}, and CHRISTIAN HEILIGER^{1,3} — ¹Institute for Theoretical Physics, Justus Liebig University, Giessen D-35392, Germany — ²Institute of Physical Chemistry, Justus Liebig University, Giessen D-35392, Germany — ³Center for Materials Research (ZfM), Justus Liebig University, Giessen D-35392, Germany — ⁴Institute of Experimental Physics I, Justus Liebig University, Giessen D-35392, Germany

The development of innovative electrochemical storage systems, such as solid-state batteries, is critical for achieving climate neutrality and sustainability goals. Several hurdles must be overcome before such technologies are ready for the market. Impedance spectroscopy is a powerful method for characterizing the electrical transport properties of new materials and for monitoring systems in operation. Although it is an older measurement technique, the interpretation of data for inhomogeneous solid-state systems lacks established concepts for reliable results. Thus, we use 3D electrical network models for spatially-resolved transport simulations and systematic investigation of the influence of sample microstructure and solid-solid interface morphology. The material-specific transport quantities derived from 1D models (e.g., brick layer model) sometimes exhibit inaccuracies of several orders of magnitude. In addition, the impedance response of the system exhibits geometric signatures that cannot be adequately represented in 1D physically motivated circuit models, e.g., current constriction.

KFM 17.9 Wed 18:05 EMH 225

Vacancies on the Lithium-Sublattice in the Solid-State Electrolyte LLZO employing Positron Annihilation Spectroscopy — DOMINIK BORAS¹, ANDREAS KOHRMANN¹, DANIEL WAGNER¹, DANIEL GÖBEL¹, JANEZ KOSIR², TANJA KALLIO², and •TORSTEN E.M. STAAB¹ — ¹Institute for Functional Materials and Biofabrication, Julius-Maximilians Universität Würzburg, D-97070 Würzburg, Röntgenring 11 — ²Department of Chemistry, Aalto University, Kemistintie 1, FIN-02015 Espoo

We characterize the electrolyte LLZO for all solid-state batteries. LLZO (Li₇La₃Zr₂O₁₂) samples have been synthesised via the mixed-oxide route, i.e. grinding and calcination, grinding again, then pressing and finally sintering the pellets. We varied the doping (Fe, Al) and the excess Li content. The formed phases (cubic and tetragonal) have been characterised by XRD, while the lattice defects have been investigated by the method of positron annihilation lifetime spectroscopy (PALS). By PALS we were able to see clear differences after calcination when varying the lithium excess. Measuring powder with increasing Li-excess a lifetime component, which could be related to the bulk crystal significantly decreases from 220ps to 190ps. This may be an indication of more and more filled Li-lattice site after the calcination step. Sintered pellets showed two different positron lifetimes (190 / 200ps and 326 / 374ps) for both un-doped / Al-doped samples. This first attempt shows the potential of PALS to characterise all solid-state electrolytes with respect to defects and the occupation of crystal lattice site influencing the mobility of Li ions.

KFM 17.10 Wed 18:25 EMH 225

Exploring Polaron Stability and Defect Structures in Li₄Ti₅O₁₂ (LTO): A Combined Theoretical and Experimental Approach — •YU-TE CHAN¹, MATTHIAS KICK², CRISTINA GROSU², CHRISTOPH SCHEURER¹, and HARALD OBERHOFER³ — ¹Fritz-Haber-Institut der MPG, Berlin — ²Massachusetts Institute of Technology, Cambridge, USA — ³University of Bayreuth

Spinel Li₄Ti₅O₁₂ (LTO) is a promising anode material for next-generation all-solid-state Li-ion batteries (ASSB) due to its "zero strain" charge/discharge behavior. Pristine, white LTO possesses poor

ionic and electronic conductivity. Through tailoring the sintering protocol, one can produce oxygen vacancies accompanied by polaron formation, resulting in a performing, blue LTO material.

By performing Hubbard corrected density-functional theory (DFT+U) calculations we are able to show that polaron formation and a possible polaron hopping mechanism play a significant role in enhancing electronic conductivity and in boosting Li^+ diffusion, in line with the experimentally observed improved conductivities.[1] We pair these findings with positron lifetime spectroscopy (PALS) to study the charge carriers' (polaron and Li^+) behavior and the defect structures produced in the sintering. We developed a machine-learned potential to study the dynamics of the polaron and the structural defects measured from PALS, reaching a rather complete picture of the bulk vs. surface defect chemistry in LTO particles.

[1] M. Kick *et al.*, J. Phys. Chem. Lett. **11**, 2535 (2020); ACS Appl. Energy Mater. **4**, 8583 (2021).

KFM 17.11 Wed 18:45 EMH 225

Partially substituted metal sulfide anodes for high-performance sodium-ion batteries — ●ZIDONG WANG — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Due to sodium resources' abundance and easy availability, sodium-ion battery technology has attracted extensive research interest and made significant progress in recent years. Among the various anode materials used for sodium-ion battery anodes, transition metal sulfides, especially bimetallic sulfides, have great potential due to their high capacity and electrochemical activity. In this work, the original bimetallic sulfide cations were partially replaced to improve the performance further. In this strategy, the synergistic effect of multi-metal cations will result in superior energy absorption and enhancement. Metal elements with different oxidation states can produce higher capacity through synergistic effects with each other. Mn-Ni-Co-S with 10% substitution showed satisfactory capacity (721.09 mAh/g at 300 mA/g and 662.58 mAh/g after 20 cycles) and excellent cycle life (85.41% capacity retention after 1000 cycles at 2000 mA/g).

KFM 18: SrTiO₃: A Versatile Material from Bulk Quantum Paraelectric to 2D Superconductor: Poster (joint session TT/KFM/MA/O)

Strontium titanate (SrTiO₃) is a paradigmatic material that plays an important role in various fields of solid-state physics, surface science and catalysis: The pure bulk phase is a wide-band-gap semiconductor that upon cooling becomes a textbook quantum paraelectric. When slightly doped, SrTiO₃ turns into a Fermi-liquid-type metal that becomes superconducting at extremely low charge carrier density. SrTiO₃-based surfaces and interfaces host un-conventional electronic states such as quasi-two-dimensional electron liquid, magnetism and superconductivity. Despite intensive studies over the past decades, SrTiO₃ continues to reveal surprising new phenomena that challenge the established views on this material. To this end achieving light-induced nonequilibrium states and the recent preparation of a 2D oxide based on SrTiO₃ opens new playgrounds for research. This Focus Session will present exciting developments in the study of electronic states that are based on the peculiar properties of SrTiO₃.

Please note that this Focus Session comprises four parts: Posters are presented within the TT poster session TT58, Wed 15:00-18:00, poster area E. Invited talks are compiled in the session TT62 (Thursday, 9:30 to 12:45, H0104), Contributed talks will be presented in sessions TT72 (Thursday 15:00-18:00, H0104) and TT83 (Fri 9:30-12:30, H0104).

Organizers: Rossitza Pentcheva, University of Duisburg-Essen, Marc Scheffler, University of Stuttgart

Time: Wednesday 15:00–18:00

Location: Poster E

KFM 18.1 Wed 15:00 Poster E

Optical conductivity of superconducting Nb:SrTiO₃ in magnetic fields at GHz frequencies — ●CENK BEYDEDA¹, MARKUS THIEMANN¹, MARTIN DRESSEL¹, HANS BOSCHKER², JOCHEN MANNHART², and MARC SCHEFFLER¹ — ¹Physikalisches Institut, Universität Stuttgart — ²Max-Planck-Institut für Festkörperforschung, Stuttgart

Doped SrTiO₃ was among the first unconventional superconductors, the application of the BCS theory is questionable due to the small Fermi energy. Here we present the optical conductivity (1 – 30 GHz) of superconducting Nb:SrTiO₃ in magnetic field. We observe features typical of an s-wave single-gap dirty type II superconductor. We attribute a kink in the magnetic field dependence to 2 distinct superconducting bands. We observe values of the real part of the optical conductivity exceeding the normal state value multiple times for rising magnetic field. Excessive losses at low frequency $hf \ll 2\Delta$ in dependence of temperature are a known feature of superconductivity and a result of coherence effects of the Cooper pairs in the superconducting state (coherence peak). The excessive losses we observe with rising magnetic field are substantially different from the coherence peak, especially in magnetic field dependence and absolute values. As far as we know, excessive losses of this type were not observed in any other superconductor. It is not clear whether Nb:SrTiO₃ is the only material that can show excessive losses of this type. We present an interpretation of our data in terms of Caroli-de Gennes-Matricon modes in the vortex state, reproducing the effect of excessive losses qualitatively.

KFM 18.2 Wed 15:00 Poster E

Ultrafast second harmonic generation spectroscopy of SrTiO₃

surfaces and interfaces — MAHENDRA KABBINAHITHLU, NEWSHA VESALIMAHMOUD, TOBIAS LOJEWSKI, PING ZHOU, KATHARINA OLLEFS, and ●ANDREA ESCHENLOHR — Faculty of Physics and CENIDE, University Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Perovskite oxide heterostructures can exhibit properties at their interfaces that are very different from the bulk, for example a two-dimensional electron gas [1]. These properties emerge from charge carrier localization or charge transfer, which motivates an interface-sensitive analysis of the charge configuration and charge carrier dynamics. Second harmonic generation (SHG) spectroscopy is an interface-sensitive probe in centrosymmetric materials, suitable for the investigation of SrTiO₃-based heterostructures [2]. We perform pump-probe SHG spectroscopy with < 30 fs time resolution in the visible wavelength range (1.9-2.5 eV) at SrTiO₃(001) surfaces as well as LaTiO₃/SrTiO₃ heterostructures, and discuss the polarization-, wavelength- and time-dependence of the observed SHG response.

[1] H. Y. Hwang, Y. Iwasa, M. Kawasaki, B. Keimer, N. Nagaosa, Y. Tokura, Nat. Mater. **11**, 103 (2012).

[2] A. Rubano, D. Paparo, Materials **16**, 4337 (2023).

KFM 18.3 Wed 15:00 Poster E

Low-temperature GHz response of quantum paraelectrics SrTiO₃ and KTaO₃ — VINCENT T. ENGL, NIKOLAJ G. EBENSBERGER, CENK BEYDEDA, LARS WENDEL, MARIUS TOCHTERMANN, ILENIA NEUREUTHER, ISHAN SARVAIYA, MARTIN DRESSEL, and ●MARC SCHEFFLER — 1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany

The low-temperature dielectric properties of SrTiO₃ and KTaO₃ are

characteristic of their quantum paraelectric nature: upon cooling, the real part ϵ_1 of the dielectric function strongly increases, but eventually levels off at high values of ≈ 20000 for SrTiO₃ and ≈ 4000 for KTaO₃. In particular for SrTiO₃ it is very demanding to combine such dielectric bulk material with conventional GHz circuitry. We present superconducting coplanar Nb resonators on SrTiO₃ and KTaO₃ substrates, where in the case of SrTiO₃ we employ a distant flip chip geometry. Taking advantage of several resonator modes, we determine the dielectric properties of the two materials at frequencies around 1 GHz and at temperatures down to 25 mK. We thus access regimes of frequency and temperatures, where the dielectric properties of SrTiO₃ and KTaO₃ have barely been studied.

For the case of SrTiO₃, we find an unexpected temperature dependence of the real part ϵ_1 of the dielectric constant: at temperatures below 5 K, where ϵ_1 is expected to vary little upon further cooling, we find a clear maximum around 3 K and a weak minimum around 200 mK. We also observe a strong suppression of microwave losses in both SrTiO₃ and KTaO₃ for temperatures down to the mK range.

KFM 18.4 Wed 15:00 Poster E

ferromagnetic two-dimensional electron gas in oxide interfaces — •YU CHEN¹, MARIA D'ANTUONO^{1,2}, MARTANDO RATH¹, CINTHIA PIAMONTEZE³, DANIELE PREZIOSI⁴, BENOIT JOUAULT⁵, DANIELA STORNAIUOLO^{1,2}, and MARCO SALLUZZO¹ — ¹CNR-SPIN, Napoli, Italy — ²Università di Napoli "Federico II", Italy — ³Photon Science Division, Paul Scherrer Institut, Switzerland — ⁴Université de Strasbourg, CNRS, IPCMS UMR, France — ⁵Laboratoire Charles Coulomb, UMR 5221, CNRS, Université de Montpellier, France

Interfacial inversion symmetry breaking triggers novel phenomena not observed in bulk materials, such as unconventional superconductivity and magnetism. Here, we report on the realization of ferromagnetic two-dimensional electron gas (2DEG) at (001) and (111) interfaces between LaAlO₃, EuTiO₃, and SrTiO₃. At variance with the octahedral and quasi-octahedral symmetry in bulk SrTiO₃ and (001) interface, trigonal crystal field is reconstructed at (111) interface. The experiments of transport, magnetic and x-ray spectroscopy indicate that the filling of Ti 3d bands in the EuTiO₃ layer and at the interface with SrTiO₃ induces an exchange interaction between Eu-4f⁷ magnetic moments. We observe carrier density-dependent ferromagnetic correlations and anomalous Hall effect, sizable in-plane orbital moment possibly related to Ti-3d electrons occupying bands with the main 3d_{xz,zy} and a_{1g} orbital characters at (001) and (111) interfaces, respectively. Our findings show intriguing interplay between ferromagnetism, spin-orbit coupling, and symmetry breaking at oxide 2DEG, serving as a guide for the materials design of advanced spintronics.

KFM 18.5 Wed 15:00 Poster E

Role of excitonic effects in optical and x-ray absorption spectroscopy of SrTiO₃: insights from a combined first principles and many-body theory approach — •V. BEGUM-HUDE¹, M. E. GRUNER², and R. PENTCHEVA² — ¹University of Illinois Urbana-Champaign, USA. — ²University of Duisburg-Essen, Duisburg, Germany.

We present a comprehensive study of the optical[1] and x-ray absorption spectrum[2] (XAS) in the paradigmatic oxide, SrTiO₃. Our results demonstrate that inclusion of the quasiparticle effects with single-shot G_0W_0 as well as the electron-hole (e-h), and electron-(core)hole interactions by solving the Bethe-Salpeter Equation (BSE) is integral to accurately describe both the valence and core electron excitations. For the optical spectra, the effect of the exchange-correlation functional is

observed to progressively reduce from 1.5 eV variance in the onset of the spectrum in the independent particle picture to 0.3 eV upon inclusion of excitonic corrections. The Ti-L_{2,3} XAS edge is concurrent with experiment w.r.t. the energetic positions of the four-peak structure which is characteristic of Ti octahedral coordination in SrTiO₃. We also analyze the origin of prominent peaks in the spectra and identify the orbital character of the relevant contributions by projecting the e-h coupling coefficients from the BSE eigenvectors on the band structure. The spatial distribution of the first bound exciton wave function of the O K edge exhibits an intriguing two-dimensional spread in the x-y plane despite the three-dimensional nature of the material.

[1] Phys. Rev. Mater. **3**, 065004 (2019)

[2] Phys. Rev. Res. **5**, 013199 (2023)

KFM 18.6 Wed 15:00 Poster E

Boosting the Edelstein effect of two-dimensional electron gases by ferromagnetic exchange — •GABRIEL LAZRAC¹, ANNIKA JOHANSSON², BÖRGE GÖBEL^{2,3}, INGRID MERTIG^{2,3}, AGNÈS BARTHÉLÉMY¹, and MANUEL BIBÈS¹ — ¹Laboratoire Albert Fert, Université Paris-Saclay, CNRS, Thales, Palaiseau, FRANCE — ²Max Planck Institute of Microstructure Physics, Halle, GERMANY — ³Martin Luther University Halle-Wittenberg, Halle, GERMANY

In this work, we show that making STO 2DEGs ferromagnetic significantly boosts the conversion efficiency of charge and spin currents through direct and inverse Edelstein effects (EE/IEE). Starting from the experimental band structure of non-magnetic SrTiO₃ 2DEGs, we mimic magnetic exchange coupling by introducing an out-of-plane Zeeman term in a tight-binding model. We then calculate the band structure and spin textures for increasing internal magnetic fields and compute the Edelstein effect using a semiclassical Boltzmann approach. The conversion efficiency initially rises with magnetic field strength, reaching a maximum before declining. This behavior results from the interplay between exchange coupling and the effective Rashba interaction. Our experimental focus is on the 2DEG at the SrTiO₃/EuO interface to introduce ferromagnetism into the system.

KFM 18.7 Wed 15:00 Poster E

Impact of a Si(001) substrate on the electronic reconstruction and two-dimensional electron gas formation at LaTiO₃/SrTiO₃(001) — •ANDRI DARMAWAN and ROSSITZA PENTCHEVA — Department of Physics, University of Duisburg-Essen

The two-dimensional electron gas (2DEG) formed at oxide interfaces e.g. between the band insulator SrTiO₃ and the Mott insulator LaTiO₃ has attracted a lot of attention [1]. However, despite the high carrier density at the interface, the carrier mobility is lower compared to semiconductor materials. A strategy to overcome this shortcoming is the integration of the oxide system on a semiconductor substrate [2]. Based on density functional theory calculations with a Hubbard U term we modeled LaTiO₃/SrTiO₃(001) with and without a Si(001) substrate. We explore systematically the sample geometry and the effect of the termination to Si(001) on the electronic reconstruction at the LaTiO₃/SrTiO₃(001) interface. The comparison between the two systems indicates lower effective masses and consequently higher mobility of the 2DEG at LaTiO₃/SrTiO₃/Si(001).

Funding by DFG within CRC1242 and computational time at the Leibniz Supercomputer Center (project pr87ro) are gratefully acknowledged.

[1] A. Ohtomo et al., Nature 419, 378 (2002)

[2] E. N. Jin et al., APL Mater. 2, 116109 (2014)

KFM 19: Topical Session: In Situ and Multimodal Microscopy in Materials Physics (joint session MM/KFM)

Time: Wednesday 15:30–18:00

Location: C 130

Topical Talk KFM 19.1 Wed 15:30 C 130
Charges, Structure, Properties - Concepts and Applications of four-dimensional electron microscopy — ●KNUT MÜLLER-CASPARY^{1,3}, BENEDIKT DIEDERICH^{1,2}, ZIRIA HERDEGEN¹, TIZIAN LORENZEN¹, FELIX DUSHIMINEZA^{1,3}, MAX LEO LEIDL^{1,3}, ACHIM STRAUCH³, and FRANK FILBIR² — ¹Ludwig-Maximilians-Universität München, Dept. of Chemistry, Butenandtstr. 11, 81377 München — ²Institute of Biological and Medical Imaging, Helmholtz Zentrum München, 85764 Neuherberg, Germany — ³Forschungszentrum Jülich, Wilhelm Johnen Str., 52425 Jülich

Scanning an electron probe across a specimen and recording a diffraction pattern at each scan point established 4D-STEM as a versatile concept to characterise materials. We start with a very brief introduction of mapping electric fields and electrostatic potentials by using direct methods such as centre-of-mass imaging and analyticalptychographic solutions to the inverse single-scattering problem. Applications to large-scale electric field mapping and 2D materials will be shown. For thicker specimens, structure retrieval needs to invert multiple scattering. In this respect, we report a parametric inverse multislice concept in which both partial coherence of the probe and multiple frozen phonon states are taken into account. In particular, we investigate the impact of thermal diffuse scattering on different inverse multislice approaches. The concept is demonstrated via simulations first, and then applied to measure ionic displacements in ferroelectrics with picometre precision.

KFM 19.2 Wed 16:00 C 130

TEM investigations of local structure and dynamics in PdNiP bulk metallic glass — ●OLIVIA VAERST¹, MARTIN PETERLECHNER², and GERHARD WILDE¹ — ¹Institute of Materials Physics, University of Münster, Münster, Germany — ²Karlsruhe Institute of Technology, Laboratory for Electron Microscopy (LEM), Karlsruhe, Germany

The bulk metallic glass PdNiP is kinetically highly stable against crystallisation and therefore often used as a model system for investigations of the glassy state. Such investigations include experiments to further explore the glass formation and the structure-property relations of metallic glasses. In this work, the focus lies on understanding the atomic structure and local mobility of PdNiP in various thermo-mechanical states. For this purpose, multimodal transmission electron microscopy (TEM) measurements are performed using advanced techniques. The main method used is electron correlation microscopy (ECM), where diffracted intensities of a time series of dark-field images are correlated to deduce structural dynamics parameters with nanometer spatial resolution. A systematic analysis of the effect of varying electron beam parameters on the dynamics is conducted and optimal measuring parameters for PdNiP are determined. 4D-STEM fluctuation electron microscopy (FEM) is used for complementary structural investigations concerning the medium-range order of the different thermo-mechanical material states. The results on local dynamics and structural properties are discussed with respect to properties measured by macroscopically averaging methods.

KFM 19.3 Wed 16:15 C 130

Strain mapping of a sigma 5(310) grain boundary in a Cu bi-crystal using scanning transmission electron microscopy — ●ANOOSHEH AKBARI¹, HARALD RÖSNER¹, ESAKKIRAJA NEELAMEGAN¹, HUI DING², CHRISTIAN.H LIEBSCHER², SERGIY DIVINSKIY¹, and GERHARD WILDE¹ — ¹Institute of Materials Physics, University of Münster, Münster, Germany — ²Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Grain boundaries play an important role in determining the physical properties of materials. With respect to diffusion, extended strain fields localized at GBs can modify atomic transport along GBs. In order to understand the effect of strain on GB diffusion in more detail, the evolution of strain along GBs under mechanical treatment is investigated. For this purpose, a Cu bi-crystal containing a sigma 5(310) GB was fabricated by a modified Bridgman technique, followed by annealing at 800 °C. The surface was mirror-like polished subsequently followed by FIB lamella target preparation of the GB in cross-sectional view. The elastic strain along and around the GB was measured on a nanometer scale, using nano-beam diffraction patterns (NBDPs) ac-

quired using a 1 nm STEM probe with grains oriented in zone axis conditions. A custom written code was employed to extract the strain maps. On the atomic scale, the strain was characterized using geometrical phase analysis applied to high resolution STEM images confirming the results obtained by NBDP. The analysis was finally extended to deformed samples.

KFM 19.4 Wed 16:30 C 130

Unfolding structural features of NaNbO₃ using atomic resolution 4D-STEM — ●HUI DING¹, YU HUANG², MAO-HUA ZHANG³, JING-FENG LI², and CHRISTIAN H. LIEBSCHER¹ — ¹Structure and Nano- / Micromechanics of Materials, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — ²School of Materials Science and Engineering, Tsinghua University, Beijing, China — ³Department of Materials Science and Engineering, Penn State University, University Park, USA

As one of the most promising lead-free antiferroelectrics, NaNbO₃ suffers from irreversibility of the phase transition, limiting further application in electronic devices. Understanding the structural complexity and establishing a well-defined structure-property relationship of NaNbO₃ is of great importance for targeted tailoring of its functionality.

Here, we employ atomic resolution HAADF-STEM and 4D-STEM to probe the local atomic structure of NaNbO₃ thin films resolving the Nb, Na and O sublattices simultaneously. Reconstructed differential phase contrast STEM images indicate either the coexistence of P4bm (tetragonal) and P2₁ma (orthorhombic) phases, instead of the intrinsic Pbcm phase, or the formation of a new hybrid phase. In particular, the O columns form a zig-zag pattern along the Nb columns in the (001) plane due to O octahedral tilting, which is the characteristic of the P2₁ma phase. However, an alternating contrast of the Na columns, characteristic for the P4bm phase, is observed and confirmed by 4D-STEM image simulations.

KFM 19.5 Wed 16:45 C 130

Machine learning-enabled tomographic imaging of chemical short-range order in Fe-based alloys — ●YUE LI and BAPTISTE GAULT — Max-Planck Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Chemical short-range order (CSRO), describing preferential local ordering of elements within the disordered matrix, can change the mechanical and functional properties of materials. CSRO is typically characterized indirectly, using volume-averaged (e.g. X-ray/neutron scattering) or through projection microscopy techniques that fail to capture the complex, three-dimensional atomistic architectures. Quantitative assessment of CSRO and concrete structure-property relationships have remained so far unachievable. Here, we present a machine-learning enhanced approach to break the inherent resolution limits of atom probe tomography to reveal three-dimensional analytical imaging of the size and morphology of multiple CSRO. We showcase our approach by addressing a long-standing question encountered in a body-centred-cubic Fe-18Al and Fe-19Ga (at.%) alloy that sees anomalous property changes upon heat treatment, supported by electron diffraction and synchrotron X-ray scattering techniques. The proposed strategy can be generally employed to investigate short/medium/long-range ordering phenomena in a vast array of materials and help design future high-performance materials.

KFM 19.6 Wed 17:00 C 130

TESCAN 4D-STEM for Multimodal Characterization of Challenging and Interesting Specimens — LARS-OLIVER KAUTSCHOR¹ and ●ROBERT STROUD² — ¹TESCAN GmbH, Zum Lonnenhohl 46, Dortmund — ²TESCAN USA, 765 Commonwealth Dr #101, Warrendale, PA 15086, USA

The all-new TESCAN TEM solution: TESCAN TENSOR - the world's first Integrated, Precession-assisted, Analytical 4D-STEM will be presented. Designed from the ground up TESCAN TENSOR's quality throughput, and robustness of 4D-STEM acquisition, analysis, and processing has been optimized with state-of-the-art technologies, such as Precession Electron Diffraction (PED), 4D-STEM computing and visualization, electrostatic beam blanking, and ultra-high vacuum

at the specimen area. Additionally, TESCAN TENSOR features real-time, automated data analysis and processing, which empowers an unprecedented level of system accessibility, utilization, and productivity. The methodology behind this advanced (electron diffraction) microscope will be explained as the solution of choice for a range of nanoscale applications.

KFM 19.7 Wed 17:15 C 130

Micro-CT goes multimodal - 3D elemental analysis with new the SPECTRAL CT, — ●LARS-OLIVER KAUTSCHOR — TESCAN GmbH, Zum Lonnenhohl 46, Dortmund

X-ray micro-computed tomography (micro-CT) has opened new avenues of research and understanding. It is now recognized as an essential technique for non-destructive 3D imaging. Extending the technique to the temporal regime, through time-resolved 3D imaging (or 4D imaging), provides a new route to better and more complete understanding of materials evolution, facilitating in situ investigations ranging from mechanical deformation to fluid flow in porous materials. With the new SPECTRAL CT, TESCAN offers the possibility to perform elemental analysis inside your sample non-destructively. In this talk we explore the general technique of micro-CT as well as the advantages of the new SPECTRAL.

Topical Talk

KFM 19.8 Wed 17:30 C 130

Unsupervised Machine Learning Analysis for Electron Mi-

croscopy Datasets — ●MARY SCOTT — Department of Materials Science and Engineering, University of California, Berkeley, Berkeley, CA 94720, USA — National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Lab, Berkeley, CA 94720, USA

Electron microscopy is the characterization method of choice to observe local atomic-scale and microstructural features within materials that play a critical role in material performance. Recently developed high frame rate electron detectors acquire diffraction patterns from nanoscale regions at frame rates of 100 kHz, an approach that enables multimodal analysis from the same dataset to create maps of crystal orientation, strain, and more. This method, termed 4D-STEM, creates datasets can contain tens of thousands of diffraction patterns from heterogeneous structural regions. The large datasets cannot be analyzed manually, and lack of prior knowledge of the crystal structure of diverse samples limits the application of supervised automated approaches, motivating the development of unsupervised analysis. Here I will overview implementation of an automated, unsupervised clustering pipeline for 4D-STEM data, emphasizing the importance of input data representation. Furthermore, I will describe an ensemble approach to generate more stable clustering results. This type of unsupervised data analysis pipeline is an important step towards incorporating rapid 4D-STEM analysis into material discovery and design efforts, particularly when evaluating defect-rich and disordered materials.

KFM 20: Structurally and Chemically Complex Alloys (joint session MM/KFM)

Time: Wednesday 17:15–18:00

Location: C 230

KFM 20.1 Wed 17:15 C 230

Synthesis and atomic transport properties in pseudo-binary ordered B2 aluminides — ●MOHAN MURALIKRISHNA GARLAPATI¹, CHRISTIAN H. LIEBSCHER², MURTY B.S.³, GERHARD WILDE¹, and SERGIY V. DIVINSKI¹ — ¹Institute of Materials Physics, University of Muenster, 48149-Muenster, Germany — ²Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — ³Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, 600036-Chennai, India.

The present study highlights a novel alloy design of HEAs to fabricate fully ordered pseudo-binary multicomponent and ordered aluminides and is focused on the underlying diffusion behaviour. Microstructure and sublattice ordering in the multicomponent alloys starting from binary to hexanary B2 aluminides are studied. A radiotracer technique using the ⁵⁷Co, ⁵⁹Fe, ⁵⁴Mn, ⁶³Ni and ⁶⁵Zn radioisotopes is employed to measure the diffusion rates of individual elements. Diffusion in the multicomponent (n>4) B2 ordered alloys is found to be enhanced in comparison to stoichiometric binary AlNi. However, the addition of Co or Fe to AlNi slows down (Co) or enhances (Fe) the diffusion rates. The measured diffusivities are compared to the literature data and the effect of chemical complexity and the B2 ordering on diffusion are discussed.

KFM 20.2 Wed 17:30 C 230

Short range order in compositionally complex NiCoMnTi alloys — DAVID KOCH¹, BENEDIKT BECKMANN¹, OLEH IVASKO², MARTIN VON ZIMMERMANN², OLIVER GUTFLEISCH¹, and ●WOLFGANG DONNER¹ — ¹Institute of Materials Science, Technical University of Darmstadt, 64287 Darmstadt, Germany — ²Deutsches Elektronen-Synchrotron DESY, D-22607 Hamburg, Germany

Analyzing the chemical order in compositionally complex alloys can be challenging and may become complicated by low elemental contrast. One such compositionally complex material is the all-d-Heusler alloy NiCoMnTi. These alloys exhibit a tunable magneto-structural

phase transition, where the high-temperature phase has a long-range B2 structure that can be adjusted through proper thermal treatment. The typical long-range *L*₂₁ structure found in classical p-metal Heusler alloys cannot be stabilized. In this report, we present data on short-range order in this system, which can be probed through diffuse X-ray scattering. To achieve this, we grew single crystals via abnormal grain growth and conducted synchrotron high-energy X-ray diffraction experiments to obtain high-quality diffuse scattering data. This data was then reconstructed into reciprocal space maps for interpretation.

KFM 20.3 Wed 17:45 C 230

Mechanical Alloying of High-Entropy Alloys: Insights from Molecular Dynamics Simulations — ●MARIE CHARRIER, YULIA KLUNNIKOVA, and KARSTEN ALBE — Technical University of Darmstadt, Materials Modelling Division, Otto-Berndt Straße 3, 64206 Darmstadt, Germany

Mechanical alloying is a promising technique for producing high-entropy alloys. In this work, we explore intermixing processes and the formation of the solid solution starting from principal elements Co, Fe, Ni, Cr and Al in their respective lattice structures.

Severe plastic deformation is mimicked in Molecular Dynamics simulations by cyclic compressive loading of nanocrystalline samples inducing a quasi-hydrostatic stress state. The influence of grain orientation, grain size and temperature on structural evolution and chemical mixing is investigated. The structural and chemical complexity is increased by varying interfaces (from planar, bicrystalline to multiple, randomly oriented grains) and the number of components, respectively.

Independent of the starting configuration, we observe grain refinement and an HCP/BCC-FCC phase transformation within a few cycles, while chemical homogeneity is reached only at higher strains. These processes strongly depend on temperature and grain size, while the grain orientation plays a minor role. The final structures exhibit a large number of defects, in agreement with experimental observations. In general, the results provide atomic level insights into the mechanisms of mechanical alloying.

KFM 21: Focus Session: SrTiO₃: A Versatile Material from Bulk Quantum Paraelectric to 2D Superconductor (joint session TT/KFM/MA/O)

Strontium titanate (SrTiO₃) is a paradigmatic material that plays an important role in various fields of solid-state physics, surface science and catalysis: The pure bulk phase is a wide-band-gap semiconductor that upon cooling becomes a textbook quantum paraelectric. When slightly doped, SrTiO₃ turns into a Fermi-liquid-type metal that becomes superconducting at extremely low charge carrier density. SrTiO₃-based surfaces and interfaces host un-conventional electronic states such as quasi-two-dimensional electron liquid, magnetism and superconductivity. Despite intensive studies over the past decades, SrTiO₃ continues to reveal surprising new phenomena that challenge the established views on this material. To this end achieving light-induced nonequilibrium states and the recent preparation of a 2D oxide based on SrTiO₃ opens new playgrounds for research. This Focus Session will present exciting developments in the study of electronic states that are based on the peculiar properties of SrTiO₃.

Please note that this Focus Session comprises four parts: Posters are presented within the TT poster session TT58 (Wed 15:00-18:00, poster area E). Invited talks are compiled in the session TT62 (Thursday, 9:30 to 12:45, H0104), Contributed talks will be presented in sessions TT72 (Thursday 15:00-18:00, H0104) and TT83 (Fri 9:30-12:30, H0104).

Organizers: Rossitza Pentcheva, University of Duisburg-Essen, Marc Scheffler, University of Stuttgart

Time: Thursday 9:30–12:45

Location: H 0104

Invited Talk KFM 21.1 Thu 9:30 H 0104
Ferroelectricity and Superconductivity in SrTiO₃ — ●SUSANNE STEMMER — University of California, Santa Barbara, USA

Polar superconductors have attracted significant interest for their potential to host unconventional superconductivity. One candidate is doped strontium titanate (SrTiO₃), which can undergo successive ferroelectric and superconducting transitions. Recent experimental observations of a factor of two enhancement of the superconducting transition temperature in ferroelectric samples and the fact that both ferroelectricity and superconductivity vanish around the same carrier density, hint at common physical interactions relevant for both phenomena. We will discuss our understanding of ferroelectricity in strained SrTiO₃ films, and experiments aimed at elucidating the connection between superconductivity and ferroelectricity.

Although the ferroelectric transition of strained, undoped SrTiO₃ is usually described as a classic displacive transition, we show that it has pronounced order-disorder characteristics. Increasing the carrier concentration causes polar nanodomains to break up into smaller clusters. (Local) polar order appears to be essential to the superconducting state. For example, in strained SrTiO₃ films, suppression of superconductivity is correlated to the destruction of the (global) ferroelectric state, either by overdoping, by decreasing the film thickness or by alloying large amounts of a rare earth ion. We discuss how the length scale of polar order emerges as an important parameter in controlling the superconductivity of SrTiO₃.

Invited Talk KFM 21.2 Thu 10:00 H 0104
Dilute superconductivity in doped strontium titanate — ●KAMRAN BEHNI — LPEM-ESPCI, Paris, France

Dilute superconductivity survives in bulk strontium titanate when the Fermi temperature falls well below the Debye temperature. The onset of the superconducting dome is dopant dependent. The threshold density for superconductivity is much lower for mobile electrons introduced by removing oxygen atoms compared to those brought by substituting Ti with Nb. Our study of quantum oscillations reveals a difference in the band dispersion between the dilute metals made by these doping routes and our band calculations demonstrate that the rigid band approximation does not hold when mobile electrons are introduced by oxygen vacancies. We identify the band sculpted by these vacancies as the exclusive locus of superconducting instability in the ultradilute limit.

Invited Talk KFM 21.3 Thu 10:30 H 0104
Polarons and Excitons in quantum-paraelectric SrTiO₃ — ●CESARE FRANCHINI — University of Vienna & Bologna

SrTiO₃ stands as one of the most extensively investigated materials, captivating attention due to its distinctive electronic properties emerging from its quantum paraelectric nature. Positioned on the cusp of various collective phases, this material holds significant potential for exploitation in electronic and optical applications. In this presenta-

tion, we delve into the biphonon collective behaviors and quasiparticle properties of SrTiO₃ in both bulk and reduced dimensions, leveraging a combination of single-particle and many-body methods supported by machine learning techniques. Our exploration commences with an examination of temperature-dependent quantum and anharmonic effects employing a synergy of machine-learned potentials and the stochastic self-consistent harmonic approximation [1,2]. Shifting focus, we investigate the electron-phonon-driven formation of polarons, scrutinizing the interplay between spatially localized small polarons and dispersive large polarons in both bulk SrTiO₃ [3,4] and on the bulk-terminated SrTiO₃(001) surface [5,6]. In conclusion, our study delves into the optical and excitonic properties, with particular emphasis on the emergence of strongly bound excitonic peaks in the monolayer limit [7,8].

- [1] Adv. Quantum Technol. 6 (2023) 2200131
- [2] Phys. Rev. Mater. 7 (2023) L030801
- [3] Phys. Rev. B 91 (2015) 085204
- [4] npj Computational Materials 125 (2022)
- [5] Phys. Rev. Mater. 3, 034407 (2019); Phys. Rev. B 103 (2021) L241406
- [6] Phys. Rev. Mater. 7 (2023) 064602
- [7] Phys. Rev. Mater. 5 (2021) 074601
- [8] arXiv:2303.14830

15 min. break

Invited Talk KFM 21.4 Thu 11:15 H 0104
Controlling ferroelectrics with light — ●ANDREA CAVALLERI — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg — Department of Physics, University of Oxford

I will discuss how irradiation of ferroelectrics with intense, far and mid-infrared pulses, which are made resonant with certain phonon modes, can be used to manipulate the ferroelectric polarization. Two cases have been identified so far. On the one side, irradiation of a low temperature ferroelectric phase (e.g. in LiNbO₃) can achieve switching of the polarization. In incipient ferroelectric phases (e.g. in SrTiO₃), can lead to the formation of a long range ordered phase with stronger ferroelectricity than the paraelectric ground state. The microscopic physics of these phenomena are only in part clear, and I will discuss progress in this area.

Invited Talk KFM 21.5 Thu 11:45 H 0104
Terahertz electric field driven dynamical multiferroicity in SrTiO₃ — ●STEFANO BONETTI — Ca' Foscari University of Venice, Venice, Italy

In recent years, the ultrafast dynamical control and creation of novel ordered states of matter not accessible in thermodynamic equilibrium is receiving much attention. Among those, the theoretical concept of dynamical multiferroicity has been introduced to describe the emergence of magnetization by means of a time-dependent electric polarization in non-ferromagnetic materials. However, the experimental verifi-

cation of this effect is still lacking. Here, we provide evidence of room temperature magnetization in the archetypal paraelectric perovskite SrTiO₃ due to this mechanism. To achieve it, we resonantly drive the infrared-active soft phonon mode with intense circularly polarized terahertz electric field, and detect a large magneto-optical Kerr effect. A simple model, which includes two coupled nonlinear oscillators whose forces and couplings are derived with ab-initio calculations using self-consistent phonon theory at a finite temperature, reproduces qualitatively our experimental observations on the temporal and frequency domains. A quantitatively correct magnitude of the effect is obtained when one also considers the phonon analogue of the reciprocal of the Einstein - de Haas effect, also called the Barnett effect, where the total angular momentum from the phonon order is transferred to the electronic one. Our findings show a new path for designing ultrafast magnetic switches by means of coherent control of lattice vibrations with light.

KFM 21.6 Thu 12:15 H 0104

Emergence of a quantum coherent state at the border of ferroelectricity in SrTiO₃ — ●MATTHEW COAK^{1,2}, CHARLES HAINES², CHENG LIU², STEPHEN ROWLEY^{2,3}, GILBERT LONZARICH², and SIDDHARTH SAXENA² — ¹School of Physics and Astronomy, University of Birmingham, Birmingham, UK — ²Cavendish Laboratory, University of Cambridge, Cambridge, UK — ³Centro Brasileiro de Pesquisas Fisicas, Rio de Janeiro, Brazil

SrTiO₃ exists on the border of ferroelectricity in the vicinity of a quantum critical point (QCP). It is this proximity to a quantum critical point and the fluctuations associated with it which are responsible for SrTiO₃'s strikingly non-classical dielectric susceptibility.

I will discuss our results utilising ultra-high precision measurements of the the dielectric susceptibility to demonstrate an unconventional quantum paraelectric state exhibiting 'order by disorder' - a fluctuation-induced enhancement of electric polarization up to a coherence temperature T^* . We show that in the vicinity of T^* this phe-

nomenon can be understood quantitatively in terms of the hybridization of the critical electric polarization field and the volume strain field of the lattice.

We argue that this coherent optical-acoustic phonon state emerges from the QCP and is critical to our understanding of the mechanisms behind the quantum criticality and the phenomena resulting from it. At still lower temperatures, well below T^* , we observe a breakdown of this unconventional form of quantum paraelectricity and the emergence of a new instanton liquid phase.

KFM 21.7 Thu 12:30 H 0104

Dynamics of the critical phonon modes in quantum paraelectric SrTiO₃ — ●SHIYU DENG^{1,2}, CHARLES S. HAINES^{1,3}, MATTHEW J. COAK^{1,4}, ALEXANDRE IVANOV², ANDREA PIOVANO², ANDREW R. WILDES², and SIDDHARTH S. SAXENA¹ — ¹Cavendish Laboratory, University of Cambridge — ²Institut Laue-Langevin — ³University of East Anglia — ⁴University of Birmingham

The proximity of SrTiO₃ to a ferroelectric quantum critical point (FE QCP) has become a promising new branch of the study of quantum critical phenomena. New forms of quantum order have been reported in SrTiO₃ different from the quantum paraelectric state via dielectric measurements.

We report our recently performed triple-axis inelastic neutron scattering experiments on single-crystal SrTiO₃ at the temperature and pressure region of interest. These were the first direct measurements deep into the enigmatic 'quantum polar-acoustic state' in the vicinity of the FE QCP. Measurements are taken at and around $q = 0$ in multiple directions in reciprocal space to explore the transverse acoustic and soft optical phonon modes and their hybridization. In addition, we explore how pressure affects the underlying phonon modes in SrTiO₃. Our observations address directly the coupling of the soft optical mode with the acoustic phonons, and its response to external pressure. We believe this could help us understand the importance of anharmonic lattice dynamics and quantum fluctuations in SrTiO₃.

KFM 22: Perovskite and Photovoltaics II (joint session HL/KFM)

Time: Thursday 9:30–13:15

Location: EW 203

KFM 22.1 Thu 9:30 EW 203

Raman spectroscopy on BaTiS₃ perovskite nanocrystals — ●SELINA NÖCKER¹, SANDRA ZECH¹, VINCENT MAURITZ², KATHARINA DEHM², RYAN CRISP², and JANINA MAULTZSCH¹ — ¹Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — ²Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Perovskites and related materials are emerging candidates for photovoltaics demonstrating promising energy conversion efficiencies. Here we study lead- and halide-free BaTiS₃, colloiddally synthesized as wire- and rod-shaped nanocrystals.

For the structural analysis of those nanocrystals, we use Raman spectroscopy and compare the results to single-crystal spectra of BaTiS₃. Our study includes temperature-dependent and excitation-wavelength dependent measurements. Moreover, we show that Raman spectroscopy can be used as a straightforward method to distinguish between the two shape types.

KFM 22.2 Thu 9:45 EW 203

Crystallization and defect properties in combinatorially synthesized BaZrS₃ thin films — ●ADRIANA RÖTTGER¹, JACK VAN SAMBEEK², MARIN RUSU¹, HANNES HEMPEL¹, RAFAEL JARAMILLO², and THOMAS UNOLD¹ — ¹Helmholtz-Zentrum Berlin, Deutschland — ²Massachusetts Institute of Technology, Cambridge, MA, USA

BaZrS₃ is a chalcogenide perovskite composed of Earth-abundant elements with potential applications for photovoltaic (PV) energy conversion. Using pulsed laser deposition, oxide precursors with a lateral [Ba]/[Zr] ratio, ranging from 0.8 to 1.3, were deposited on 50 x 12 mm² large samples, which were then sulfurized in a tube furnace using different concentrations of H₂S in Ar gas at temperatures ranging from 800°C to 1000°C. The combinatorial nature of the thin films allows the study of crystallization behavior dependent on the composition of the material. A considerable increase in crystallite size was observed from the Zr-rich side to the Ba-rich side of all samples using grazing incidence x-ray diffraction and scanning electron microscopy. We hy-

pothesize that Ba excess leads to liquid phase assisted growth, similar to a low temperature growth mechanism reported recently by Yang et al.^[1] We demonstrate control over the kinetics of crystallization by varying temperature and/or H₂S partial pressure. We find that band-edge photoluminescence (PL) increases from the Ba-rich to the Zr-rich side, while defect state PL probed at low temperatures show a reverse trend. This suggests that careful control of the metals ratio will be key to achieving thin films with large crystals and good PV performance.

[1] Yang et al., Chemistry of Materials 2023 35 (12), 4743-4750

KFM 22.3 Thu 10:00 EW 203

Combining transient photoluminescence and transient surface photovoltage experiments: insights from drift-diffusion modeling — ●ORESTIS KARALIS, HANNES HEMPEL, and THOMAS UNOLD — Helmholtz-Zentrum Berlin, Berlin, Deutschland

The combination of transient surface photovoltage (trSPV) and transient photoluminescence (trPL) can help to distinguish charge transfer and recombination at the interfaces between photo-absorbers and charge-selective layers (I. Levine, 2021). This distinction is particularly crucial for the optimization of halide perovskite solar cells, as their power conversion efficiency is mainly limited by interfacial losses. However rate-equation models previously employed for trSPV (I. Levine, 2021) or trPL (F. Staub, 2016) are unable to simultaneously describe both experiments, which raises concerns about the validity of their findings. To address this limitation, we perform drift-diffusion modeling utilizing the open-source SIMsalabim algorithm (M. Koopmans, 2022). Our investigation reveals that strong charging of the sample with repetitive pulsed illumination, a factor overlooked in previous models, can strongly change the shape of the transients. Based on the improved model, we explore the impact of various parameters, such as charge-transfer velocity, bulk trap density, energy level alignment between absorber and charge transport layer, on the trPL and trSPV transients, as well as on overall solar cell performance. Finally, comparison of these simulations allows a simple phenomenological interpretation of trPL and trSPV. This insight can serve as a valuable guide in the pursuit of optimizing halide perovskite solar cells.

KFM 22.4 Thu 10:15 EW 203

Impact of different substrates and annealing treatments on the formation of fully evaporated perovskite — ●MOHAMED MAHMOUD^{1,2}, MARTIN BIVOURE¹, YASHIKA GUPTA^{1,2}, OUSSAMA ER-RAJI^{1,2}, and JULIANE BORCHERT^{1,2} — ¹Fraunhofer ISE, Freiburg, Germany — ²University of Freiburg, Freiburg, Germany

Perovskite solar cells have the advantages of a strong absorption edge, defect tolerance, and potential cheap production. In the industry, a great interest is shown towards perovskite-silicon tandem solar cells to overcome the single junction limit. Double-sided textured (micrometer sized pyramid) silicon is commonly produced to decrease reflection losses and improve light trapping. Solution-based processing methods of perovskite on top of the textured silicon showed low conformality, which resulted in shunts and non-working solar cells. To overcome this issue, physical vapor deposition (PVD) is used for the different precursors to conformally coat the perovskite on the silicon pyramids. Therefore, we study distinct vacuum-based methodologies for perovskite processing, specifically the hybrid route and the fully evaporated route. In this study, we investigate the effect of different substrates, that includes different materials and different Si pyramid heights, on the formation of fully evaporated perovskite. The results show that different surfaces (i.e. different materials) affects not only the morphology of the evaporated perovskite, but also the crystal structure. In addition to that, we compare planar Si surfaces to nano structured as well as micro structured on the formation of fully evaporated perovskite.

KFM 22.5 Thu 10:30 EW 203

Room temperature exciton-polaritons in quasi-2D Ruddlesden-Popper perovskites — ●HAMID PASHAEI ADL^{1,2}, CHRISTOPH BENNENHEI¹, JENS CHRISTIAN DRAWER¹, LUKAS LACKNER¹, MARTI STRUVE¹, ANTHONY ERNZERHOF¹, NADIYA MATUKHNO¹, SIGALIT AHARON³, DAVID CAHEN³, MARTIN ESMANN¹, and CHRISTIAN SCHNEIDER¹ — ¹Institute for Physics, Carl von Ossietzky University of Oldenburg, 26129 Oldenburg, Germany. — ²Instituto de Ciencia de Materiales (ICMUV) Universidad de Valencia/Catedrático José Beltrán, 2, Paterna E-46980, Spain. — ³Weizmann Institute of Science 234 Herzl Street, Rehovot 7610001, Israel.

Ruddlesden-Popper (RP) layered perovskites [1] with high oscillator strength and large exciton binding energy are promising materials for photonic applications. The crystalline form of these perovskites can be used as excitonic medium in optical microcavities, allowing for the study of their optical properties in the strong light-matter coupling regime. Here, using angle resolved reflection spectroscopy, we show tunable strong coupling of light modes to mechanically exfoliated quasi-2D RP flakes in an open access microcavity under ambient conditions [2], which is supported by transfer matrix calculations. In ongoing experiments, we introduce structured photonic lattices to the open cavity to study the coupling of the polaritons to tailored topological features and investigate Bose-Einstein condensation.

[1] J. C. Blancon, et al., *Nat Nanotechnology* 15, 969 (2020). [2] L. Lackner, et al., *Nat Commun* 12, 4933 (2021).

KFM 22.6 Thu 10:45 EW 203

Predicting Optoelectronic Performance: A First-Principles Analysis of Carrier Recombination in Metal Halide Perovskites — UTKARSH SINGH and ●SERGEI I. SIMAK — Department of Physics, Chemistry and Biology (IFM), Linköping University, SE-581 83, Linköping, Sweden

Unveiling the full potential of Metal Halide perovskites (MHPs) for optoelectronic applications depends on understanding factors influencing device performance, specifically the interplay between radiative and non-radiative recombination at various carrier densities. We explore these processes, laying the foundation for enhanced device functionality and tailored design approaches. We implement the calculation of carrier recombination facilitated through direct and phonon-assisted mechanisms via a first-principles approach. Using methods at and beyond the level of density functional theory, we highlight the role of MHP constituents and the contribution of various factors towards carrier dynamics. The primary focus is on MHPs CsPbI₃ and its lead-free counterpart CsSnI₃, where high radiative and low non-radiative recombination rates are favorable for potential use as LEDs. We reveal how these processes depend on the material's electronic structure, dictating the phase space available for charge carrier interactions [1]. An in-depth understanding of principles governing recombination dynam-

ics, implemented in a predictive framework, may significantly impact advancements in this field.

[1] F. Yuan et al., "Bright and stable near-infrared lead-free perovskite light-emitting diodes", *Nature Photonics* (2023, accepted).

KFM 22.7 Thu 11:00 EW 203

Additive engineering for high bandgap perovskite absorber for application in triple-junction solar cells — ●ATHIRA SHAJI¹, MINASADAT HEYDARIAN¹, MARYAMSADAT HEYDARIAN¹, PATRICIA S. C. SCHULZE¹, JULIANE BORCHERT^{1,2}, and ANDREAS BETT¹ — ¹Fraunhofer Institute for Solar Energy Systems — ²INATECH, University of Freiburg

Multi-junction solar cells can overcome the theoretical efficiency limit of state-of-the-art silicon single-junction solar cell. Recently, perovskite-silicon tandem solar cells have achieved high power conversion efficiency (PCE) of 33.9% on small area. By adding a third junction this PCE can be further increased. For a top cell in a triple-junction solar cell, a high band gap (HBG) perovskite is required. However, there are several challenges associated with such HBG perovskites such as photo-induced phase segregation and high V_{OC} deficit¹. In addition, the high Br content in the HBG perovskite composition has been lead to poor perovskite film formation and morphology which can exacerbate the mentioned issues¹. Suppression of phase segregation and increased grain size can be achieved by improving the perovskite crystallization via additive engineering¹. Here, we employ a triple cation perovskite composition with general formula $Cs_{0.05}(FA_{1-x}MA_x)_{0.95}Pb(I_{1-x}Br_x)_3$ ($E_g > 1.83$ eV) which is used as the top cell absorber². We investigate the effects of additives on this perovskite crystallization and grain size¹.

1.Chen, B. et al. *Joule* 2019, 3(1), 177-190.

2.Heydarian, M. et al. *ACS Energy Lett.* 2023, 8(10), 4186-4192.

15 min. break

KFM 22.8 Thu 11:30 EW 203

Thermodynamics and kinetics of silver in Cu(In,Ga)Se₂ solar cell absorbers — MARKUS MOCK, ●DELWIN PERERA, and KARSTEN ALBE — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Cu(In,Ga)Se₂ (CIGS) is at the moment the most efficient absorber material in thin-film solar cells. Its efficiency can be further enhanced by substituting copper with silver which increases the band gap and turns CIGS into a wide-gap semiconductor with potential application in tandem solar cells.

In this contribution, we investigate the impact of silver on structural and electronic properties of CIGS. Using semi-grand canonical Monte Carlo simulations, we explore the CIGS phase diagram as a function of silver content. In particular, we map out the phase transition between solid solution and phase decomposition as well as the spinodal region. Based on a cluster expansion model, our Monte Carlo simulations reveal the microstructure evolution within the binodal region. We supplement the thermodynamic analysis with kinetic considerations by calculating defect migration barriers and defect association energies. Finally, we investigate the effect of silver on the band gap employing hybrid density functional theory calculations.

KFM 22.9 Thu 11:45 EW 203

Photon echo spectroscopy of CsPbI₃ nanocrystals — ARTUR V. TRIFONOV^{1,2}, ●MARIO ALEX HOLLBERG¹, STEFAN GRISARD¹, ELENA V. KOLOBKOVA^{3,4}, MARIA S. KUZNETSOV², MIKHAIL O. NESTOKLON¹, JAN KASPARI⁵, DORIS REITER⁵, DMITRI R. YAKOVLEV^{1,6}, MANFRED BAYER¹, and ILYA A. AKIMOV¹ — ¹Experimentelle Physik 2, Technische Universität Dortmund — ²St. Petersburg, Russia — ³St. Petersburg, Russia — ⁴St. Petersburg, Russia — ⁵Condensed Matter Theory, Technische Universität Dortmund — ⁶St. Petersburg, Russia

All-inorganic halide perovskite nanocrystals hold potential for future optoelectronic technologies. One of the paths to fully unlock their capabilities, is a deeper understanding of coherent exciton dynamics in these materials. In this work, we investigated a caesium lead tri-iodide (CsPbI₃) nanocrystal ensemble using time-resolved photon echo spectroscopy at cryogenic temperatures (1.5 K). We observed a long exciton lifetime T_1 of about 1 ns and an exciton coherence time T_2 of up to approximately 300 ps. The initial tens of picoseconds in the photon echo decay exhibited oscillatory behavior with two most pronounced frequencies of 3.2 meV and 5.1 meV, which we attribute to the interac-

tion between excitons and optical phonons. The exciton fine structure manifests itself at lower oscillation frequencies of 0.2 meV and 1.1 meV.

KFM 22.10 Thu 12:00 EW 203

Damping the phase segregation in mixed halide perovskites: Influence of X-site anion — ●MARIA AZHAR — Universitz of Konstanz, Konstanz, Germany

This study reveals that phase segregation becomes more prominent on decreasing bromine content in mixed halide CsPbBr_{3-x}Cl_x perovskites, when bromine content is 50NCs have been synthesized to mitigate the phase segregation. The grain size of the synthesized NCs exists in the range of 20*25 nm. The selected area electron diffraction exhibits the faint rings of the CsPbBr_{1.5}Cl_{1.5} indicating the presence of defects in NCs and the X-rays diffraction analysis confirms the NCs exist in monoclinic crystal structure. Mixed halides perovskites have same crystal structure but exhibit a slight shift in 2θ values. The trend in stability follows the order as, CsPbBr_{3-x}Cl_x > CsPbCl₃ > CsPbBr₃ that is estimated by the values of octahedral factor (μ) and tolerance factor (t). The UV*Vis and steady-state photoluminescence (PL) analysis depict a blue-shift in the spectra by substituting bromine with chlorine in CsPbBr₃. The PL kinetics analysis predicts the CsPbBr_{2.5}Cl_{0.5} exhibits the longest average PL lifetime amongst all other CsPbBr_{3-x}Cl_x perovskites NCs. Our study provides insights in designing stable mixed halides perovskites by suppressing the phase segregation.

KFM 22.11 Thu 12:15 EW 203

Extrinsic doping and compensating defects in the 2D hybrid perovskite PEA₂PbI₄ — GABRIELLE KOKNAT¹, HAIPENG LU^{2,3}, YI YAO¹, JI HAO², XIXI QIN¹, CHUANXIAO XIAO², RUYI SONG¹, FLORIAN MERZ⁴, MARKUS RAMPP⁵, ●SEBASTIAN KOKOTT⁶, CHRISTIAN CARBOGNO⁶, TIANYANG LI¹, GLENN TEETER², MATTHIAS SCHEFFLER⁶, JOSEPH J. BERRY², DAVID B. MITZI¹, JEFFREY L. BLACKBURN², VOLKER BLUM¹, and MATTHEW C. BEARD² — ¹Duke University, Durham, NC, USA — ²NREL, Golden, CO, USA — ³Hong Kong University of Science and Technology, Hong Kong, China — ⁴Lenovo HPC Innovation Center, Stuttgart, Germany — ⁵MPCDF, Garching, Germany — ⁶NOMAD laboratory at FHI, Berlin, Germany

2D hybrid organic-inorganic perovskites are exciting materials for optoelectronic device applications due to their higher chemical and structural adjustability. Precise control over carrier concentrations necessitates the electronic doping of these materials through the incorporation of extrinsic dopants. Conversely, the undesirable presence of intrinsic defects can adversely affect electronic doping efficiencies. In this study, we investigate intrinsic point defects and extrinsic dopants (e.g., Bi, Sn [PRX Energy, 2, 023010 (2023)]) both in isolation and as combined defects in phenylethylammonium lead iodide (PEA₂PbI₄). Employing spin-orbit-coupled hybrid density functional theory (DFT) and supercell models scaling up to 3,383 atoms, we identify the anticipated positions of dopant-derived electronic levels within the bandgap. Complementary experimental findings reinforce hypotheses of compensation mechanisms and limiting factors derived from DFT.

KFM 22.12 Thu 12:30 EW 203

Growth and Investigation of Sequentially Evaporated Mixed Halide (Cs,FA)Pb(I,Br)₃ Perovskites — ●TOBIAS SCHULZ¹, KARL HEINZE¹, PAUL PISTOR², and ROLAND SCHEER¹ — ¹Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle (Saale), Germany — ²Universidad de Pablo de Olavide, Carretera de Utrera 1, 41013 Sevilla, Spain

Perovskite films were grown via thermal evaporation and characterized via in situ XRD which give structural information in real-time. Besides the growth of FAPbI₃ and (Cs,FA)PbI₃ also bromine incorporation into the perovskite to prepare (Cs,FA)Pb(I,Br)₃ was investigated [1].

The substitution of iodine with bromine increases the band gap, which is interesting for tandem applications, and improves the thermal stability. In contrast to co-evaporation, the less studied sequential evaporation route was employed which allows a more precise process control. Sequential perovskite formation in vacuum in general proceeds via diffusion of the reactants CsI, FAI, PbI₂, and PbBr₂ which are assembled in different layer stacks. With the in situ XRD setup, the diffusion of these materials during the necessary annealing step was observed. In combination with SEM images, the reactant's diffusion speed was quantified. Additionally, the perovskites show no unfavourable delta-phase during our experiments, allowing the assumption, that sequential evaporation can fully suppress this non-photoactive phase. [1]: K. Heinze, T. Schulz et al., "Structural Evolution of Sequentially Evaporated (Cs,FA)Pb(I,Br)₃ Perovskite Thin Films via In Situ XRD", Physica Status Solidi A, accepted for publication

KFM 22.13 Thu 12:45 EW 203

Impact of ion migration on the performance and stability of perovskite-based tandem solar cells — ●SAHIL SHAH and MARTIN STOLTERFOHT — Physik weicher Materie, Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany

Mobile ions play a significant role in perovskite photovoltaics, yet their impact on the overall performance and stability of tandem solar cells (TSCs) remains largely unexplored. In this study, we present a comprehensive study that combines an experimental analysis of ionic losses in Si/perovskite and all-perovskite TSCs, drift-diffusion simulations, and sub-cell-selective measurements on all-perovskite TSCs during aging. Our findings demonstrate that mobile ions have a significant influence on the hysteresis of Si/perovskite tandem solar cells at high scan speeds (400 V/s) during current-voltage measurements, as well as on performance degradation due to field screening. Additionally, subcell-dominated measurements reveal more pronounced ionic losses in the wide-bandgap subcell during aging, which we attribute to its tendency for halide segregation. Drift-diffusion simulations fully corroborate the results. Overall, this work provides valuable insights into ionic losses in perovskite solar cells and discloses new opportunities for their optimization toward more efficient and stable perovskite-based tandem cells.

KFM 22.14 Thu 13:00 EW 203

Why copper oxide is not a reliable hole transporting layer for perovskite solar cells — ●MALGORZATA KOT¹, LUDWIG MARTH², ZBIGNIEW STAROWICZ³, PAUL PLATE², JAN INGO FLEGE¹, and KATARZYNA GAWLINSKA-NECEK³ — ¹APhLS, BTU Cottbus-Senftenberg, Konrad-Zuse-Str. 1, 03046 Cottbus, Germany — ²SENTECH INSTRUMENTS GmbH, Schwarzschildstr. 2, 12489 Berlin, Germany — ³IMMS PAS, Photovoltaic Laboratory, 22 Krakowska St., 43-340 Kozy, Poland

One approach, among many others, to increase the stability of perovskite solar cells is to replace an organic hole transporting layer (HTL), which becomes highly unstable when exposed to air for a long time, with more stable inorganic materials. The material that seems to be very promising is copper oxide. In our investigation we however found, that the formamidinium lead iodide perovskite deposited directly on copper oxide in the p-i-n structure degrades within tens of minutes due to the migration of copper ions under X-ray exposure and creation of CuI and Cu. Furthermore, an application of an ultrathin atomic layer deposited Al₂O₃ film on the copper oxide substrate, that in our previous work [1] succesively blocked the migration of perovskite ions into the HTL in the n-i-p structure, does not sufficiently block the migration of copper ions through the perovskite film. Therefore, in order for copper oxide to be a reliable HTL for perovskite solar cells, an effective method must be still developed to block the migration of copper ions into other layers. [1] C. Das et al., Cell Rep. Phys. Sci. 2020, 100112.

KFM 23: Focus Session: Fermi level engineering of functional ceramics

We will discuss the role of the Fermi level as key quantity for predicting and controlling properties of functional ceramics. The focus will be on doping and compensation effects in functional ceramics, including i.e. fuel cells, batteries, membranes, piezoceramics and electroceramics. Experimental and theoretical contributions, which focus on the interplay of compensation effects by electrons, holes, polarons and ions, as well as the role of grain boundaries, surfaces and heterogeneous interfaces are invited to contribute to this special symposium.

Chair: Karsten Albe (TU Darmstadt)

Time: Thursday 9:30–11:50

Location: E 124

Invited Talk KFM 23.1 Thu 9:30 E 124
The Research Center FLAIR: Fermi Level Engineering of Oxide Electroceramics — ●ANDREAS KLEIN — Technical University of Darmstadt, Institute of Materials Science

Chemical substitution is the primary strategy to tailor material properties. Isovalent substitution changes the density of states while heterovalent substitution, i.e. doping, can induce electronic compensation, ionic compensation, valence changes of cations or anions, or result in the segregation or neutralization of the dopant. While all these can, in principle, occur simultaneously, it is often desirable to select a certain mechanism in order to determine material properties. Being able to predict and control the individual compensation mechanism should therefore be a key target of materials science. This contribution outlines the perspective that this could be achieved by taking the Fermi energy as a common descriptor for the different compensation mechanisms. This generalization becomes possible since the formation enthalpies of the defects involved in the various compensation mechanisms do all depend on the Fermi energy. In order to control material properties, it is then necessary to adjust the formation enthalpies and charge transition levels of the involved defects. Understanding how these depend on material composition will open up a new path for the design of materials by Fermi level engineering. This is the target of the research center FLAIR (www.mawi.tu-darmstadt.de/flair), which has been established in January 2023 by the German Research Foundation. The scientific concept of the center is published in [1]. [1] A. Klein et al., *J. Electroceramics*, doi: 10.1007/s10832-023-00324-y

KFM 23.2 Thu 10:00 E 124
Operando XPS Study with electrochemical cell setup — ●SAVITA CHAUDHARY, PENGCHENG HU, BINXIANG HUANG, KIM ALEXANDER CREUTZ, YUE LIU, GERO JOHANNES PICKEL, VINIT AGARWALLA, ALEXANDER FREBEL, and ANDREAS KLEIN — Technical University of Darmstadt, Darmstadt, Germany

The change of the oxygen content in a material using an electrochemical cell is an important asset to understand the variation of the Fermi energy in materials, paving the way for Fermi level engineering as a versatile toolkit for designing a broad range of materials according to specific applications. The electrochemical cell is constructed by top and bottom electrodes deposited on an oxygen ion conducting electrolyte. The reduction or increase of the oxygen content in the electrodes by cathodic or anodic polarization, is accompanied by an increase or lowering of the Fermi energy, respectively. The latter can be monitored together with chemical changes of the sample if the electrochemical cell is operated in an X-ray photoelectron spectrometer. We will present experiments using Y-stabilized zirconia, Fe-doped SrTiO₃, (1-x)Pb(Mg_{1/3}Nb_{2/3})O_{3-x}PbTiO₃(PMN-PT), Na_{1/2}Bi_{1/2}TiO₃-BaTiO₃ (NBT-BT) or (Pb,La)(Zr,Sn,Ti)O₃ (PLZST) as electrolytes, and (Sn-doped) In₂O₃, SrFeO_{3-δ} and Sr-doped LaCoO_{3-δ} as electrode materials. The use of the setup to quantify the Fermi energies of charge transition levels in either the electrolyte or the electrode will be demonstrated.

KFM 23.3 Thu 10:20 E 124
Machine Learning Potential for BaTiO₃ — ●AMIT SEHRAWAT — Materials Modelling Division, Otto-Berndt-Str. 3 64206 Darmstadt

Barium titanate (BaTiO₃, BTO), a well-known perovskite oxide, undergoes intricate ferroelectric phase transitions. These transitions are characterized by a shift from a paraelectric cubic phase at high temperatures to a sequence of low-temperature phases (Cubic → Tetragonal → Orthorhombic → Rhombohedral), predominantly driven by anti-ferrodistortive modes. Although *ab-initio* molecular dynamics is used to explore the finite-temperature properties, the high computational

cost and scaling to only a few hundred atoms restricts the study for a longer time and length scale. Conversely, classical molecular dynamics simulations, though efficient in understanding atomic-scale dynamics, often lack accuracy compared to first-principles-based methods. To overcome these limitations, we develop a machine learning interatomic potential (MLIP) for BaTiO₃, based on Atomic Cluster Expansion (ACE) formalism using data from density functional theory (DFT) calculations. The ML potential achieves DFT-level accuracy while facilitating simulations over significantly longer time and length scales. Using trained potential, our research investigates the temperature-driven cubic-to-Rhombohedral phase transition in BTO and examines the influence of pressure on the transition temperature.

KFM 23.4 Thu 10:40 E 124
Fermi-level Engineering of Ba-rich perovskite oxide materials by introducing fluorine — ●SYLVIA LORRAINE KUNZ, LAXMIPRIYA SAHOO, and OLIVER CLEMENS — Institute for Materials Science, University of Stuttgart, 70569 Stuttgart, Germany

Perovskite compounds ABO₃ are renowned for their structural and compositional flexibility. They exhibit variations on both the cation A and B sites, as well as on the anion sublattice [1]. The introduction of anions in the host lattice has an impact on the coordination sphere of the cations, influencing their oxidation states and consequently affecting the Fermi energy [2]. By investigating the substitutional effects, a Fermi-level guided synthesis approach could be derived to tailor specific electronic properties.

In this contribution, we systematically exemplify the relationship between the Fermi energy and sample synthesis in the context of the topochemical fluorination of Ba-rich transition metal oxides BaFe_{1-x}Co_xO_{3-d}F_y, BaFe_{1-x}Ti_xO_{3-d}F_y, BaCo_{1-x}Ti_xO_{3-d}F_y with varying amount of fluorine (0 ≤ y ≤ 1). The fluorination of Ba-rich transition metal oxides was achieved through a topochemical reaction route at 370 °C, utilizing PVDF as fluorination agent [3]. We will discuss the potential impact on structural and compositional changes on the Fermi-Level of these compounds.

References [1] Kobayashi, Y.; Tsujimoto, Y.; Kageyama, H.. *Annu. Rev. Mater. Res.* 2018, 48, 303-326. [2] Clemens, O.; Slater, P. *Rev. Inorg. Chem.* 2018, 33 (2-3), 105-117. [3] Perween et al, *Inorg. Chem.* 2023, 62, 40, 16329-16342.

KFM 23.5 Thu 11:00 E 124
fermi-level involved phase field modeling of grain growth in the perovskite oxide SrTiO₃ — KAI WANG and ●BAIXIANG XU — Mechanics of Functional Materials (MFM), TU-Darmstadt, Darmstadt, Germany

The grain boundary (GB) distribution and the interaction between GB with point defects in polycrystalline ceramics significantly determine the macro properties of the materials. In order to investigate the GB properties, we developed an electro-chemo phase field model to reproduce space charge effects and the distribution of different point defects in bulk and along GB. The performance of this phase field model is benchmarked with sharp interface calculations by simulating the Fe-doped perovskite oxide SrTiO₃ (STO) at the equilibrium state when iron defects in STO are immobile and mobile. Moreover, through considering the influence of fermi-level, different dopants with various valencies are taken into account in the phase field simulations. Then, the corresponding space charge effects are studied.

Invited Talk KFM 23.6 Thu 11:20 E 124
Designing Transition Metal Oxynitrides for Photoelectrochemical Applications — ●VERENA STREIBEL^{1,2}, LAURA I. WAGNER^{1,2}, JOHANNA L. SCHÖNECKER^{1,2}, ELISE SIROTTI^{1,2}, JOHANNA EICHHORN^{1,2}, SASWATI SANTRA^{1,2}, and IAN D. SHARP^{1,2}

— ¹Walter Schottky Institut, TU München, Garching, Germany —
²Physics Department, TUM School of Natural Sciences, TU München,
 Garching, Germany

Transition metal oxynitrides are an emerging class of functional materials with tunable electronic and optical properties. They offer a high potential for tailored materials development since their Fermi levels, energy band gaps, valence/conduction band positions, and surface chemistry can be controlled by adjusting the cation and anion composition. These design opportunities are especially important for photoelectrochemical applications. Here, we discuss our approach to

developing transition metal oxynitride thin films as photoelectrodes using reactive sputter deposition. First, we focus on the influence of the anion ratio in the zirconium oxynitride system. At sufficiently high oxygen concentrations, we observe the opening of a band gap in the UV-visible range and the emergence of photoelectrochemical activity for oxidation reactions. Second, we focus on cation substitution in the titanium tantalum (oxy)nitride system.[1] We demonstrate that controlled Ti-doping of Ta₃N₅ thin films dramatically reduces the concentration of deep-level defects and thereby enhances the photoelectrochemical activity.

[1] Wagner, Streibel, Sharp, et al., Adv. Func. Mat., 2023, 2306539.

KFM 24: Focus Session: Battery Materials – Ion Transport, Impurity Effects and Modelling (joint session KFM/MM)

The focus session is dedicated to the characterization of microstructure, electrochemical, thermal and safety properties of Lithium-ion and Post-Lithium cells and their individual active and passive materials. This is required to obtain quantitative and reliable data, which are necessary to improve the current understanding in order to design and develop better and safer materials and cells. Potential topics include, but are not limited to electrochemical characterization techniques, thermal characterisation techniques, safety testing, development of safer materials and cell designs, thermodynamic modelling of materials, modelling of thermal runaway and propagation.

Chair: Ilyas Mohsin (KIT Karlsruhe)

Time: Thursday 9:30–13:35

Location: EMH 225

Invited Talk KFM 24.1 Thu 9:30 EMH 225
Ion transport in battery electrolytes and related interphases
 — ●JELENA POPOVIC-NEUBER — University of Stavanger, Norway

The development of next generation batteries depends heavily on the capability of electrolytes to quickly and selectively transport alkali and alkaline earth metal cations, and form stable electrochemical interfaces. In the first part of my talk, current understanding of ion transport mechanisms and related electrochemical measurement techniques (impedance spectroscopy, galvanostatic polarization) in soft matter battery electrolytes including liquids, polymers and hybrid materials will be discussed. According to this discussion, I will give guidelines and examples of improvements of the relevant electrochemical properties including ionic conductivity and the cationic transference number. In the second part of my talk, I will show recent findings related to the electrochemical and chemical growth and transport in SEIs on several alkali and alkaline earth metal anodes in contact with liquid and solid-state electrolytes. The multitechnique approach involving the measurement of activation energy for ion transport showed that such SEIs are complex composite liquid/solid materials, with sometimes predominant ionic pathways in the liquid phase. The relevance of the native passive layer on alkali and alkaline earth metals, possibility of forming artificial SEIs and electrodeposition through porous SEI will be discussed. Finally, I will show a new modelling approach for treatment of impedance spectroscopy data of symmetric alkaline and alkaline earth metal cells.

KFM 24.2 Thu 10:00 EMH 225
NASICON as solid electrolyte for Mg- and Ca-ion batteries
 — ●KATHARINA HELMRECHT¹ and AXEL GROSS^{1,2} — ¹Institute of Theoretical Chemistry, Ulm University, Ulm, Germany — ²Helmholtz-Institute Ulm (HIU) for Electrochemical Energy Storage, Ulm, Germany

In Na-ion batteries, NASICON has been used as a solid-electrolyte material. Here we present a density functional theory study in which we investigate whether NASICON can also be a suitable solid electrolyte for bivalent charge carriers such as Mg and Ca. We have in particular chosen Ca_{0.5}Ti₂(PO₄)₃, Ca_{0.5}Zr₂(PO₄)₃, Mg_{0.5}Sn₂(PO₄)₃, and Mg_{0.5}Zr₂(PO₄)₃ for our investigation. We find that these phases indeed show promise as solid electrolytes.

Unlike the classic NASICON phase, which often undergoes a phase transition from rhombohedral to monoclinic within the battery's operating range, this issue does not arise with Ca and Mg. However, only half of the sites occupied by Na (specifically, the Na1 sites) become occupied by the bivalent carriers. We investigate the energetic ordering of the occupied positions inside and the diffusion mechanism inside the phase as well as bottleneck sizes and compare this to the classic

NASICON phase.

KFM 24.3 Thu 10:20 EMH 225
Rhombohedral (R-3) Prussian white cathode material: An ab-initio study — ●SEBASTIAN BAUMGART¹, MOHSEN SOTOUDEH¹, and AXEL GROSS^{1,2} — ¹Institute of Theoretical Chemistry, Ulm University, Ulm, Germany — ²Helmholtz-Institute Ulm (HIU) for Electrochemical Energy Storage, Ulm, Germany

The demand for efficient and sustainable cathode materials for alternative battery chemistries is ever more increasing. Prussian Blue analogues (PBAs) exhibit a long cycling life and a high rate capability, which makes them a promising cathode material for next-generation battery technologies. Notably, Prussian White (PW) exhibits a phase transition at high sodium and low vacancy content, transitioning to a rhombohedral (R-3) phase.

However, the detailed exploration of the rhombohedral modification and its electronic structure remains incomplete. In this study, we provide insights into why the rhombohedral structure manifests itself only at high sodium contents, employing atomistic first-principles calculations.

Our findings reveal the stabilization of the rhombohedral structure by sodium atoms. Additionally, we elucidate the changes in the sodium ion minimum energy position during the phase transition and analyze the sodium migration barrier within the cubic and rhombohedral phases, offering a comprehensive theoretical assessment of its viability as a battery material.

KFM 24.4 Thu 10:40 EMH 225
Advancing Post-Lithium Batteries: Insights into Cathode Material Design and Electrochemical Stability — ●MOHSEN SOTOUDEH¹ and AXEL GROSS^{1,2} — ¹Institute of Theoretical Chemistry, Ulm University, Oberberghof 7, 89081 Ulm — ²Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm

In the search for sustainable alternatives to the prevailing Li-ion batteries, key features that influence the activation energy barrier and electrochemical stability are investigated using periodic density functional theory calculations. The study employs a novel descriptor to determine the ionic mobility and highlights the critical role of ionic radii, oxidation state, and electronegativity on the mobility as well as the stability of crystalline materials, providing practical guidelines for the selection of promising solid materials. At the same time, the potential of Mg batteries with oxide cathodes is explored, recognizing the challenges posed by the sluggish kinetics of Mg²⁺ migration. Promising candidates, guided by theoretical insights, have been synthesized and structurally characterized, paving the way for the exploitation of functional cathode materials with improved Mg²⁺ transport proper-

ties. In addition, the electrochemical stability of binary and ternary spinel compounds is investigated, with potential applications as protective coatings, and solid electrolytes in batteries. This comprehensive study provides critical insights into the development of new battery technology for high-performance energy storage solutions.

The work has been supported by the DFG through Excellence Cluster EXC-2154, project No. 422053626.

KFM 24.5 Thu 11:00 EMH 225

Remodeling interfacial electrical field for superhigh capacity and ultralong lifespan aqueous zinc-ion batteries — ●YAN RAN¹, YUDE WANG², HUAPING ZHAO¹, and YONG LEI¹ — ¹Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²Yunnan Key Laboratory of Carbon Neutrality and Green Low-carbon Technologies, Yunnan University, 650091 Kunming, China

Herein, density functional theory (DFT) calculations studied the NH4V4O10@carbon cloth (NVO@CC) as a high-performance cathode material at the heterostructure interface for AZIBs. The electronic structure, adsorption energy, and migration energy barrier prove there are additional active sites at the interface due to the built-in electric field between NVO and CC, which improves the conductivity and stability of the NVO@CC electrode material. Accordingly, the designed binder-free NVO@CC cathode exhibits high specific capacity (607.1 mAh/g at 0.1 A/g), an outstanding energy density (443.6 Wh/kg at 0.3 A/g), and an excellent long-term cyclability (the capacity retention rate is 81.24% after 10,000 ultra-long cycles at 5 A/g). This excellent electrochemical performance is attributed to enhanced conductivity and fast electrochemical kinetics by a series of ex-situ characterizations. This work reveals a binder-free self-grown flexible cathode on carbon cloth, which is promising for high-performance aqueous zinc ion batteries.

15 min. break

KFM 24.6 Thu 11:35 EMH 225

Computational Screening of Chloride Perovskites as Cl⁻ Ion Solid Electrolyte — ●JOHANNES DÖHN¹ and AXEL GROSS^{1,2} — ¹Institute of Theoretical Chemistry, Ulm University, Germany — ²Helmholtz Institute Ulm, Germany

The intermittency of wind and solar power - the solely sustainable energy sources which are considered to be abundantly available - leaves only one consequence: For the transition towards renewable energy systems, efficient and reliable storage technologies are needed. Batteries are one of the most widely used storage devices but current technology based on the transfer of Li-ions faces several challenges including their dependence on critical materials with respect to both, scarcity and toxicity.

In our contribution, we will present atomic-scale investigations of potential future battery materials carried out using density functional theory (DFT). We employed a high-throughput approach in order to screen the well known materials' class of chloride perovskites as solid electrolyte material for chloride ion batteries and we derived several properties as electrochemical stability and diffusion barrier for in total 148 compounds. Our screening focusses on the highly symmetric cubic perovskite structure but for the most promising candidates also the less symmetric distorted phases are investigated, additionally shedding some light on potential property-structure relationships.

Such in silico investigations significantly narrow down the potential materials space for our experimental coworkers and, thereby, contribute to finding green, cheap and reliable devices for energy storage.

KFM 24.7 Thu 11:55 EMH 225

The role of the SEI for lithium whiskers in lithium metal batteries — ●MARTIN WERRES^{1,2}, ARNULF LATZ^{1,2,3}, and BIRGER HORSTMANN^{1,2,3} — ¹Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Ulm, Deutschland — ²Helmholtz Institut Ulm (HIU), Ulm, Deutschland — ³Universität Ulm, Ulm, Deutschland

Lithium metal (Li) batteries are promising due to their high specific energy. However, safety concerns and non-optimal cycle stability hold back Li anodes paired with liquid electrolytes.[1] A major challenge is the growth of Li whiskers. Li whiskers come with cycling inefficiencies, e.g., enhanced formation of isolated Li.[2] Understanding why Li whiskers emerge can help find design rules for safer Li batteries. We study plating/stripping of Li under the aspect of the mechanical properties of Li and the role of the covering solid-electrolyte interphase

(SEI).[3] We consider a Li nucleus covered by SEI, which grows continuously during plating. Once the stress in the SEI exceeds a threshold, the SEI breaks. Due to the softness of Li and significant creep under the expected stress conditions, Li can extrude through the hole in the SEI. We model this by approximating Li as a Herschel-Bulkley liquid. Our predicted shapes and growth rates are consistent with the experimental observation of Li whiskers. We deduce that the SEI is the most important design parameter to achieve safe Li batteries.

[1] B. Horstmann et al., Energy Environ. Sci. 2021, 14(10), 5289-5314. [2] M. Werres et al., ACS Nano 2023, 17(11), 10218-10228. [3] L. von Kolzenberg et al., Phys. Chem. Chem. Phys. 2022, 24(31), 18469-18476.

KFM 24.8 Thu 12:15 EMH 225

Elucidating the Silicon Voltage Hysteresis by Mechanical Coupling of Anode Particles and SEI — ●LUKAS KÖBBING^{1,2}, ARNULF LATZ^{1,2,3}, and BIRGER HORSTMANN^{1,2,3} — ¹German Aerospace Center (DLR), Ulm, Germany — ²Helmholtz Institute Ulm (HIU), Ulm, Germany — ³Ulm University, Ulm, Germany

Silicon promises to be a superior next-generation anode material. However, a major challenge of silicon anodes is the significant voltage hysteresis reducing efficiency and leading to detrimental heat generation. Additionally, the hysteresis hinders precise state-of-charge estimation. Our recent research identifies the chemo-mechanical coupling of silicon and the Solid-Electrolyte Interphase (SEI) as the reason for the substantial voltage hysteresis. The SEI is a thin passivating film that grows on negative electrode particles due to electrolyte decomposition [1]. For silicon particles, volume changes lead to significant strains and plastic deformation within the SEI [2]. As anode particle and SEI are mechanically coupled, the stress generated inside the SEI impacts the stress inside the anode, affecting its potential. Our chemo-mechanical model reproduces the observed open-circuit voltage hysteresis [3]. Furthermore, our visco-elastoplastic SEI model reproduces the voltage difference between slow cycling and the relaxed voltage. This detailed physical understanding can improve the performance of silicon anodes. [1] L. Köbbing et al. J. Power Sources 2023, DOI: 10.1016/j.jpowsour.2023.232651. [2] L. Kolzenberg et al. Batter. Supercaps 2022, 5, DOI: 10.1002/batt.202100216. [3] L. Köbbing et al. Adv. Funct. Mater. 2023, DOI: 10.1002/adfm.202308818.

KFM 24.9 Thu 12:35 EMH 225

Understanding SEI formation in Alkali Metal Batteries — ●DANIEL STOTTMEISTER¹ and AXEL GROSS^{1,2} — ¹Institut für Theoretische Chemie, Ulm University, Ulm, Germany — ²Helmholtz Institute Ulm, Ulm, Germany

Batteries have established themselves as one of the prime energy storage devices in modern times. Due to the relative scarcity of lithium and the ever-increasing demand for safe, efficient, and affordable energy storage solutions, post-lithium battery systems have emerged as promising future energy storage solutions. Other more common alkali metals like sodium and potassium are of particular interest. However, like their lithium predecessors, sodium and potassium batteries suffer from various issues, some of which originate from the formation of an instable solid electrolyte interphase (SEI). The formation mechanisms of said SEI are yet to be fully understood. Density Functional Theory (DFT) is a well-established method for the description of systems at the atomic level and can help to unravel some of the reaction mechanisms relevant to the formation of the SEI. This contribution uses ab initio molecular dynamics (AIMD) and DFT simulations to investigate and compare the electrolyte decomposition and the resulting SEI formation mechanisms of lithium, sodium, and potassium metal batteries at the atomistic level.

KFM 24.10 Thu 12:55 EMH 225

Effects of Aluminum trifluoride impurities on NMC811 /Graphite Lithium-ion battery performance. — ●SLAHEDDINE JABRI — Institute of Applied Physics, Technische Universität Braunschweig, 38106 Braunschweig, Germany

The effects of aluminum trifluoride (AlF₃) impurities in the electrolyte of full cell lithium-ion batteries has been studied using NMC811/Graphite electrodes. A strong decline of the retention capacity is observed when the cells are cycled at 50 °C in the presence of AlF₃ impurities in the electrolyte. The AlF₃ accelerates the cell degradation by the generation of various compounds during battery operation. The NMC811 cathode and the Graphite anode are characterized with different techniques. Scanning electron microscopy SEM, including cross-section- Focus Ion Beam FIB, Raman spectroscopy and

X-ray photoelectron spectroscopy XPS methods are employed to investigate the effect of the degradation on the electrolyte due to the AlF_3 impurities. We found modified chemical components and morphology of the surface electrolyte interface (SEI) and cathode electrolyte interface (CEI) layers of anode and cathode after cell aging with polymer layers on the both surfaces. Pathways to understand the AlF_3 impact are proposed.

KFM 24.11 Thu 13:15 EMH 225

Impurity Effects of AlCl_3 on the Performance of Polyamide-Ionic-Liquid-based Polymer Electrolytes for Aluminium Batteries — ●MOHAMMAD MOSTAFIZAR RAHMAN, AMIR MOHAMMAD, SHUVRODEV BISWAS, HARTMUT STÖCKER, and DIRK C. MEYER — Institute of Experimental Physics, TU Bergakademie Freiberg

The AlCl_3 - Et_3NHCl ionic liquid (IL) has emerged as a promising and cost-effective option for the rechargeable Al-ion battery system. The

polyamide-based solid polymer electrolyte (SPE) derived from this IL was utilized for the present investigation. Six different purities of AlCl_3 salts (ranging from 98 % to 99.999 %) with variable prices were used to prepare the SPEs and their performance was evaluated using various electrochemical characterization techniques. The results indicate good reversibility and Al stripping/plating behavior without impurity effects. Conductivities range from 0.19 mS/cm to 0.21 mS/cm, while stability windows span 2.70 V to 2.83 V. In addition, specific capacities range from 28 mAh/g to 39 mAh/g with no systematic effect of impurities. Overall, the electrochemical analysis shows that impurities in AlCl_3 salts have minimal impact on the SPE electrochemical properties. A cost-benefit analysis indicates that utilizing a low-cost AlCl_3 salt (0.027 €/g) yields comparable electrolyte performance as a higher-priced (6.198 €/g) high-purity salt. This discovery enables a reduction in electrolyte cost by approximately a factor of 17, consequently leading to a decrease in the overall cost of Al batteries.

KFM 25: Materials for Storage and Conversion of Energy (joint session MM/KFM)

Time: Thursday 11:45–13:00

Location: C 264

KFM 25.1 Thu 11:45 C 264

Unraveling, with *ab initio* modeling, the connection between electronic structure and dynamical properties of the sodium bismuth titanate. — ●MARCIN KRYŃSKI — Warsaw University of Technology, Warsaw, Poland

Oxide ion solid electrolytes has have drawn significant attention as they find applications in many electrochemical devices like oxygen sensors, oxygen pumps and solid oxide fuel cells [1]. Recently, ceramic compounds based on the perovskite $\text{Na}_0.5\text{Bi}_0.5\text{TiO}_3$ (NBT) attracted major attention due to its high Curie temperature ($\sim 325^\circ\text{C}$), large remnant polarization ($38 \mu\text{C}\cdot\text{cm}^{-2}$) and exceptional fast oxygen-ion conduction. Interestingly, NBT shows high ionic conductivity only if the molar ration between Na and Bi atoms is above unity. Below this value, a sudden drop of conductivity is observed. In this project we employ state of the art Density Functional Theory, using Strongly Constrained and Appropriately Normed functional (SCAN) together with Dudarev approach of on-site Coulombic interaction to model oxide ion dynamics of NBT electrolyte. For the first time, we correlate dynamical properties of mobile ions with the composition-dependent presence of small polarons. Furthermore, we look at the charge transfer during dynamical processes, change of the dipole moment as well as the bond strength. All this allows us to form a coherent picture of the diffusion processes being strongly correlated to the electronic structure of the NBT and how those two aspects of this compound are modulated by the composition. This work was supported by the National Science Centre, Poland under grant number UMO-2018/30/M/ST3/00743.

KFM 25.2 Thu 12:00 C 264

Exploration of Cathode-Stable Layered Solid-State Electrolytes — ●SINA ZIEGLER, KARSTEN REUTER, and CHRISTOPH SCHEURER — Fritz-Haber-Institut der MPG, Berlin

Promising higher safety and capacity, all-solid-state lithium batteries are envisioned to replace standard lithium-ion batteries in the near future. Lithium thiophosphates achieve the highest lithium-ion conductivities of all solid-state electrolytes (SSE) known to date, but their instability towards high-performance electrodes remains a critical challenge. To address this issue, we investigate the concept of rare-earth lithium halides as a material-efficient, nanometer thick cathode coating in contact with thiophosphate electrolytes. Halides provide wide electrochemical stability windows as well as good chemical and thermodynamic stability.

To determine a suitable halide/thiophosphate combination, we aim to identify an energetically feasible reaction pathway in the multidimensional phase diagram between the two materials. The corresponding stabilities of the emerging SSE/halide interfaces are examined by *ab initio* thermodynamics to screen reaction free enthalpies of possible interface reactions. Next, an end member analysis is performed to analyze possible compositions of interface products and possible secondary phases. Machine-learning interatomic potentials are trained on promising material combinations to validate the approach.

KFM 25.3 Thu 12:15 C 264

Understanding Anion-trapping in composite solid-state elec-

trolytes with active ceramic fillers — ●MAURICIO BONILLA¹, HENRY CORTES¹, ERNESTO MARINERO², JAVIER CARRASCO^{3,4}, and ELENA AKHMATSKAYA^{1,4} — ¹BCAM - Basque Center for Applied Mathematics, Bilbao, Spain — ²School of Materials Engineering, Neil Armstrong Hall of Engineering, Purdue University, West Lafayette, IN, USA — ³Centre for Cooperative Research on Alternative Energies (CIC energiGUNE), Basque Research and Technology Alliance (BRTA), Vitoria-Gasteiz, Spain — ⁴IKERBASQUE, Basque Foundation for Science, Bilbao, Spain

Developing high-performance solid-state electrolytes (SSEs) is a key step in the development of safe and efficient solid-state batteries. Composite SSEs (cSSEs) comprising active particles dispersed in an ion-conducting polymer matrix constitute a promising strategy to obtain higher ionic conductivity (IC), and interfacial and mechanical stability than single-phase SSEs. Recent experiments showed that garnet particles enhance the IC of cSSEs and that this effect can be tuned through aliovalent doping. However, the underlying mechanism is not well understood. Here, we use an enhanced hybrid Monte Carlo technique and MD simulations to bridge this gap. By focusing on the cSSEs comprising Ga-doped $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ particles in a polyethylene oxide (PEO) + $\text{LiC}_2\text{F}_6\text{NO}_4\text{S}_2$ (LiTFSI) matrix, we show how the dynamic electrostatic trapping of TFSI⁻ anions leads to IC enhancement by increasing the Li⁺ transference number. Moreover, we show that such enhancement can be modulated through the Ga dopant content.

KFM 25.4 Thu 12:30 C 264

Can Migrating Ions Block and Deactivate the Active Sites in Solid Oxide Cells? — ●PATRICIA KÖNIG, HANNA TÜRK, THOMAS GÖTSCH, FRANZ-PHILIPP SCHMIDT, AXEL KNOP-GERICKE, ROBERT SCHLÖGL, THOMAS LUNKENBEIN, KARSTEN REUTER, and CHRISTOPH SCHEURER — Fritz-Haber-Institut der MPG, Berlin

Degradation of the air electrode in electrolysis mode during the oxygen evolution reaction severely limits the commercial adoption of solid oxide cells. Up to now, the atomistic structure of this active catalyst region is essentially unknown, which prevents a detailed analysis of the actual degradation mechanisms.

In prior research, we identified a complexion at the solid/solid interface of the sintered anode [1], featuring partial amorphization and varying elemental distributions deviating from the confining bulk phases. Located around the complexion area, we propose deactivation mechanisms driven by strong cation inter-diffusion. To assess if these cation migrations impede active sites and cell functionality, we conduct a large-scale study on possible active site structural motifs. We sample structures with polarons near oxygen defects, altering ion dopant concentrations to simulate ion migration effects. By employing density-functional theory to compute EELS spectra, we link oxygen defects and their proximity to polarons to distinctive peaks in experimentally recorded EELS spectra. Ultimately, this approach aids in identifying active site structures and deactivation mechanisms, enhancing future cell design with improved efficiency and durability.

[1] H. Tuerk *et al.*, Adv. Mater. Interfaces **8**, 2100967 (2021).

KFM 25.5 Thu 12:45 C 264

Anharmonic Lattice Dynamics of Solid-State Ion Conduc-

tors from Machine-Learning Molecular Dynamics — •TAKERU MIYAGAWA, MANUEL GRUMET, NAMITA KRISHNAN, WALDEMAR KAISER, and DAVID A. EGGER — Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

Solid-state ionic conductors (SSICs) are playing an important role in electrification of transport and energy industries. Recent studies suggested that the host lattice dynamics play a critical role in the ionic conduction mechanisms [1]. Several SSICs exhibit anharmonic lattice vibrations taking mobile ions into anharmonic regions of their potential energy surface [2, 3]. Here, we investigate the role of anharmonic host lattice vibrations and their impact on the conduction of mobile cations

in SSICs by using machine-learning molecular dynamics (MLMD). Particularly, we focus on different classes of superionic conductors that all exhibit anharmonicities: AgI, a strongly disordered Ag-conductor [2]; Na₃PS₄, a Na vacancy conductor [3]; and Li₁₀GeP₂S₁₂, showing concerted Li migration [4]. Our results demonstrate the potential of MLMDs in understanding coupled host lattice-mobile ion dynamics and show guidelines for the design of novel SSICs with higher ionic conductivities.

[1] Zhang; *Natur. Rev. Mater.* 7, 389-405 (2022). [2] Brenner et al. *Phys. Rev. Mater.* 4, 115402 (2020). [3] Brenner et al. *J. Phys. Chem. Lett.* 13, 25, 5938-5945 (2022). [4] Fang; *Jena, Nat. Comm.* 13, 2078 (2022)

KFM 26: SrTiO₃: A Versatile Material from Bulk Quantum Paraelectric to 2D Superconductor II (joint session TT/KFM/MA/O)

Strontium titanate (SrTiO₃) is a paradigmatic material that plays an important role in various fields of solid-state physics, surface science and catalysis: The pure bulk phase is a wide-band-gap semiconductor that upon cooling becomes a textbook quantum paraelectric. When slightly doped, SrTiO₃ turns into a Fermi-liquid-type metal that becomes superconducting at extremely low charge carrier density. SrTiO₃-based surfaces and interfaces host un-conventional electronic states such as quasi-two-dimensional electron liquid, magnetism and superconductivity. Despite intensive studies over the past decades, SrTiO₃ continues to reveal surprising new phenomena that challenge the established views on this material. To this end achieving light-induced nonequilibrium states and the recent preparation of a 2D oxide based on SrTiO₃ opens new playgrounds for research. This Focus Session will present exciting developments in the study of electronic states that are based on the peculiar properties of SrTiO₃.

Please note that this Focus Session comprises four parts: Posters are presented within the TT poster session TT58 (Wed 15:00-18:00, poster area E). Invited talks are compiled in the session TT62 (Thursday, 9:30 to 12:45, H0104), Contributed talks will be presented in sessions TT72 (Thursday 15:00-18:00, H0104) and TT83 (Fri 9:30-12:30, H0104).

Organizers: Rossitza Pentcheva, University of Duisburg-Essen, Marc Scheffler, University of Stuttgart

Time: Thursday 15:00–18:00

Location: H 0104

KFM 26.1 Thu 15:00 H 0104

Origin of unconventional normal-state transport and superconductivity in electron-doped SrTiO₃ — •STEPHEN ROWLEY — Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge, CB3 0HE, United Kingdom

Quantum phase transitions may be reached in many ferroelectric systems by suppressing the Curie temperature to absolute zero using a control parameter such as chemical substitution or hydrostatic pressure. In electron-doped specimens of quantum critical ferroelectrics such as SrTiO₃, unconventional superconductivity and unusual normal-state transport have been detected. In the latter case, a resistivity varying as temperature-squared is observed over a wide range of temperatures above the Fermi temperature. We present new experimental and model results that provide insight into the nature of the mechanisms for both superconductivity and normal-state transport. We find in experiments and quantitative models without adjustable parameters, that both effects are connected and enhanced in samples tuned to the ferroelectric quantum critical point. Superconductivity appears to arise near the critical point due to the virtual exchange of longitudinal hybrid-polar-modes, even in the absence of a direct coupling to the transverse-optical phonon modes.

KFM 26.2 Thu 15:15 H 0104

Dilute superconductivity in the vicinity of a ferroelectric quantum critical point coupled via the "vector coupling": The case of SrTiO₃ — •SUDIP KUMAR SAHA^{1,2}, AVRAHAM KLEIN¹, JONATHAN RUHMAN², and MARIA NAVARRO GASTIASORO³ — ¹Ariel University, Israel — ²Bar-Ilan University, Israel — ³Donostia International Physics Center, Spain

Lightly doped SrTiO₃ (STO) is one of the most studied examples of quantum ferroelectric metal (QFEMs), where superconductivity coexists with ferroelectric order. Pristine STO is paraelectric naturally close to a ferroelectric quantum critical point (QCP). Strain or chemical substitution (for example, doping with Ba/Ca instead of Sr) drives STO through the QCP to the ferroelectric phase, which manifests itself

in the softening of the transverse optical (TO) phonon mode. Doped samples are superconducting, where the T_c vs. density dome extends to very low density. To date, there is no consensus on the mechanism leading to superconductivity at such low density. Edge et al. have proposed that the ferroelectric QCP and dilute superconductivity are related [*Phys. Rev. Lett.* 115, 247002 (2015)]. In this work we explore the possible origin of low-density superconductivity from coupling linearly to the TO mode via a "vector coupling". We solve the critical-Eliashberg theory numerically, including fermionic and bosonic self-energy corrections, which allows us access all the way to the QCP. Notably, all our calculations are justified within standard approaches. We find the existence of a superconducting dome with magnitude and dependence on the distance from the QCP that resembles experiments.

KFM 26.3 Thu 15:30 H 0104

Dislocation-based filamentary superconductivity in reduced SrTiO₃ — •CHRISTIAN RODENBÜCHER¹, GUSTAV BIHLMAYER², CARSTEN KORTE¹, and KRISTOF SZOT³ — ¹Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research (IEK-14), 52425 Jülich, Germany — ²Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-1), 52425 Jülich, Germany — ³University of Silesia, Institute of Physics, 41-500 Chorzów, Poland

Exposure of SrTiO₃ single crystals to reducing conditions at elevated temperatures leads to the generation of metallic filaments forming along of dislocations, which act as preferential reduction sites. This effect can be enhanced when stimulating the local deoxidation by electric fields. This results in an agglomeration of metallic filaments in nano-bundles, which are embedded in the insulating surrounding crystal matrix. Despite removing only 10¹⁴⁻¹⁵ oxygen atoms from the dislocation network, electro-reduced crystals are superconducting with a transition temperature of 0.2 K, and their residual resistance is lower than that of purely thermally-reduced crystals. As the total amount of oxygen removed during electro-reduction is much smaller than the smallest reported carrier concentration for superconducting SrTiO_{3-x} so far, our findings challenge traditional explanations of superconduc-

tivity in metal oxides. Combining conductivity characterization by atomic force microscopy with theoretical analysis of the dislocation cores, we propose a model explaining the superconducting properties by the coexistence of metallic dislocation cores with polar insulating regions allowing for polaronic coupling in the bundles.

KFM 26.4 Thu 15:45 H 0104

Dislocation-Induced Photoconductivity Enhancement in Fe-Doped SrTiO₃: compensation of low mobility by high carrier density through the emergence of a sub-band gap level — ●MEHRZAD SOLEIMANY^{1,2}, TILL FRÖMLING¹, JÜRGEN RÖDEL¹, and MARIN ALEXE² — ¹Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany — ²Department of Physics, University of Warwick, Coventry, UK

Owing to the remarkable properties of SrTiO₃ (STO), such as quantum paraelectric state below 37 K, negative differential resistance under illumination, and significant alteration of properties by doping, STO stands out among perovskite oxides. Until recently, little attention had been paid to the tunability of its properties - especially optical properties - via the introduction of dislocations. In this study, we introduce the method of dislocation imprint, which allows us to induce high densities of dislocations ($> 1 \times 10^{14} \text{ m}^{-2}$) into a large volume of Fe-doped STO. Low-temperature I-V measurements indicated an about one order of magnitude increase in the photoconductivity of dislocation-rich samples. Photo-Hall measurements revealed that while dislocations might decrease the mobility, they could enhance the photoconductivity by increasing the number of carriers. Spectral responsivity measurements demonstrated that the higher carrier density could stem from the emergence of a sub-band gap level. Complementary C-AFM measurements conducted under illumination confirmed the local enhancement of photoconductivity at dislocations, which fitted well to the Electron Channeling Contrast Images of dislocations.

KFM 26.5 Thu 16:00 H 0104

IR and THz studies on (Ba_{0.45}Sr_{0.55}TiO₃)₂₄Ba_{0.45}Sr_{0.55}O and (Ba_{0.45}Sr_{0.55}TiO₃)₈Ba_{0.45}Sr_{0.55}O thin films — VERONICA GOIAN¹, MATTHEW BARONE², NATALIE DAWLEY², CHRISTELLE KADLEC¹, ●DARRELL SCHLOM^{2,3}, and STANISLAV KAMBA¹ — ¹Institute of Physics ASCR, Prague, Czech Republic — ²Department of Materials Science and Engineering, Cornell University, Ithaca, NY, USA — ³Kavli Institute at Cornell for Nanoscale Science, Ithaca, NY, USA

(SrTiO₃)_nSrO and (n=1..6) films crystallizing in the Ruddlesden-Popper (RP) structure are well known for low dielectric loss and large microwave permittivities which are highly tunable with electric field.^{1,2} Bulk (SrTiO₃)_nSrO is paraelectric, but the tensile strained thin films deposited on (110)DyScO₃ with $n \geq 3$, become ferroelectric at low temperatures. (ATiO₃)₂₄AO and (ATiO₃)₈AO, A= Ba_{0.45}Sr_{0.55} films deposited on (110)DyScO₃ exhibit no strain and yet become ferroelectric. Here we performed infrared and THz studies of phonon dynamics down to 10 K and compared it with above mentioned thin films and (Sr,Ba)TiO₃. The effect of soft mode and central mode on microwave dielectric properties and electric field tunability of permittivity will be discussed.

[1] C. H. Lee et al., Nature, 502 (2013) 532

[2] N. M. Dawley et al., Nat. Mater. 19 (2020) 176

KFM 26.6 Thu 16:15 H 0104

Polar phonon behaviour in polycrystalline Bi-doped strontium titanate thin films — ●OLEKSANDR TKACH¹, OLENA OKHAY², DMITRY NUZHNY³, JAN PETZELT³, and PAULA M. VILARINHO¹ — ¹Department of Materials and Ceramic Engineering, CICECO, University of Aveiro, Aveiro, Portugal — ²TEMA-Centre for Mechanical Technology and Automation, Department of Mechanical Engineering, University of Aveiro, Aveiro, Portugal — ³Institute of Physics of the Czech Academy of Sciences, Prague, Czechia

Among strontium titanate (STO) based materials, Bi-doped STO have been intensively studied as for dielectric as for resistance-switching memory and thermoelectric applications. Here, we enhance the dielectric characterisation by a lattice dynamics study of sol-gel-derived Sr_{1-1.5x}Bi_xTiO₃ thin films with $x = 0.0053$ and 0.167 , deposited on Al₂O₃ substrates, using a variable-temperature far-infrared spectroscopy in a transmittance mode. Bi doping, known to induce a low-frequency dielectric relaxation in STO ceramics and films, due to off-centre dopant ion displacements generating electric dipoles, is shown to affect the polar phonon behaviour of thin films. We show that in weakly Bi-doped films, the low-frequency polar TO1 mode softens on

cooling but less than in undoped STO. In heavily Bi-doped STO films, this mode displays no significant frequency variation with temperature from 300 to 10 K. The polar phonon behaviour of polycrystalline Bi-doped STO thin films is comparable with that of Bi-doped STO ceramics, which exhibit dielectric relaxations and harden soft-mode behaviour instead of the ferroelectric phase transition.

15 min. break

KFM 26.7 Thu 16:45 H 0104

Emergence of strain-Induced magnetism in plastically-deformed SrTiO₃ at low temperature — ●ANIRBAN KUNDU¹, XI WANG², AVRAHAM KLEIN¹, and BEENA KALISKY² — ¹Department of Physics, Ariel University, Israel — ²Institute of Nanotechnology & Advanced Materials, Bar-Ilan University, Israel

It is well established that SrTiO₃ (STO) can possess ferroelectric states alongside observed superconducting states. However, so far, the phenomena of magnetism have not been established. In our collaborative work, in a plastically deformed bulk STO sample; SQUID measurements reveal strong magnetic signals which are completely absent in pristine samples. This strain-induced magnetism has two salient features. First, the magnetic moment is seen only with applied strain and increases with applied strain. Second, it also increases with temperature. Using Ginzberg Landau theory we show that these properties may be the result of coupling terms between strain, polar, and magnetic orders centered around dislocation walls induced by the plastic deformation. Our analysis implies that deformed STO is a quantum multiferroic.

KFM 26.8 Thu 17:00 H 0104

Mobility in SrTiO₃ Mediated by Machine Learning Predicted Anharmonic Phonons — ●LUIGI RANALLI¹, CARLA VERDI², and CESARE FRANCHINI¹ — ¹University of Vienna, Vienna, Austria — ²University of Queensland: Brisbane, Queensland, Australia

The anharmonic corrections to ionic motion play a crucial role in influencing the electron-phonon interaction, a phenomenon typically addressed through harmonic dynamical matrices at the ground state. By combining machine learning methodologies [1] and the stochastic self-consistent harmonic approximation [2], we achieve a precise depiction of the temperature-dependent evolution of phonon frequencies and the onset of ferroelectricity in the quantum paraelectric perovskites SrTiO₃ [3] and KTaO₃ [4]. In this presentation, anharmonic dynamical matrices are incorporated into the Boltzmann transport equation calculations for SrTiO₃ up to 300K using the EPW code [5] and fixing the derivatives of the Kohn-Sham potential computed through density functional perturbation theory [6]. This approach yields a coherent interaction vertex, ensuring that the temperature-dependent ferroelectric soft mode explains and recovers the observed trend in experimental mobility, akin to the behavior observed in KTaO₃.

[1] R. Jinnouchi et al., Phys. Rev. Lett. 122 (2019) 225701

[2] L. Monacelli et al., J. Phys.: Condens. Matter 33 (2021) 363001

[3] C. Verdi et al., Phys. Rev. Materials 7 (2023) L030801

[4] L. Ranalli et al., Adv. Quantum Technol. 6 (2023) 2200131

[5] H. Lee et al., 10.1038/s41578-021-00289-w (2023)

[6] J. Zhou et al., Phys. Rev. Research 1 (2019) 033138

KFM 26.9 Thu 17:15 H 0104

Machine-learning-backed evolutionary exploration of the SrTiO₃(110) surface phase diagram — ●RALF WANZENBÖCK¹, FLORIAN BUCHNER¹, MICHELE RIVA², JESÚS CARRETE^{3,1}, and GEORG K. H. MADSEN¹ — ¹Institute of Materials Chemistry, TU Wien, A-1060 Vienna, Austria — ²Institute of Applied Physics, TU Wien, A-1040 Vienna, Austria — ³Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, 50009 Zaragoza, Spain

We use CLINAMEN2, a modern functional-style Python implementation of the covariance matrix adaptation evolution strategy (CMA-ES), to gain insights into the lesser-known regions of the complex SrTiO₃(110) surface phase diagram. To speed up the process, we leverage the transferability of a neural-network force field (NNFF) implemented on top of the state-of-the-art JAX framework.

Starting from smaller reconstructions in well-explored phases, such as the 4×1 surface reconstruction [Wanzenböck et al., Digit Discov 1, 703-710 (2022)], the NNFF is iteratively refined using an active learning workflow that relies on uncertainty estimation techniques [Carrete et al., J. Chem. Phys 158, 204801 (2023)]. We show how this work-

flow and the underlying uncertainty metric lead to a flexible NNFF, highlighted by the exploration of out-of-sample SrTiO₃(110)-(2 × n) reconstructions.

KFM 26.10 Thu 17:30 H 0104

Quasiparticle and excitonic properties of monolayer SrTiO₃ — ●LORENZO VARRASSI¹, PEITAO LIU², and CESARE FRANCHINI^{1,3} — ¹Dipartimento di Fisica e Astronomia, Università di Bologna, Bologna — ²Shenyang National Laboratory for Materials Science, Institute of Metal Research — ³University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna.

Recently, a breakthrough has been achieved with the synthesis of free-standing SrTiO₃ ultrathin films down to the monolayer limit[1]; its optical and excitonic properties remain however largely unexplored. This talk will provide insights on the quasiparticle and excitonic properties of monolayer SrTiO₃, employing many-body perturbation theory.

Our analysis[2] emphasizes the need to go beyond the diagonal GW approximation and include off-diagonal self-energy elements in order to obtain correct description of the orbital hybridizations. A fully satisfying description is achieved by treating non-locality in both exchange and correlation.

The optical properties are studied through the solution of the Bethe-Salpeter equation. We observe a significant enhancement of the excitonic effects with respect to the bulk phase, with a binding energy at the optical gap about four times greater. Furthermore, the two-dimensional polarizability at the long wavelength limit is dominated by two strongly bound excitonic peaks; their character is determined

through the analysis of the excitonic wavefunctions.

[1] D. Ji et al., Nature 570 (2019) 87

[2] L. Varrassi et al., arXiv:2303.14830 (2023)

KFM 26.11 Thu 17:45 H 0104

SrTiO₃: Thoroughly investigated but still good for surprises — ●ANNETTE BUSSMANN-HOLDER¹, REINHARD K. KREMER¹, KRYSZTIAN ROLEDER², and EKHARD K. H. SALJE³ — ¹Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany — ²Institute of Physics, University of Silesia, ul. 75 Pułku Piechoty 1, 41-500 Chorzów, Poland — ³Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, United Kingdom

For decades SrTiO₃ is in the focus of research with seemingly never-ending new insights regarding its ground state properties, its application potentials, its surface and interface properties, the superconducting state, the twin boundaries and domain functionalities, etc. Here, we focus on the already well-investigated lattice dynamics of STO and show that four different temperature regimes can be identified which dominate the elastic properties, the thermal conductivity and the birefringence. These regimes are the low-temperature quantum fluctuation dominated one, followed by an intermediate regime, the region of the structural phase transition at 105 K and its vicinity, and at high temperatures a regime characterized by precursor and saturation effects. They can all be elucidated by lattice dynamical aspects. The relevant temperature dependencies of the soft modes are discussed and their relationship to lattice polarizability is emphasized.

KFM 27: Polar oxides: Lithium niobate and lithium tantalate

Chair: Manuel Zahn (Uni Augsburg)

Time: Thursday 15:00–16:20

Location: EMH 025

KFM 27.1 Thu 15:00 EMH 025

The role of domain wall conductivity in ferroelectric domain inversion — ●MICHAEL RÜSING^{1,2}, BORIS KOPPITZ², IULIA KISELEVA², LAURA PADBERG¹, CHRISTOF EIGNER¹, CHRISTINE SILBERHORN¹, and LUKAS M. ENG^{2,3} — ¹Paderborn University, Integrated Quantum Optics, Institute for Photonic Quantum Systems (PhoQS), Warburger Str. 100, 33098 Paderborn, Germany — ²TU Dresden, Institute of Applied Physics, Nöthnitzer Strasse 61, 01187 Dresden, Germany — ³ct.qmat: Dresden-Würzburg Cluster of Excellence EXC 2147, TU Dresden, 01062 Dresden, Germany

During electric field poling of single-domain, single-crystals, like lithium niobate, it is observed that the nucleation and growth of spike domains predominantly starts from one crystallographic side. This phenomenon is often explained by different surface barriers at the crystal's surface. The conductivity of ferroelectric DWs is suggested to be central to general domain reversal, e.g. by assisting and allowing screening processes [1]. In this work we will discuss how the directionality of DW conductivity, as well as the observed dominance of only sign of charge carrier in conductive DWs [2], can explain the preference of one of the crystal surfaces for initial domain reversal independent of the surface's properties. This work shows that DW conductivity can play a key role when explaining macroscopic ferroelectric material properties. [1] B. Sturman and R. Podivilov, JETP Letters, 116, 246 (2022); [2] H. Beccard et al., ACS Appl. Nano Mater. 5, 8717 (2022).

KFM 27.2 Thu 15:20 EMH 025

Theoretical Modelling of Domains and Domain Walls in Ferroelectric Oxides — ●LEONARD VERHOFF and SIMONE SANNA — Institut für Theoretical Physics, Justus Liebig University, Giessen, Germany

Ferroelectric domain walls (DW) in lithium niobate (LN) and lithium tantalate (LT), i.e. interfaces between regions of different polarization, present a compelling field of study with diverse emergent functionalities. DW not only exhibit unique electronic and optical properties but also present a rich avenue for tailoring and manipulating the material's behaviour for advanced applications in optoelectronics and information processing.

We employ various methods to model DW parallel to the *z*-axis in the ferroelectric oxides LN and LT. Beginning with a symmetry-based description, we utilize Ginzburg-Landau-Devonshire theory for qualita-

tive insights. We delve into specific, high-symmetry DW orientations through density functional theory (DFT) calculations to investigate the ionic structure around the DW and the respective formation energies in detail. These energies, interpreted as interaction strengths of neighboring domains, are then incorporated into a 2D Ising model to simulate the formation of DW on a larger scale lattice, that would be inaccessible through DFT due to the large number of atoms. Special emphasis is placed on understanding the shape of emerging ferroelectric domains, with a focus on the anisotropy of formation energy that leads to hexagonal domain shapes in LN, while LT forms triangular domains.

KFM 27.3 Thu 15:40 EMH 025

Ab initio investigation of the ferroelectric phase transition in LiNbO₃ and LiTaO₃ — ●ALEXANDER KAPP, WAFAA AL NACHWATI, and SIMONE SANNA — Institute for Theoretical Physics, Justus Liebig University, Giessen, Germany

Lithium niobate (LN, LiNbO₃) and Lithium tantalate (LT, LiTaO₃) are synthetic, isomorph solids. Both crystallize in a trigonal lattice, belonging to the space group R3c for the ferroelectric state and R3c for the paraelectric states. These materials display several favorable properties such as ferroelectricity, piezoelectricity and the Pockels effect, just to name some examples. For this reason, these crystals are used in many applications e.g., in the telecommunication market for mobile telephones or optical modulators, and also for laser uses like Q-switching or frequency doubling. In this work, we model the transition from the paraelectric to the ferroelectric state and determine the Curie temperature in both crystals using ab initio molecular dynamics, as implemented in the Vienna Ab initio Simulation Package (VASP). Within this approach, atoms in the supercell can move according to existing forces, estimated by density functional theory (DFT). In our calculations, we take into account the expansion of cell volume with increasing temperature. Moreover, very large supercells are used to reduce finite-size effects. Within this approach, we obtain transition temperatures in close agreement with the measured values.

KFM 27.4 Thu 16:00 EMH 025

Vibrational and optical properties of LiNbO₃ and LiTaO₃ under uniaxial stress — ●MIKE PIONTECK¹, MATTHIAS ROEPER², EKTA SINGH², BORIS KOPPITZ², SVEN REITZIG², MICHAEL LANGE², SAM SEDDON², MICHAEL RÜSING^{2,3}, LAURA PADBERG³, SIMONE

SANNA¹, and LUKAS ENG^{2,4} — ¹Institut für Theoretische Physik, Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — ²Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany — ³Paderborn University, Integrated Quantum Optics, Institute for Photonic Quantum Systems (PhoQS), Warburger Str. 100, 33098 Paderborn, Germany — ⁴ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Our work provides, for the first time, a theoretical description of phonon frequencies of LiNbO₃ and LiTaO₃ under uniaxial stress along

Cartesian axes using density functional theory (DFT). The calculations show a roughly linear dependence of the Raman frequencies on the applied uniaxial stress, which is confirmed by corresponding Raman measurements [1]. Additionally, we model linear and non-linear optical properties of LiNbO₃ in dependence on uniaxial stress using time-domain DFT. We find roughly linear changes for all components of the second harmonic generation under uniaxial stress. From the calculated dielectric tensor under stress, the dispersion of the piezo-optic and photoelastic coefficients are obtained. [1] E. Singh *et al.* Phys. Rev. Mat. **7**, 024420 (2023).

KFM 28: Focus Session: (Multi-)Ferroic States IV

The focus session is dedicated to (multi)ferroic states at interfaces and in heterostructures. The design of (emergent) properties at interfaces, modelling methods and advanced characterization tools will be of interest. Typical examples may include electrostatic and strain boundary conditions at interfaces, domains and domain walls in (multi)ferroics and applications in nano-electronic device.

Chair: Morgan Trassin (ETH Zürich)

Time: Thursday 15:00–17:45

Location: EMH 225

Invited Talk KFM 28.1 Thu 15:00 EMH 225
Every (ferroelectric) wall is a door - exploring the links between structure, dynamics, and emergent functionalities — ●PATRYCJA PARUCH — DQMP, University of Geneva, Switzerland

Ferroelectric materials can host a wide range of unusual structural features, often linked to novel functional properties. One such feature are the domain walls separating regions with different polarisation orientation, providing an intrinsically nanoscale, powerful model system for the rich physics of pinned elastic interfaces. Understanding their structure, geometry, and nonlinear dynamics is key for controlling polarisation switching and domain size, shape, and stability in memory, electro-optic, electro-mechanical and catalytic devices. In addition, at such domain walls the complex interaction between polarisation, electrostatics, and strain can lead to localised chiral polarisation textures, electrical conductivity, local mechanical responses, and charge or chemical segregation, potentially useful for nanoelectronics applications. We use a broad spectrum of primarily scanning probe microscopy techniques, coupled with machine learning analysis to investigate and disentangle the many complex and correlated physical phenomena in these materials. Considering the dual role of defects for both domain wall pinning and local electrical conduction modulation in Pb(Zr_{0.2}Ti_{0.8})O₃ and PbTiO₃ thin films, with both 180° and 90° domain walls, I will emphasise the interactions between the statistical physics approach and new insights into emergent functional properties at domain walls.

KFM 28.2 Thu 15:30 EMH 225
Nanoscale electrostatic control of polarization in ferroelectric thin films using lattice chemistry — ●IPEK EFE¹, ALEXANDER VOGEL², WILLIAM S. HUXTER¹, ELZBIETA GRADAUSKAITE¹, CHRISTIAN L. DEGEN¹, MARTA D. ROSSELL², MANFRED FIEBIG¹, and MORGAN TRASSIN¹ — ¹ETH Zurich — ²Empa, Switzerland

Nanoscale electrostatic control of oxide interfaces enables functionalities beyond the realm of the bulk material, including superconductivity, multiferroicity, and topological properties. Here, by exploiting spontaneously forming charged interfaces in layered materials, we control the electrostatic boundary conditions in ferroelectric oxide heterostructures. Using in-situ optical second harmonic generation during the growth of layered Aurivillius Bi₅FeTi₃O₁₅ films, we correlate, in real-time, the stacking of highly charged fluorite-like (Bi₂O₂)²⁺ layers with the formation of the out-of-plane antipolar ordering of electric dipoles in the unit-cell. Next, we insert multiferroic BiFeO₃ into the Aurivillius scaffold and show that the resulting charged layering stabilizes the ferroelectric-like ordering of the electric dipoles. Our work brings the use of polarizing charged layers of layered oxides as an additional degree of freedom towards the design of technologically relevant electric dipole orderings in epitaxial thin films.

KFM 28.3 Thu 15:50 EMH 225
First-principles predictions of HfO₂-based ferroelectric superlattices — ●BINAYAK MUKHERJEE¹, NATALYA S. FEDOROVA¹, and JORGE ÍÑIGUEZ-GONZÁLEZ^{1,2} — ¹Department of Materials Research

and Technology, Luxembourg Institute of Science and Technology, L-4362, Esch-sur-Alzette, Luxembourg — ²Department of Physics and Materials Science, University of Luxembourg, L-4422, Belvaux, Luxembourg

The metastable nature of the polar phase of HfO₂ is a significant impediment to its industrial application as a functional ferroelectric material. In fact, no polar phases exist in the bulk phase diagram of HfO₂, which shows a non-polar monoclinic ground state, and this requires polar orthorhombic HfO₂ to be kinetically stabilized. Here, we propose an alternative approach, demonstrating the feasibility of thermodynamically stabilizing polar HfO₂ through superlattices with other simple oxides. Using the composition and stacking direction of the superlattice as design parameters, we obtain heterostructures that can be fully polar, fully antipolar or mixed, with improved energetics compared to the orthorhombic polar HfO₂ in bulk form. Our results suggest that combining HfO₂ with an oxide that does not have a monoclinic ground state generally drives the superlattice away from this non-polar phase, favoring the stability of the ferroelectric structures that minimize the elastic and electrostatic penalties. As such, these diverse and tunable superlattices hold promise for various applications in thin-film ferroelectric devices.

KFM 28.4 Thu 16:10 EMH 225
Localized oxygen reorganization under sub-millisecond switching in ferroelectric epitaxial hafnia-based films — ●NIVES STRKALJ^{1,2}, MEGAN O. HILL², JI SOO KIM², MORITZ L. MÜLLER², MAXIMILIAN T. BECKER², DIBYA PHUYAL^{2,3}, SUNIL TAPER², MANISHA BANSAL⁴, BABAK BAKHIT³, TUHIN MAITY⁴, GIULIANA DI MARTINO³, and JUDITH L. MACMANUS-DRISCOLL³ — ¹IoP, Zagreb, Croatia — ²UCAM, UK — ³KTH, Sweden — ⁴IISER TVM, India

The discovery of ferroelectricity in nanoscale films of binary oxides based on hafnia spurred renewed interest in the emergence of ferroelectric properties on the nanoscale. The unusual size dependence of polarization in hafnia is a topic of intense research with explanations including flat phonon bands, and coupling to an antipolar phase or an electrochemical state. Though polarization switching and electrochemical reactions have been shown to co-occur in hafnia-based films, their relationship remains unclear.

To elucidate the relationship between the polarization state and the electrochemical state, we perform direct observations of the electrochemical state in areas with preset polarization directions for hafnia-based films using hard x-ray photoelectron spectroscopy (HAXPES). Because we observe more pronounced electrochemical changes in films with lower polarization, we propose that the polarization and the electrochemical change are not directly linked. Our results present a step forward in disentangling the origin of the ferroelectric response in hafnia-based films.

15 min. break

KFM 28.5 Thu 16:45 EMH 225

Conduction mechanisms in $\text{Al}_{1-x}\text{Sc}_x\text{N}$ -based thin-film ferroelectric capacitors — ●VINAY LULLA¹, GEORG SCHÖNWEGER^{2,3}, SIMON FICHTNER^{2,3}, HERMANN KOHLSTEDT^{1,4}, and ADRIAN PETRARU¹ — ¹Chair of Nanoelectronics, Institute of Electrical and Information Engineering, Faculty of Engineering, Kiel University, Kaiserstraße 2, D-24143 Kiel, Germany — ²Chair of Microsystems and Technology Transfer, Institute of Material Science, Faculty of Engineering, Kiel University, Kaiserstraße 2, D-24143 Kiel, Germany — ³Fraunhofer Institute of Silicon Technology, Fraunhoferstraße 1, 25524 Itzehoe, Germany — ⁴Kiel NanoSurface and Interface Science KiNSIS, Kiel University, Christian-Albrechts-Platz 4, D-24118 Kiel, Germany

Current $\text{Al}_{1-x}\text{Sc}_x\text{N}$ based devices are limited by the high electric switching fields that require to operate the capacitors in a regime where the breakdown is highly likely, i.e., close to 4 MV/cm. In this work, ferroelectric capacitors with the layer sequence Pt/ $\text{Al}_{1-x}\text{Sc}_x\text{N}$ /Pt have been investigated. The electrodes and the $\text{Al}_{1-x}\text{Sc}_x\text{N}$ were deposited by DC sputtering and pulsed DC sputtering, respectively. These devices exhibit high leakage currents, especially for films thinner than 100 nm. In order to understand the transport mechanisms, the electric field dependence and temperature dependence (300 K - 77 K) of the leakage currents were investigated. The experiments showed that Richardson-Schottky conduction is likely to dominate the transport in high electric field regime (4 MV/cm), while domain wall conduction and Poole-Frenkel were valid mechanisms in the low-field regime (2 MV/cm).

KFM 28.6 Thu 17:05 EMH 225

Point Defects and Domain Walls in Soft Ferroelectric CsGeX_3 ($X = \text{Cl}, \text{Br}, \text{I}$) — ●KRISTOFFER EGGESTAD, BENJAMIN ALBERT DOBSON WILLIAMSON, DENNIS GERHARD MEIER, and SVERRE MAGNUS SELBACH — Department for Materials Science and Engineering - NTNU

Conductive domain walls (DWs) hold promise for nanoscale, energy-efficient multi-level diodes and neuromorphic circuitry. In CsGeX_3 , caesium and halogen vacancies are intrinsic point defects that can induce electrons and holes, respectively. Controlling the formation and position of vacancies can in principle give switchable local n-type or

p-type conductivity at DWs and enable new concepts for DW-based circuitry. This requires a material where mobile point defects of both positive and negative charge can accumulate at DWs. CsGeX_3 is here chosen as our model system due to the possibility of having mobile caesium and halogen vacancies.

Using hybrid density functional theory (DFT) we investigate electronic structure and defect formation energies in bulk, showing highly mobile holes and free electrons, as well as relatively shallow defect levels. Moreover, a study on point defect mobility in bulk, reveals exceptionally mobile anion vacancies with migration barriers comparable to Li vacancies in the best solid-state electrolytes. Furthermore, we show that Y-type 71-degree DWs are the most stable and that they are extremely mobile, implying that polarisation can easily be switched. Finally, the possibility of reversible p- and n-type conductivity in DWs in CsGeX_3 and other similar materials is discussed.

KFM 28.7 Thu 17:25 EMH 225

Ferroelectricity in epitaxially strained thin films of a binary oxide — ●ZHUOTONG SUN, NIVES STRKALJ, SUNIL TAPER, ATIF JAN, CHUCK WITT, BARTOMEU MONSERRAT, GIULIANA DI MARTINO, and JUDITH DRISCOLL — University of Cambridge, Cambridge, UK

Interest in ferroelectric materials for processing, memory and sensing devices has been spurred by the discovery of nanoscale ferroelectricity in insulating binary oxides based on HfO_2 and ZrO_2 . However, stabilizing the ferroelectric phase and achieving good ferroelectric performance in these materials is challenging because several non-ferroelectric phases have similar formation energy to the ferroelectric phase. The search for other binary oxide ferroelectrics which can be achieved by industry-friendly processes is therefore still ongoing. Here, we report the stabilization of epitaxial films of a binary oxide at temperatures below 400°C using atmospheric pressure chemical vapor deposition. In these films, strain imposed by the substrate gives rise to the spontaneous polarization evidenced by piezo-response force microscopy. Exploring ferroelectricity in binary oxide films could provide a new platform for polarization-controlled memory applications and allow combining ferroelectric and photosensitive properties for photo-ferroelectrics applications.

KFM 29: Members' Assembly

Time: Thursday 18:10–19:00

Location: EMH 225

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

KFM 30: SrTiO_3 : A Versatile Material from Bulk Quantum Paraelectric to 2D Superconductor III (joint session TT/KFM/MA/O)

Strontium titanate (SrTiO_3) is a paradigmatic material that plays an important role in various fields of solid-state physics, surface science and catalysis: The pure bulk phase is a wide-band-gap semiconductor that upon cooling becomes a textbook quantum paraelectric. When slightly doped, SrTiO_3 turns into a Fermi-liquid-type metal that becomes superconducting at extremely low charge carrier density. SrTiO_3 -based surfaces and interfaces host un-conventional electronic states such as quasi-two-dimensional electron liquid, magnetism and superconductivity. Despite intensive studies over the past decades, SrTiO_3 continues to reveal surprising new phenomena that challenge the established views on this material. To this end achieving light-induced nonequilibrium states and the recent preparation of a 2D oxide based on SrTiO_3 opens new playgrounds for research. This Focus Session will present exciting developments in the study of electronic states that are based on the peculiar properties of SrTiO_3 .

Please note that this Focus Session comprises four parts: Posters are presented within the TT poster session TT58 (Wed 15:00-18:00, poster area E). Invited talks are compiled in the session TT62 (Thursday, 9:30 to 12:45, H0104), Contributed talks will be presented in sessions TT72 (Thursday 15:00-18:00, H0104) and TT83 (Fri 9:30-12:30, H0104).

Organizers: Rossitza Pentcheva, University of Duisburg-Essen, Marc Scheffler, University of Stuttgart

Time: Friday 9:30–12:30

Location: H 0104

KFM 30.1 Fri 9:30 H 0104

High-mobility two-dimensional electron gases based on strain engineered ferroelectric SrTiO_3 thin films — ●RUCHI TOMAR¹,

TATIANA KUZNETSOVA², SRIJANI MALLIK¹, LUIS M. VICENTE-ARCHE¹, FERNANDO GALLEGO¹, MAXIMILIEN CAZAYOUS³, ROMAN ENGEL-HERBERT^{2,4}, and MANUEL BIBES¹ — ¹Unité Mixte de

Physique, CNRS, Thales, Université Paris-Saclay, 91767 Palaiseau, France. — ²Pennsylvania State University, University Park, PA 16802, USA. — ³Laboratoire Matériaux et Phénomènes Quantiques (UMR 7162 CNRS), Université de Paris, 75205 Paris Cedex 13, France. — ⁴Paul Drude Institute for Solid State Electronics, Leibniz Institute within Forschungsverbund Berlin eV, Hausvogteiplatz 5-7, 10117, Berlin, Germany.

Two-dimensional electron gases (2DEGs) based on the quantum paraelectric SrTiO₃ display fascinating properties such as large electron mobilities, superconductivity, and efficient spin-charge interconversion owing to their Rashba spin-orbit coupling. Here, we use oxide molecular beam epitaxy to grow high-quality strain-engineered SrTiO₃ films that are ferroelectric up to 170 K. We then generate a 2DEG by sputtering a thin Al layer and demonstrate an increase in mobilities compared to earlier literature. Furthermore, through Raman spectroscopy and magneto-transport measurements, we show that the ferroelectric character is retained after 2DEG formation. These results thus qualify our samples as ferroelectric 2DEGs up to temperatures well above previous results based on Ca-SrTiO₃ substrates, opening the way towards ferroelectric 2DEGs operating at room temperature.

KFM 30.2 Fri 9:45 H 0104

Two-dimensional electron liquids at truly bulk-terminated SrTiO₃ — ●IGOR SOKOLOVIC^{1,2}, EDUARDO B. GUEDES³, THOMAS VAN WAAS⁴, SAMUEL PONCÉ^{4,5}, CRAIG M. POLLEY⁶, MICHAEL SCHMID², ULRIKE DIEBOLD², MILAN RADOVIĆ³, MARTIN SETVÍN^{2,7}, and J. HUGO DIL^{3,8} — ¹Institute of Microelectronics, TU Wien, Vienna, Austria — ²Institute of Applied Physics, TU Wien, Vienna, Austria — ³Photon Science Division, PSI, Villigen, Switzerland — ⁴ETSF, Institute of Condensed Matter and Nanosciences, UCLouvain, Louvain-la-Neuve, Belgium — ⁵WEL Research Institute, Wavre, Belgium — ⁶MAX IV laboratory, Lund University, Lund, Sweden — ⁷Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — ⁸Institut de Physique, ÉPFL, Lausanne, Switzerland

A truly bulk-terminated SrTiO₃(001) surface prepared by cleaving *in situ* was investigated with angle-resolved photoemission spectroscopy (ARPES) and noncontact atomic force microscopy (ncAFM). The (1×1) SrTiO₃(001) surfaces were achieved through our cleaving procedure that exploits the strain-induced ferroelectric transition in SrTiO₃, and provides both possible surface terminations, TiO₂ and SrO. Each hosts a specific two-dimensional electron liquid (2DEL): the first with split and the other with degenerate bands. The origin of the 2DELs and the band-splitting mechanisms are elucidated by correlating the observed reciprocal- and real-space electronic and atomic structure.

KFM 30.3 Fri 10:00 H 0104

Low-energy excitations at SrTiO₃(001) surfaces in absence and presence of a two-dimensional electron gas — ●HANNES HERRMANN, ANNE OELSCHLÄGER, and WOLF WIDDRA — Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

The low-energy excitations of SrTiO₃, a large-bandgap oxide perovskite, are dominated by phonons and phonon polaritons. At the surface they couple to dipole-active surface phonon polaritons that are bound to the SrTiO₃-vacuum interface. These excitations can be addressed by surface vibrational spectroscopy techniques as, e.g., high-resolution electron energy loss spectroscopy (HREELS).

Here we will present HREELS studies that identify all SrTiO₃(001) dipole-active excitations, including their specific line shapes and will discuss the electron-phonon coupling to a two-dimensional electron gas. The latter are prepared with variable charge-carrier concentrations either by annealing under ultrahigh-vacuum condition or by growth of an ultrathin layers of EuO on top. With formation of the 2DEGs, the discrete surface phonon polaritons couple to the electron-hole pair continuum as is witnessed by a substantial line broadening and asymmetric Fano-like line shapes. A quantitative description that accounts for all details of the line shape paves the way for an *in-situ* analysis of the 2DEG charge carrier dynamics.

KFM 30.4 Fri 10:15 H 0104

Confined ionic-electronic systems based on SrTiO₃ — ●FELIX GUNKEL, MARCUS WOHLGEMUTH, MORITZ L. WEBER, and REGINA DITTMANN — Peter Gruenberg Institute, Forschungszentrum Juelich SrTiO₃ reflects a a prototype ionic-electronic oxide, in which the physical properties are significantly affected by the ionic defect structure. [Gunkel et al., APL 2020] At the same time, spatial confinement of

electronic charge carries led to unexpected electronic and magnetic phenomena, including 2DEG formation, magnetoresistance and localization phenomena. Here we will discuss, how spatial confinement also affects the ion-dynamics and defect-equilibria of SrTiO₃, yielding interfacial defect structures and ion-dynamics that significantly differ from the bulk. [Rose et al., Adv. Mater. (2023); Weber et al., Nature Mater., to be published (Jan 2 2024)]. New opportunities to tailor such confined ionic-electronic systems arise from synthesis advances in generating transferable, free-standing SrTiO₃ sheets. These reflect ideally-confined nanosheets of SrTiO₃ and can serve as model system for ionic-electronic confinement phenomena as well as template for the synthesis of functional bilayer structures. We discuss the state-of-the-art of controlled bilayer synthesis and derive the required finite-size corrections in the thermodynamic description of the defect chemistry of SrTiO₃, indicating that the average reduction enthalpy of SrTiO₃ can be effectively reduced via confinement.

KFM 30.5 Fri 10:30 H 0104

Origin of spin-polarized 2DEG at the EuTiO₃(001) surface and LaAlO₃/EuTiO₃/SrTiO₃(001) interface — ●MANISH VERMA and ROSSITZA PENTCHEVA — Department of Physics, Universität Duisburg-Essen

Since the discovery of a two-dimensional electron gas (2DEG) at the interface between the LaAlO₃ and SrTiO₃ band insulators, studies on oxide surfaces and interfaces uncovered an intriguing and rich physics, such as possible magnetism in 2DEG. Using density functional theory with an on-site Coulomb repulsion term U , we find a spin-polarized 2DEG at the EuTiO₃(001) surface arising from the interplay of ferromagnetic (FM) order of Eu-4*f* magnetic moments and the localization of electrons released from oxygen divacancies at the surface Ti sites, in agreement with *in situ* high-resolution angle-resolved photoemission [1]. The 2DEG at the LaAlO₃/EuTiO₃/SrTiO₃(001) interface is formed due to the polar discontinuity. The spin-polarization is due to the FM exchange interaction between Eu 4*f* and Ti 3*d* states and steers the occupation of d_{xz}/d_{yz} orbitals [2].

- [1] R. Di Capua *et al.*, Phys. Rev. Research **3** (2021) L042038
[2] R. Di Capua *et al.*, npj Quantum Mater. **7** (2022) 41

KFM 30.6 Fri 10:45 H 0104

A multiferroic STO-based 2D-electron gas — ●MARCO SALLUZZO¹, YU CHEN¹, MARTANDO RATH¹, DANIELA STORNAIUOLO², JULIEN BREHIN³, MANUEL BIBES³, JULIEN VARIGNON⁴, and CINTHIA PIAMONTEZE⁵ — ¹Cnr-Spin Complesso Monte S. Angelo via Cinthia 80126, Napoli, Italy — ²Università "Federico II" di Napoli, Dipartimento di Fisica "Ettore Pancini", Complesso Monte S. Angelo via Cinthia 80126, Napoli, Italy — ³Unité Mixte de Physique, CNRS, Thales, Université Paris Saclay, Palaiseau, France — ⁴Crismat, CNRS, Ensicaen, Normandie Université, Caen, France — ⁵Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland.

The fabrication of artificial materials combining different functional properties is a powerful method to create novel quantum states. Here we demonstrate the realization of a 2D electron gas exhibiting a co-existence of ferroelectric and ferromagnetic order parameters, by heteroepitaxy.

The novel 2DEG is realized by inserting few unit cells of the antiferromagnetic insulator EuTiO₃ between a LaAlO₃ band insulating thin film (10 unit cells) and a Ca-doped SrTiO₃ single crystal.

By using Ti-L_{2,3} and Eu M_{4,5} edges x-ray linear dichroism and x-ray magnetic circular dichroism, we provide evidences of a switchable polarization, non-volatile tuning of Ti3*d* orbital splitting, and of a modulation of Eu-4*f* magnetic moment of the 2DEG by the FE-polarization[1]. The result is of interest for quantum spin-orbitronic applications.

- [1] J. Bréhin et al., Nat. Phys. **19** (2023) 823

KFM 30.7 Fri 11:00 H 0104

Magnetotransport properties of a spin polarized STO-based 2D electron system tuned by visible light — MARIA D'ANTUONO^{1,2}, YU CHEN², ROBERTA CARUSO^{1,2,3}, BENOIT JOUAULT⁴, MARCO SALLUZZO², and ●DANIELA STORNAIUOLO^{1,2} — ¹Department of Physics, University of Naples Federico II, Italy. — ²CNR-SPIN, Naples, Italy. — ³Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory, NY, USA. — ⁴Laboratoire Charles Coulomb, CNRS, Université de Montpellier, France

Two-dimensional electron systems (2DES) developing in STO-based heterostructures possess a wide range of properties which are largely

tunable thanks to the systems band structure and carrier density. In $\text{LaAlO}_3/\text{EuTiO}_3/\text{SrTiO}_3$ (LAO/ETO/STO) heterostructure, for instance, the charge carriers, above a critical value, start to fill Ti-3d bands with $d_{xz,yz}$ character, leading to the stabilization of a ferromagnetic order of Ti and Eu magnetic moments, and to a spin polarization of the 2DES. In this work we show that such mechanism can be achieved not only using electric field effect, but also using visible light irradiation. Furthermore, the analysis of the Anomalous Hall effect and of magnetocconductance curves demonstrate that visible light irradiation leads to enhanced stabilization of ferromagnetic correlations in the 2DES. Our results establish the combined use of visible light and gate voltage as a straightforward way to access unexplored regions of the LAO/ETO/STO 2DES phase diagram.

15 min. break

KFM 30.8 Fri 11:30 H 0104

All-electrical measurement of the spin-charge conversion effect in nanodevices based on SrTiO_3 two-dimensional electron gases — ●FERNANDO GALLEGO¹, FELIX TRIER^{1,2}, SRIJANI MALLIK¹, JULIEN BREHIN¹, SARA VAROTTO¹, LUIS MORENO¹, TANAY GOSAVY³, CHIA-CHING LIN³, JEAN-RENÉ COUDEVYLLE⁴, LUCÍA IGLESIAS¹, FÉLIX CASANOVA^{5,6}, IAN YOUNG³, LAURENT VILA⁷, JEAN-PHILIPPE ATTANÉ⁷, and MANUEL BIBES¹ — ¹Unité Mixte de Phys, CNRS-Thales, Univ. Paris-Saclay, 91767 Palaiseau, France. — ²Dept of Energy Conservation and Storage, Univ. of Denmark, 2800 Kgs. Lyngby, Denmark. — ³Comp. Res. Intel Corp., Hillsb., OR 97124, USA. — ⁴Centre de Nanosciences et de Nanotech., CNRS, Université Paris-Sud, Université Paris-Saclay, France. — ⁵CIC nanoGUNE BRTA, 20018 Donostia, Spain. — ⁶IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain. — ⁷Univ. Grenoble Alpes, CNRS, CEA, SPINTEC, Grenoble, France.

We report all-electrical spin-injection and spin-charge conversion experiments in nanoscale devices harnessing the inverse Edelstein effect of SrTiO_3 2DEGs. We have designed, patterned and fabricated nanodevices in which a spin current injected from a cobalt layer into a $\text{LaAlO}_3/\text{SrTiO}_3$ 2DEG is converted into a charge current. We optimized the spin-charge conversion signal by back-gating. We further disentangled the inverse Edelstein contribution from spurious effects. The combination of non-volatility and high energy efficiency of these devices could potentially lead to new technology paradigms for beyond-CMOS computing architectures.

KFM 30.9 Fri 11:45 H 0104

Effect of confinement and coulomb interactions on the electronic structure of the (111) $\text{LaAlO}_3/\text{SrTiO}_3$ interface — ●MATTIA TRAMA^{1,2,3}, VITTORIO CATAUDELLA^{4,5}, CARMINE ANTONIO PERRONI^{4,5}, FRANCESCO ROMEO¹, and ROBERTA CITRO^{1,2} — ¹Università degli Studi di Salerno, Fisciano, Italy — ²INFN Sezione di Napoli, Naples, Italy — ³Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany — ⁴Università degli Studi di Napoli Federico II, Naples, Italy — ⁵CNR-SPIN Napoli Unit, Naples, Italy

A tight-binding supercell approach is used for the calculation of the electronic structure of the (111) $\text{LaAlO}_3/\text{SrTiO}_3$ interface. The confinement potential at the interface is evaluated solving a discrete Poisson equation by means of an iterative method. In addition to the effect of the confinement, local Hubbard electron-electron terms are included at the mean-field level within a fully self-consistent procedure. The calculation carefully describes how the two dimensional electron gas arises from the quantum confinement of electrons near the interface

due to the band bending potential. The resulting electronic sub-bands and Fermi surfaces show full agreement with the electronic structure determined by angle-resolved photoelectron spectroscopy experiments. In particular, we analyse how the effect of local Hubbard interactions change the density distribution over the layers from the interface to the bulk. Interestingly, the two-dimensional electron gas at the interface is not depleted by local Hubbard interactions which indeed induce an enhancement of the electron density between the first layers and the bulk.

KFM 30.10 Fri 12:00 H 0104

Enhanced Non-linear Response by Manipulating the Dirac Point in the (111) $\text{LaTiO}_3/\text{SrTiO}_3$ Interface — ●YORAM DAGAN, GAL TUVIA, AMIR BURSHEIN, ITAI SILBER, AMNON AHARONY, ORA ENTIN-WOHLMAN, and MOSHE GOLDSTEIN — School of Physics and Astronomy, Tel Aviv University

Tunable spin-orbit interaction (SOI) is an important feature for future spin-based devices. In the presence of a magnetic field, SOI induces an asymmetry in the energy bands, which can produce non-linear transport effects ($V \sim I^2$). Here, we focus on such effects to study the role of SOI in the (111) $\text{LaTiO}_3/\text{SrTiO}_3$ interface. This system is a convenient platform for understanding the role of SOI since it exhibits a single-band Hall-response through the entire gate-voltage range studied. We report a pronounced rise in the non-linear longitudinal resistance at a critical in-plane field H_{cr} . This rise disappears when a small out-of-plane field component is present. We explain these results by considering the location of the Dirac point formed at the crossing of the spin-split energy bands. An in-plane magnetic field pushes this point outside of the Fermi contour, and consequently changes the symmetry of the Fermi contours and intensifies the non-linear transport. An out-of-plane magnetic field opens a gap at the Dirac point, thereby significantly diminishing the non-linear effects. We propose that magnetoresistance effects previously reported in SrTiO_3 -based interfaces could be comprehended within our suggested scenario.

KFM 30.11 Fri 12:15 H 0104

Tunable 2D Electron- and 2D Hole States Observed at Fe/SrTiO_3 Interfaces — ●PIA MARIA DÜRING¹, PAUL ROSENBERGER^{1,2}, LUTZ BAUMGARTEN³, FATIMA ALARAB⁴, FRANK LECHERMANN⁵, VLADIMIR N. STROCOV⁴, and MARTINA MÜLLER¹ — ¹FB Physik, Universität Konstanz, 78457 Konstanz — ²TU Dortmund, 44221 Dortmund — ³FZ Jülich, PGI-6, 52425 Jülich — ⁴PSI, SLS, CH-5232 Villigen — ⁵TP III, RU Bochum, 44780 Bochum

Oxide electronics provide the key concepts and materials for enhancing silicon-based semiconductor technologies with novel functionalities. However, a crucial property of semiconductor devices remains undisclosed in their oxide counterparts: the ability to set or even switch between negatively (n) charged electrons or positively (p) charged holes. Using resonant angle-resolved photoelectron spectroscopy, we provide direct evidence for individually emerging n- or p-type 2D band dispersions in SrTiO_3 (STO)-based heterostructures [1]. The key to setting the carrier character is the oxidation state of a Fe-based interface layer: For Fe and FeO, hole bands emerge in the empty band gap region of STO, while for Fe_3O_4 overlayers, an 2D electron system (2DES) is formed. Unexpected oxygen vacancy characteristics arise for the hole-type interfaces, which as of yet had been exclusively assigned to the emergence of 2DESs. In general, this study unveils the potential to seamlessly alter the conductivity type at STO interfaces by manipulating the oxidation state of a redox overlayer.

[1] P. M. Düring et al., Adv. Mater. (accepted)

KFM 31: Perovskite and Photovoltaics III (joint session HL/KFM)

Time: Friday 9:30–13:00

Location: EW 203

KFM 31.1 Fri 9:30 EW 203

Data-efficient machine learning for perovskite alloys — ●JARNO LAAKSO, HENRIETTA HOMM, and PATRICK RINKE — Department of Applied Physics, Aalto University, Espoo, Finland

Perovskite solar cells are highly efficient, but their commercialization has been hindered by toxicity and lack of stability. Compositional engineering can mitigate these problems [1], but the complexity of the perovskite materials space makes the search for an optimal solar cell material challenging. We previously demonstrated how machine learning (ML) can accelerate property predictions for the perovskite alloy CsPb(Cl/Br)₃ [2]. However, the extensive density functional theory (DFT) calculations required for model training prevent applications to more complex materials. Here, we facilitate model training with a data-efficient scheme, validated on CsPb(Cl/Br)₃ data and extended to the ternary alloy CsSn(Cl/Br/I)₃.

Our approach employs clustering to build a compact but diverse initial data set of atomic structures. We then apply a two-stage active learning approach to first improve the robustness of the ML-based structure relaxations and then fine-tune the accuracy near equilibrium structures. Tests for CsPb(Cl/Br)₃ reveal that our scheme reduces the number of required DFT calculations during model training by up to 50%. The fitted model for CsSn(Cl/Br/I)₃ is robust, with all ML-based structure relaxations converging in our tests. The relaxations are also highly accurate, having an average error of 0.5 meV/atom.

[1] *iScience* **23**, 101359 (2020). [2] *Phys. Rev. Mater.* **6**, 113801 (2022).

KFM 31.2 Fri 9:45 EW 203

Passivation and Charge Carrier Selectivity Optimization for Narrow Bandgap Perovskite Solar Cells — ●ATHANASIA VICHA, GEORGIOS LOUKERIS, MARKUS KOHLSTÄDT, ULI WÜRFEL, and ANDREAS BETT — Fraunhofer ISE, Freiburg im Breisgau, Germany

This study aims to enhance narrow bandgap perovskite solar cells for all-perovskite tandem applications. Initial efforts focused on bulk passivation of the perovskite layer. The combination of two additives, Methylammonium chloride and Lead thiocyanate, increased Voc up to 0.82V and Jsc to 31mA/cm². Glycine hydrochloride improved result reproducibility leading to a favourable FF, and increasing Thiourea concentration simultaneously raised Jsc. Further optimizations and the effects of additive combinations will be presented. Concurrently, this study investigates the selectivity of the hole transport layer/perovskite interface. Thus, we examined substituting an aqueous PEDOT:PSS formulation for a solvent-based one to address water-induced degradations in the underlying perovskite layer in all-perovskite tandem devices. Preliminary assessments on single-junction narrow bandgap solar cells using solvent-based PEDOT yielded a notable 16% Voc increase compared to aqueous PEDOT:PSS. However, this rise in Voc results in a significant 23% Jsc reduction. In response, we explored strategies to boost Jsc by varying the PEDOT thickness. In thinner layers, Jsc exceeds the one of PEDOT:PSS-based cells, aligning with simulations. This research outcome provides valuable insights into optimizing passivation and enhancing selectivity in narrow bandgap perovskite solar cells.

KFM 31.3 Fri 10:00 EW 203

Understanding and mitigating atomic oxygen-induced degradation of Perovskite solar cells for near-earth space applications — ●BIRUK SEID — Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam-Golm, Germany

Atomic oxygen (AtOx) in low-Earth orbit is known to etch, corrode, and form metal oxide on the metal contact with PSC devices. To mitigate this issue, we report the applicability of thermally evaporated 0.7 μ m silicon oxide (SiOx) encapsulation as an AtOx barrier for triple-junction PSC. Moreover, the AtOx-induced degradation mechanism of phenethylammonium iodide (PEAI)-passivated and non-passivated devices are discussed and analyzed. We found that after a total exposure duration of 120 minutes, the SiOx-encapsulated cells maintained over 97% of their initial power conversion efficiency (PCE), regardless of the device type (passivated or non-passivated). In contrast, in the case of unencapsulated devices, PCEs for non-passivated and PEAI-passivated devices the PCE declined to a maximum value of 43% and 62%, respectively. In non-passivated and unencapsulated devices, AtOx has

no impact on the short-circuit current density (JSC) but degrades the fill factor (FF) and open circuit voltage (VOC). In PEAI-passivated devices, the JSC additionally degrades by almost 35%. Perovskite was not the origin of PCE degradation. Instead, inefficient charge extraction and mobile ions, due to a swiftly degrading PEAI interlayer are the primary causes of AtOx-induced device performance degradation in passivated devices, whereas a large ionic FF loss limits non-passivated devices.

KFM 31.4 Fri 10:15 EW 203

Understanding and mitigating atomic oxygen-induced degradation of Perovskite solar cells for near-earth space applications — ●BIRUK SEID — Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam-Golm, Germany

Atomic oxygen (AtOx) in low-Earth orbit is known to etch, corrode, and form metal oxide on the metal contact with PSC devices. To mitigate this issue, we report the applicability of thermally evaporated 0.7 μ m silicon oxide (SiOx) encapsulation as an AtOx barrier for triple-junction PSC. Moreover, the AtOx-induced degradation mechanism of phenethylammonium iodide (PEAI)-passivated and non-passivated devices are discussed and analyzed. We found that after a total exposure duration of 120 minutes, the SiOx-encapsulated cells maintained over 97% of their initial power conversion efficiency (PCE), regardless of the device type (passivated or non-passivated). In contrast, in the case of unencapsulated devices, PCEs for non-passivated and PEAI-passivated devices the PCE declined to a maximum value of 43% and 62%, respectively. In non-passivated and unencapsulated devices, AtOx has no impact on the short-circuit current density (JSC) but degrades the fill factor (FF) and open circuit voltage (VOC). In PEAI-passivated devices, the JSC additionally degrades by almost 35%. Perovskite was not the origin of PCE degradation. Instead, inefficient charge extraction and mobile ions, due to a swiftly degrading PEAI interlayer are the primary causes of AtOx-induced device performance degradation in passivated devices, whereas a large ionic FF loss limits non-passivated devices with no change in transit time.

KFM 31.5 Fri 10:30 EW 203

Passivating Inorganic Interlayers at the Perovskite/C₆₀ Interface in Monolithic Perovskite Silicon Tandem Solar Cells — ●JOHANNA MODES^{1,2}, PATRICIA S.C. SCHULZE¹, CARL ERIC HARTWIG⁴, STEFAN LANGE⁴, ARMIN RICHTER¹, JULIANE BÖRCHERT^{1,3}, and ANDREAS BETT^{1,2} — ¹Fraunhofer ISE — ²Albert-Ludwigs-Universität — ³NATECH — ⁴Fraunhofer CSP

Metal halide perovskites emerged in recent years as promising absorber materials for solar cells that can combine high power conversion efficiency with low production costs. Significant non-radiative charge carrier recombination occurs at the perovskite interface with the electron contact C₆₀, which prevents the full exploitation of the solar cell's potential. C₆₀ induces states within the band gap, lowers the quasi-Fermi level splitting, and limits the open circuit voltage (V_{OC}). Ultra-thin passivation layers at the perovskite/C₆₀ interface are used to reduce those losses. To enable industrial upscaling, our focus lies on inorganic passivation layers deposited via atomic layer deposition. An AlO_x interlayer was developed that increases the iV_{OC} up to 50 mV and improves the V_{OC} for single-junction and tandem devices. To better understand the effects involved in this passivation, photoluminescence quantum yield (PLQY), angle-resolved X-ray photoelectron spectroscopy (ARXPS) and surface photovoltage (SPV) measurements were carried out. State-of-the-art perovskite solar cells using a LiF_x passivation layer suffer from device degradation over time. Initial stability testing indicates that a thin AlO_x passivation layer can improve device stability and can serve as an alternative to LiF_x.

KFM 31.6 Fri 10:45 EW 203

Analyzing defect thermodynamics of (Ag,Cu)GaSe₂ solar cell absorbers using a machine-learning interatomic potential — ●VASILIOS KARANIKOLAS, DELWIN PERERA, and KARSTEN ALBE — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

One of the most widely used absorber materials for thin-film solar cells is Cu(In,Ga)Se₂ (CIGS). Currently, CIGS yields the highest efficiencies within this technology and the addition of Ag has been found to

further improve the efficiency. The performance of the CIGS absorber, however, is also governed by defects, especially by the type and density of grain boundaries (GBs) [1].

In this work, we investigate the thermodynamic properties of GBs for $(\text{Ag}_{1-x}\text{Cu}_x)\text{GaSe}_2$ structures based on a machine learning interatomic potential (MLIP)[2]. The training dataset for the regression machine learning model is created by density functional theory (DFT) calculations. The MLIP allows us to perform molecular dynamics simulations for structurally complex GBs that are inaccessible by conventional electronic structure methods. In particular, we investigate the thermodynamic properties of symmetric GBs beyond $\Sigma 3$ and include an analysis of silver segregation at the interfaces.

[1] D. Abou-Ras *et al.*, *Acta Materialia* **118**, 244-252 (2016).

[2] Y. Lysogorskiy *et al.*, *npj Computational Materials* **7**, 1 (2021).

15 min. break

KFM 31.7 Fri 11:15 EW 203

Halide segregation and ionic motion in lead-halide perovskites — ●FRANCISCO PEÑA-CAMARGO, FELIX LANG, and MARTIN STOLTERFOHT — Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany

Halide segregation is a photoinduced phenomenon observed in perovskites with multiple halides at the X site of the ABX_3 lattice. The evidence shows that the photoluminescence spectrum of the mixed phase red-shifts and increases its intensity in a timescale of minutes. On the other hand, it has been proven that mobile ions are present in cells in densities around 10^{16} cm^{-3} , which is sufficient to screen the internal electric field, generating, among other effects, the hysteresis in the forward and reverse JV scans. The scan-speed dependence of hysteresis suggests that mobile ions have an effect on the cell performance mostly at a determined condition when the voltage sweep matches the ionic timescales. Here, by measuring the JV characteristic at different speeds with a novel technique called fast hysteresis (FH) from 10-2 to 10^4 V s^{-1} , we quantify the ionic diffusion coefficient and conclude that the ionic motion happens in the seconds to minutes timescales. Moreover, using bias-assisted charge extraction (BACE) we are able to quantify the ionic volumetric density and confirm the ionic transient timescales. Based on that experimental evidence, it is plausible to link the ionic motion to halide segregation, particularly when it comes to the timescales which appear to match very well. This is also supported by the correlation of the ionic losses with the increasing Br/I ratio in triple-cation lead-based perovskite solar cells.

KFM 31.8 Fri 11:30 EW 203

Halide segregation and ionic motion in lead-halide perovskites — ●FRANCISCO PEÑA-CAMARGO, FELIX LANG, and MARTIN STOLTERFOHT — Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany

Halide segregation is a photoinduced phenomenon observed in perovskites with multiple halides at the X site of the ABX_3 lattice. The evidence shows that the photoluminescence spectrum of the mixed phase red-shifts and increases its intensity in a timescale of minutes. On the other hand, it has been proven that mobile ions are present in cells in densities around 10^{16} cm^{-3} , which is sufficient to screen the internal electric field, generating, among other effects, the hysteresis in the forward and reverse JV scans. The scan-speed dependence of hysteresis suggests that mobile ions have an effect on the cell performance mostly at a determined condition when the voltage sweep matches the ionic timescales. Here, by measuring the JV characteristic at different speeds with a novel technique called fast hysteresis (FH) from 10^{-2} to 10^4 V s^{-1} , we quantify the ionic diffusion coefficient and conclude that the ionic motion happens in the seconds to minutes timescales. Moreover, using bias-assisted charge extraction (BACE) we are able to quantify the ionic volumetric density and confirm the ionic transient timescales. Based on that experimental evidence, it is plausible to link the ionic motion to halide segregation, particularly when it comes to the timescales which appear to match very well. This is also supported by the correlation of the ionic losses with the increasing Br/I ratio in triple-cation lead-based perovskite solar cells.

KFM 31.9 Fri 11:45 EW 203

Assessing machine-learning force fields for defect calculations in halide perovskites — ●FREDERICO DELGADO¹, FREDERICO SIMÕES¹, LEEOR KRONIK², and DAVID A. EGGER¹ — ¹Physics Department, TUM School of Natural Sciences, Technical University of

Munich, Germany — ²Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

The excellent optoelectronic properties exhibited by bulk halide perovskites (HaPs) are important for their photovoltaic performance and have been extensively investigated. Despite this, the ubiquity of both point defects and extended ones like surfaces requires further careful examination of their impact on such properties. Precise investigations of dynamic effects in this context via ab-initio molecular dynamics imply large computational costs, especially when the need for accurate exchange correlation functionals arises. Therefore, in order to sample sufficiently long time scales and sufficiently large supercells, usage of on-the-fly machine learning (ML) forces fields appears to be particularly appealing. In this study, we investigate such defects and their dynamical properties in CsPbBr_3 using ML force fields. Our results can aid rationalizing the correlations between local structural dynamics and the observed optoelectronic behavior.

KFM 31.10 Fri 12:00 EW 203

Nanospectroscopy and ultrafast out-of-plane carrier dynamics in metal halide perovskites — ●MARTIN ZIZLSPERGER¹, SVENJA NERRETER¹, QIMU YUAN², KILIAN B. LOHMANN², FABIAN SANDNER¹, FELIX SCHIEGL¹, CHRISTIAN MEINEKE¹, YAROSLAV GERASIMENKO¹, LAURA M. HERZ², THOMAS SIDAY^{1,2}, MARKUS A. HUBER¹, MICHAEL B. JOHNSTON², and RUPERT HUBER¹ — ¹Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, 93040 Regensburg, Germany — ²Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, UK

The high efficiencies of metal halide perovskite solar cells have been associated with effective charge-carrier diffusion. Still, the characteristic nanograins and crystallographic disorder entailed in perovskite films hindered unraveling details of the vertical transport, calling for simultaneous experimental access to chemical composition, structural phase and ultrafast out-of-plane dynamics. Here, we promote depth-sensitive terahertz near-field nanospectroscopy to extreme subcycle time scales. In $\text{FA}_{0.83}\text{Cs}_{0.17}\text{Pb}(\text{I}_{1-x}\text{Cl}_x)_3$ films, we discern domains of the α -phase from δ -phase and PbI_2 nano-islands. Based on deep-subcycle time shifts of the scattered terahertz waveform after photoexcitation, we access the single-grain vertical diffusion. Despite topographic irregularities, diffusion is surprisingly homogeneous on sub-micrometer length scales, only varying between mesoscopic regions. Our approach linking nano-morphology with carrier dynamics may benefit all future optoelectronic devices using nanocrystalline materials.

KFM 31.11 Fri 12:15 EW 203

Comparison of the application of the TRMC technique for the characterization of crystalline silicon and perovskite solar cell absorber material and efficient surface passivation — ARPANA SINGH¹, BIRUK ALEBACHEW SEID², FELIX LANG², MARINUS KUNST³, and ●HEINZ-CHRISTOPH NEITZERT¹ — ¹DIIN, Salerno University, 84084 Fisciano, Italy — ²ROSI Freigeist Group, Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam-Golm, Germany — ³Helmholtz-Zentrum Berlin, 14109 Berlin, Germany

Time Resolved Microwave Conductivity (TRMC) as a contactless technique for the characterization of the charge carrier kinetics in photoconductive materials has been recently successfully applied for the characterization of perovskite thin films [1]. Charge carrier lifetimes depend strongly on excitation conditions, such as light intensity and wavelength. It is shown, how TRMC-measurements performed with excitation at low laser intensities and different wavelengths can give valuable information on the quality of the surface passivation of triple-cation, triple-anion Perovskite films by PEAI layers. A good correlation of the observed lifetime increase in the absorber films and the performance of the completed solar cells has been found. The results are compared to the characterization under identical measurement conditions of crystalline silicon wafers. Also in this case the influence of different passivation schemes on the charge carrier lifetime and on solar cell properties have been compared. [1] A. Marchioro, J. Teuscher, D. Friedrich, M. Kunst, R. van de Krol, T. Moehl, M. Grätzel and J. E. Moser, *Nature Photonics* **8**, 250-256 (2014).

KFM 31.12 Fri 12:30 EW 203

The detrimental role of PbI_2 at the interface between absorber and electron-transport layer in halide-perovskite solar cells — ●DAN RALF WARGULSKI, KE XU, STEVE ALBRECHT, and DANIEL ABOU-RAS — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

There is an ongoing discussion in the halide-perovskite community about the beneficial or harmful effects of PbI₂ in halide-perovskite solar cells (HPSCs). One school praises PbI₂ for its passivating and stabilizing properties, while the other aims at getting rid of excess PbI₂, because it leads to decreased cell efficiencies and degraded long-term stability. How can such a contradiction exist? The effect of PbI₂ depends on its location in the solar-cell stack and on the specific HPSC architecture used. When applied as top cells in tandem devices, HPSCs do not exhibit a n-i-p structure but an p-i-n structure, often called *inverted* HPSC structure. As a result, the top surface where PbI₂ forms is not situated at the interface between the absorber and the hole-transport layer anymore, but at the interface to the electron-transport layer. This modifies considerably the effects of PbI₂ on the device performance. The present work discusses the formation of PbI₂ in HPSCs with slot-die-coated, triple-halide perovskite absorbers, which was investigated by means of correlative electron microscopy. Studying the changing PbI₂ coverage of the halide-perovskite absorbers with varying annealing temperature, a model will be presented that explains the effects of the PbI₂ precipitates on the open-circuit voltages and the fill factors of the HPSCs with inverted cell architecture.

KFM 31.13 Fri 12:45 EW 203

Stability Enhancement of Mixed-Cation Hybrid Halide Perovskites combining DFT-1/2 with SOC — ●MOHAMMAD

KFM 32: Crystal Structure Defects / Real Structure / Microstructure II

Chair: Theo Scherer (KIT Karlsruhe)

Time: Friday 9:30–11:40

Location: E 124

KFM 32.1 Fri 9:30 E 124

Novel class of rubrene single crystals with enhanced stability — ●MOHA NAEIMI, KATHARINA ENGSTER, REGINA LANGE, TIM VÖLZER, STEFAN LOCHBRUNNER, INGO BARKE, and SYLVIA SPELLER — University of Rostock, Institute of physics, Rostock, Germany

Rubrene is an organic semiconductor recognized for its favorable properties, including high charge carrier mobility and excellent thermal stability. Its conjugated structure makes it a promising material for use in organic electronic devices. The precise control of rubrene crystallization, evolving from an amorphous to the stable orthorhombic phases enables comprehensive study of optical and electronic properties [1], as well as the investigation of exciton distribution and dynamics [2]. Through precise control of amorphous rubrene deposition on the substrate, high-rate heating and enhanced partial pressure [3], we introduce a novel class of rubrene single crystals in orthorhombic phase with different crystal orientations. Distinguished by ultra-flat and smooth surfaces with an hourglass shaped signature exhibiting four different zones of two types (i.e., diamond and triangle shaped), we characterize their optical properties and investigate their surface potential.

[1] Kathryn A. McGarry et al., Chem.Mater.2013, 25, 2254-2263

[2] Pavel Irkhin and Ivan Biaggio, Phys. Rev. Lett. 2011, 107, 017402

[3] Xin Ye et al. Chem. Mater. 2018, 30, 2, 412-420

KFM 32.2 Fri 9:50 E 124

Hidden structural transition upon dehydration of Prussian Blue analogues (PBAs) — ●YEVHENIIA KHOLINA and ARKADIY SIMONOV — ETH Zurich, Switzerland, Department of Materials, Laboratory for Disordered Materials

Prussian blue analogues (PBAs) are a diverse family of transition metal cyanide materials with chemical formula $M[M'(CN)_6]_{1-x}\square_y \cdot nH_2O$, which we abbreviate here as $M[M']$ (M and M' =transition metal ions, \square =vacancy). These materials are known for their highly connected porous network, enabled by structural vacancies of $M'(CN)_6$ with sufficiently large channels to transport or store small molecules and ions. Currently, these systems are actively investigated for application as hydrogen storage media, humidity sensors, and alkali ion sieves. One step that is often overlooked in the research is drying. PBAs are typically grown from water solutions and water has to be removed by heating the sample either in a vacuum or in a dry atmosphere. Since drying doesn't change the average structure, it is generally assumed that this step doesn't alter the porous network of PBAs. We demonstrate that the dehydration step in fact causes a hidden structural transition that

MOADDELI¹, MANSOUR KANANI^{1,2}, and ANNA GRUNEBOHM³ — ¹Department of Materials Science and Engineering, School of Engineering, Shiraz University, Shiraz, Iran — ²Solar Energy Technology Development Center, Shiraz University, Shiraz, Iran — ³Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany

Tunable band gaps, easy processing, composition engineering, and enhanced performance make mixed-cation perovskites promising as light absorbers in third generation solar cells. However, stability challenges remain in understanding the underlying mechanisms. This study emphasizes the importance of accurately predicting structural and electronic properties. While density functional theory (DFT) is the preferred method for addressing these, standard exchange-correlation functionals often fail to reproduce the band structure. Therefore, we propose the DFT-1/2 method, which is applied to single- and mixed-cation systems. We explore how the choice of the A-cation modifies the Pb-I scaffold. We find that the addition of Cs and MA to FAPbI₃ reduces the dispersion in the scaffold, which has a high potential to reduce the migration of iodide and thus improves the structural stability. Additionally, we compare Born effective charges with and without the SOC effect and the DFT-1/2 approach [1]. [1] M. Moaddeli et al, Phys. Chem. Chem. Phys. 25, 25511 (2023).

involves irreversible rearrangements of vacancies. Such rearrangements modify the pore-network characteristic, like the fraction of accessible volume and conductance of matter through the channels. We collect diffuse scattering from Mn[Co] single crystals and use 3D- Δ PDF analysis to characterize their local structure and monitor structural changes upon water removal.

KFM 32.3 Fri 10:10 E 124

EXAFS study of exfoliated MoS₂ nanoflakes in ALBA Synchrotron — ●NAJME TAGHAVI — Independent Researcher

Using an ultrasonic probe in a water-ethanol solution, MoS₂ 2D nanoflakes were prepared with varying ultrasonic powers and sonication times. The resulting samples were analyzed using EXAFS spectroscopy, which revealed that the oxidation-state of the Mo atom remained unchanged. However, increasing the power of the ultrasonic probe and sonication time led to changes in the Mo-S1 and Mo-Mo bond distances, with a decrease in the Mo-S2 bond distance. Additionally, longer sonication times resulted in a higher Debye-waller parameter. While increasing the sonication probe power significantly reduced the amplitude reduction parameter (S02), a slight increase was observed with longer sonication times.

10 min. break

KFM 32.4 Fri 10:40 E 124

Finding models of disorder using Inverse Ising methods — ●ARKADIY SIMONOV — ETH Zürich, Zürich, Switzerland

Many functional materials, such as thermoelectrics or superconductors, exhibit disorder. Consequently, their properties depend crucially not only on their average structure but also on the details of their real structure. Experimentally, the real structure can be probed using single-crystal diffuse scattering; however, the analysis of this data currently relies on modeling methods like Monte Carlo and their subsequent refinement, which is very time-consuming. In this talk, we will present faster methods for constructing trial models consistent with experimental diffuse scattering based on the family of approximate solutions to the Inverse Ising problem, including susceptibility propagation and density consistency techniques. The methods naturally work well for structures with a high amount of disorder. Interestingly, they also perform well for certain cases with strong disorder correlations

KFM 32.5 Fri 11:00 E 124

Amplitude phase-field quasicrystal — ●MARCELLO DE DONNO¹, MARCO SALVALAGLIO^{1,2}, LUIZA ANGHELUTA³, and KEN ELDER⁴ —

¹Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — ²Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany — ³Njord Centre, Department of Physics, University of Oslo, 0371 Oslo, Norway — ⁴Department of Physics, Oakland University, Rochester, Michigan 48309, USA

Quasicrystals challenge classical crystallography with their atypical atomic arrangements, characterized by a lack of periodicity while retaining long-range order. They represent a unique state of matter, lying between crystalline and amorphous structures. Since their discovery in 1982, quasicrystals have been shown to be capable of improving the mechanical properties of alloys, offering heightened strength, hardness, and resistance to wear. Additionally, their propensity for low friction makes them excellent candidates for coatings aimed at diminishing wear in moving parts.

The study of quasicrystals requires understanding the interaction between the exotic microscopic arrangement and the macroscopic properties of the material. We propose a novel mesoscale theory for quasicrystals, taking advantage of an extension we designed to the amplitude phase-field crystal model. We characterize the topological defects forming in the structure, and we discuss their kinematics. Finally, we derive self-consistent laws for linear elasticity in the quasicrystal.

KFM 32.6 Fri 11:20 E 124

Quantum sensing for materials testing — ●SIMON PHILIPP¹,

NIKLAS MATHES², MARVIN FEUERHELM¹, ALI RIZA DURMAZ¹, XAVIER VIDAL³, RUDOLF SCHÄFER⁴, THOMAS STRAUB¹, and CHRISTIAN ELSÄSSER¹ — ¹Fraunhofer IWM, Wöhlerstrasse 11, 79108 Freiburg — ²Fraunhofer IAF, Tullastraße 72, 79108 Freiburg — ³Tecnalia, Parque Científico y Tecnológico de Gipuzkoa Mikeletegi Pasealekua, 2, E-20009 Donostia-San Sebastián (Gipuzkoa) — ⁴Leibniz-Institut für Festkörper- und Werkstoffforschung, Helmholtzstraße 20, 01069 Dresden

Micromagnetic materials testing has been utilized for the measurement of a variety of relevant properties for material sciences and engineering, some of which being residual stress, micro-structure, or hardness. Recently, it has been shown [1] that the inverse magneto-strictive, or Villari effect [2] can potentially be exploited to retrieve a magnetic signature of fatigue and early-stage crack initiation in micro-mechanical specimens.

In this work, we demonstrate magneto-mechanical testing of ferromagnetic materials as a novel use case for quantum magnetometry at the interface of basic research and industry. As an example, we show recent data on magneto-mechanical testing of Fe and FeSi microspecimen under ambient conditions, using a combination of different quantum sensors.

[1] P. A. Koss et al., Applied Sciences 12, 1329 (2022). [2] G. Riesgo et al., Materials (Basel, Switzerland) 13 (2020). [3] S. C. Scholten et al., Journal of Applied Physics 130, 150902 (2021).

KFM 33: Focus Session: (Multi-)Ferroic States V

The focus session is dedicated to (multi)ferroic states at interfaces and in heterostructures. The design of (emergent) properties at interfaces, modelling methods and advanced characterization tools will be of interest. Typical examples may include electrostatic and strain boundary conditions at interfaces, domains and domain walls in (multi)ferroics and applications in nano-electronic device.

Chair: Nives Strkalj (Institute of Physics, Zagreb)

Time: Friday 9:30–12:25

Location: EMH 225

KFM 33.1 Fri 9:30 EMH 225

Landau free energy of PbTiO₃ from atomistic simulations — ●MAURO PULZONE^{1,2}, NATALYA S. FEDOROVA¹, HUGO ARAMBERRI¹, and JORGE ÑIGUEZ-GONZÁLEZ^{1,2} — ¹Luxembourg Institute of Science and Technology, Esch-sur-Alzette, Luxembourg — ²University of Luxembourg, Esch-sur-Alzette, Luxembourg

In this study we introduce a methodology to identify and compute, from atomistic simulations, the simplest Landau potential that accurately describes the static properties of PbTiO₃ as a function of temperature. The free energy of the system is expanded around the reference cubic phase in powers of the polarization. We consider all possible combinations of symmetry-allowed terms from 2nd up to 10th order. We fit all these models using the approach of Ref. [Phys. Rev. B 63, 144103 (2001)], taking as input the data obtained from Monte Carlo simulations based on the atomistic second-principles model for PbTiO₃ proposed by Wojdel et al. [Phys.: Condens. Matter 25, 305401 (2013)].

We find that a 6th-order expansion is sufficient to capture the system's behavior, including the first-order character of the transition. Moreover, as the temperature increases (hundreds of Kelvins above the phase transition) a 4th-order model is enough to reproduce the atomistic data accurately.

Presently we are extending this work to explicitly consider the strain as an order parameter, as the elastic deformation of the cell is known to play an essential role in the first-order character of the phase transition of PbTiO₃ [Phys. Rev. B 55, 6161 (1997)].

KFM 33.2 Fri 9:50 EMH 225

Reversible thermal conductivity switching in barium titanate ceramics — ●LUCILE FÉGER, NASSIMA RADOUANE, FABIEN GIOVANNELLI, JULIEN BUSTILLO, NATHALIE POIROT, GUILLAUME F. NATAF, and ISABELLE MONOT-LAFFEZ — GREMAN UMR7347, CNRS, University of Tours, INSA Centre Val de Loire, 37000 Tours, France

Control of charge flows led to the invention of the transistor and all related electronic devices of our daily life. In contrast, manipulating heat flows is still a challenge and this trend is driven by the constant pursuit of novel properties, efficiency, and functionality in technological applications. Yet, heat management is essential in electronic circuits and may lead to the development of a new paradigm of logic (phononics)

[1]. Ferroelectric materials are a promising class of materials to design thermal switches, due to the strong dependence of their properties to an applied electric field. Here we investigate the evolution under an electric field of the thermal conductivity of barium titanate. For this purpose, we adapted a laser flash system to be able to apply a voltage in-situ. We then measured at different temperatures the thermal conductivity of ceramics of barium titanate with different grain sizes: 0.5, 5, 50 and 100 micrometers. We show reversible changes in thermal conductivity under the application of an electric field in-situ, which are compared to measurements where the electric field is applied ex-situ [2]. We discuss our results based on changes in polarization and domain structures induced by the electric field. [1] Li, N. et al. Reviews of Modern Physics, 84 (2012). [2] Lin, Y. et al. ACS Applied Materials & Interfaces, 14 (2022).

KFM 33.3 Fri 10:10 EMH 225

An extended phase-field-drift-diffusion model for oxygen vacancy migration in single-crystal barium titanate — ●XUEJIAN WANG and FRANK WENDLER — Institute of Materials Simulation (WW8), Friedrich-Alexander-Universität Erlangen-Nürnberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany

Barium titanate (BTO) and its solid solutions are attractive materials for replacing lead-based piezoelectrics, exhibiting a high density of point defects. Here, we present an extended phase-field model that includes the migration of oxygen vacancies (Vo), a crucial type of point defect in ferroelectric materials, within single-crystal BTO. The model bases on the Landau-Ginzburg-Devonshire theory, considers a continuous concentration of Vo (Cv) and incorporates the drift-diffusion equation for its migration. The Finite Element Method is used to simulate domain formation with varying Cv values, where a range of phenomena is discovered. Initially, the existence of Vo induces a modification in the orientation of polarization in comparison to the defect-free crystal. The level of Cv significantly affects the evolution and structure of domain/domain walls (DWs). Systems possessing a larger Cv will generate domains of higher density and a greater variety of DWs in comparison to systems with lesser Cv. The migration of Vo occurs on both sides of the DWs and along the polarization orientation. Moreover, defect clustering is observed at the junctions of domain walls at

higher C_V levels. The influence of Vo concentrations on electromechanical loading are shown, and results are compared to experimental data from literature.

KFM 33.4 Fri 10:30 EMH 225

Parametrization of a ferroelectric phase-field model from MD including nucleation data — ●FRANK WENDLER¹, DILSHOD DURDIEV¹, MICHAEL ZAISER¹, TAKAHIRO TSUZUKI², HIKARU AZUMA², SHUJI OGATA², RYO KOBAYASHI², and MASAYUKI URANAGASE² — ¹Institute of Materials Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany. — ²Graduate School of Engineering, Nagoya Institute of Technology, Nagoya 466-9555, Japan

Phase-field models based on the Landau-Ginzburg-Devonshire theory extend the time and length scales in comparison to molecular dynamics (MD) simulations, and enable a bottom-up approach to generate a complete energy landscape purely from atomistic information. Crucial material parameters such as elastic and piezoelectric properties, kinetic coefficients, as well as domain wall characteristics are extracted from MD data to adjust anisotropic gradient energy. To bridge the gap between the atomistic and continuum model, a proposed parametrization workflow involves determining all coefficients for the 6th order Landau polynomial from polarization reversal characteristics. Polarization switching in ferroelectric barium titanate (BTO) involves localized nucleation and subsequent domain growth, driven by an applied electric field. MD simulation data proves the role of thermal activation in domain nucleation, resulting in a notable scatter in coercive fields within small systems. From this data we calculate the activation parameters for BTO that govern polarization switching at coercive fields not only for perfect, but also those containing vacancy defects.

15 min. break

KFM 33.5 Fri 11:05 EMH 225

Field dependence of the electrocaloric effect in ferroelectrics with first order and diffuse phase transitions — ●JAN FISCHER, DANIEL HAEGELE, and JOERG RUDOLPH — Ruhr University Bochum

The electrocaloric effect (ECE) in ferroelectrics is currently in the focus of interest for energy efficient cooling technologies. The field dependence $\Delta T_{ad}(E)$ of the adiabatic caloric temperature change as a key parameter of caloric materials is highly relevant both for the fundamental understanding of the ECE and for the design of caloric coolers. Traditionally, $\Delta T(E)$ has been measured only for discrete values of the electric field and the low-field range is often left unexplored.

Here, we present high-resolution measurements of the electric field dependence $\Delta T(E)$ by dynamic measurements of the IR radiation emitted by the sample [1]. We find characteristic changes of $\Delta T(E)$ within a few Kelvin as a fingerprint of the first order phase transition in BaTiO₃. In contrast, investigations of Ba(Zr_{0.12}Ti_{0.88})O₃ show only a slow and gradual change of the field dependence over a broad temperature range as a consequence of the diffuse phase transition. Simultaneous measurements of the polarization P further allow to compare the polarization dependence $\Delta T(P)$ to predictions of Landau-Devonshire theory. In addition, single-shot measurements of the dynamics $\Delta T(t)$ for few-cycle bursts of the electric field allow, e.g., to separate hysteresis heating from the pure caloric temperature change.

[1] Fischer *et al.*, Rev. Sci. Instrum. 94, 043906 (2023)

KFM 33.6 Fri 11:25 EMH 225

Towards precise domain-wall engineering in BaTiO₃-based materials — ●SHENG-HAN TENG¹, ARIS DIMOU¹, CHINWENDU NANCY ANABARAONYE^{2,3}, and ANNA GRÜNEBOHM¹ — ¹Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany — ²Institute for Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany — ³International Graduate School for Battery Chemistry, Characterization, Analysis, Recycling and Application (BAC-CARA), University of Münster, Corrensstraße 40, 48149 Münster, Ger-

many

Domain walls in ferroelectric oxides are promising for new nanoelectronic device concepts [1]. However, precise control of domain walls and their dynamics remains a challenge [2]. In the present work, we use *ab initio* based effective Hamiltonian [3] to explore how local point defects and nanoscale inclusions can affect phase and domain structure as well as wall pinning, bowing, and roughness in BaTiO₃-based materials.

[1] D. Meier, S. M. Selbach, *Nat. Rev. Mater.* **7**(3), pp. 157–173 (2022)

[2] A. Grünebohm, M. Marathe, R. Khachatryan, R. Schiedung, D. C. Lupascu, V. V. Shvartsman, *J. Phys. : Condens. Matter.* **34**(7), p. 073002 (2021)

[3] W. Zhong, D. Vanderbilt, K. M. Rabe, *Phys. Rev. B* **52**(9), pp. 6301–6312 (1995)

KFM 33.7 Fri 11:45 EMH 225

Direct probing of dislocation-controlled domain nucleation and domain-wall pinning in single-crystal BaTiO₃ by multi-stimuli MEMS-based in situ TEM — ●TIANSHU JIANG¹, FANGPING ZHUO¹, OSCAR RECALDE-BENITEZ¹, YEVHENYI PIVAK², and LEOPOLDO MOLINA-LUNA¹ — ¹Institute of Materials Science, Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany — ²DENSsolutions, Informaticalaan 12, Delft, The Netherlands

Engineering domain walls to control their nanoscale mobility influences macroscopic properties, crucial for electromechanics and electronics. This is evident in imprinting topological defects in materials, highlighting the field's potential. However, despite the critical role of defect-mediated domain nucleation and domain wall mobility, our comprehensive understanding of these phenomena remains limited. Here, we explore the dislocation-mediated domain nucleation and domain wall mobility in single-crystal BaTiO₃ at nanoscale by applying multi-stimuli MEMS-based in situ transmission electron microscopy (TEM). A dense, well-aligned "forest" of dislocations, intentionally imprinted, serves to selectively nucleate in-plane domain variants. Utilizing multi-stimuli in situ TEM, we highlight the direct observation of the pinning of ferroelastic domain walls by these imprinted dislocations. This strong pinning of domain walls results from the stress fields associated with the imprinted dislocations. Our findings advance domain wall engineering in ferroelectrics, offering a novel strategy for advanced nanoelectronics and bulk applications over a broad temperature range.

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Intrinsic strain engineering by dislocation imprint in single-crystal BaTiO₃ — ●FANGPING ZHUO and JÜRGEN RÖDEL — Department of Materials and Earth Sciences, Technical University of Darmstadt, 64287 Darmstadt, Germany

Dislocations exert significant control over strain, and charge in ferroelectrics, extending beyond the constraints of traditional bulk doping. In these materials, they not only act as nucleation sites for domain formation and pinning centers for the motion of domain walls, but also offer underappreciated potential in bulk ferroelectrics.

Our focus will be on a novel approach to manipulate the mobility of ferroelectric domain walls and piezoelectricity of single-crystal BaTiO₃. By employing controlled high-temperature plastic deformation along the [110] direction, we have effectively enhanced the dielectric and piezoelectric coefficient. This was achieved by harnessing the anisotropic interactions between 1D dislocations and 2D domain walls. We will delve into means of minimizing domain instability and extrinsic degradation processes through strategic strain adjustment, balancing in-plane and out-of-plane domain variants. Direct observation of domain-wall pinning of 90° domain walls by dislocations was documented using in situ transmission electron microscopy. We will highlight the innovative application of intrinsic strain engineering in bulk ferroelectrics, demonstrating plastic deformation as a key technique to customize microstructures and functionalities in these materials.