KFM 14: Poster

Chairs: Jan Schultheiß (NTNU, Norway) Anna Grünebohm (RUB)

Time: Wednesday 17:00–18:30 Location: P1

KFM 14.1 Wed 17:00 P1

Stability of Machine-Learned Interatomic Potentials in Molecular Dynamics Simulations for Organic Semiconductors and Metal-Organic Frameworks — •Martin Tritthart and Egbert Zojer — Institute for Solid State Physics, Graz, Austria

Organic semiconductors (OSCs) and metal-organic frameworks (MOFs) are two classes of materials that have garnered significant interest in materials science. To optimize their performance, it is crucial to understand the physical properties of these crystalline polymer materials, such as heat transport and mechanical stability. This understanding can lead to improvements in properties like thermal stability. Molecular dynamics (MD) simulations are commonly used for this purpose, as they are orders of magnitude less computationally expensive than first-principles calculations. While machine learning interatomic potentials (MLIPs) are much faster than ab initio methods, they approximate the true potential energy surface, which can result in significant errors for atomic configurations outside the training data space. Such shortcomings lead to incorrect predictions of forces and energies in MD simulations, potentially causing molecular instability during simulations. To address this issue and improve the robustness of MLIPs, a reliable estimation of their uncertainty is necessary. This enables the identification of uncertain structures, which can then be incorporated into the training set to enhance accuracy. With this iterative approach, larger and more complex molecules can be simulated with relatively efficient computational effort.

KFM 14.2 Wed 17:00 P1

Assessment of new cocrystals of amphotericin B and miltefosine (leishmanicidal pharmaceuticals) via powder X-ray diffraction analysis. — •Memoona Bibi, muhammad Iqbal Choudhary, and Sammer Yousuf — H.E.J. Research Institute of Chemistry, ICCBS, University of Karachi, Pakistan.

Cocrystals and other cutting-edge technologies offer substantial opportunities for patents that present multiple strategies for managing the life cycle of existing and novel drugs. The creation of cocrystals by employing suitable coformers represents a valuable approach toward stability, enhancement, and bio availability of pharmaceutical medications. The focal point of current study was co-crystallization of well-known commercially available anti-leishmanial drugs i.e. Amphotericin B and Miltefosine. Multiple cocrystals of amphotericin B and miltefosine were successfully synthesized. To prepare the co-crystals neat grinding method via mixer mill was applied. The characterization was conducted through powder X-ray diffraction revealing unique crystallinity and significant variation in 2θ values of cocrystals. DSC/TGA, UV, FTIR and melting point were also proceeded for further evaluation. The solubility studies of amphotericin B at pH 6.8, 7.4 and in distilled H2O in comparison with their co-crystals revealed promising results. Invitro testing of all co-crystals against L. major, L. donovani, and L. tropica demonstrated potent anti-leishmanial activity in comparison with reference standard drugs i.e. amphotericin B and miltefosine. However, cytotoxicity results revealed none of them exhibited cytotoxic effect against MTT (3T3) cell line.

KFM 14.3 Wed 17:00 P1

High-temperature properties of $LiNbO_3$ and $LiTaO_3$ — •Eva Westenferlder Gil, 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, extending from piezoelectric sensors [1] to integrated photonics [2]. Both, LN and LT, undergo a phase transition towards a paraelectric (PE) phase at around 1400K and 870K, respectively. Since devices employing LN and LT as functional materials are often operated at high temperatures, extensive research has been conducted in order to describe the materials high-temperature properties [3,4]. Here, we show that the high symmetry PE structure for both LN and LT is energetically favoured, which is in contrast to previously suggested models representing the PE phase as a superposition of differently oriented ferroelectric phases [5]. The electronic band structures indicate that both crystals remain electronic insulators in the PE phase. Furthermore, we provide thermal expansion coefficients and elastic constants, calculated from machine-learned potentials. Our results show a good agreement to recent experimental measurements.

[1] M. Xu *et al*, ACS Appl. Mater. Interfaces **9**, 40, (2017)
[2] W. Sohler *et al*, Optics & Photonics News **19**, 1, (2008)
[3] P. Gaczyński *et al*, Phys. Status Solidi A, 2300972, (2024)
[4] C. Kofahl *et al*, Solid State Ionics **409**, 116514 (2024)
[5] F. Bernhardt *et al*, Phys. Rev. Mat. **8**, 054406 (2024).

KFM 14.4 Wed 17:00 P1

Optimizing pre-annealing growth for obtaining pattern fidelity of highly ordered GaAs nanowires — •Juliane Koch[1], Jiajia Qiu[2], Chris Bohlemann[1], David Ostheimer[1], Peter Kleinschmidt[1], Huaping Zhao[2], Yong Lei[2], and Thomas Hannappel[1] — [1]TU Ilmenau, Institute for Physics, Fundamentals of Energy Materials, Ilmenau, Germany — [2]TU Ilmenau, Institute for Physics, Applied Nanophysics, Ilmenau, Germany

Bottom-up grown III-V semiconductor nanowires (NWs) offer significant potential for advanced electrical and optoelectronic device applications. This study presents a fabrication strategy for highly ordered GaAs NW arrays by combining a non-lithographic nanostructuring technique with metalorganic vapor phase epitaxy (MOVPE). Uniform Au nano-disk arrays, created using anodic aluminum oxide templates, act as catalysts for the subsequent NW growth. The special fabrication process of the Au nano-disks prevents undesired substrate imprinting, which leads to a different behavior than previously utilized methods, namely to an Au particle diffusion during the MOVPE process. The nucleation duration, optimized in terms of the Au particle volume, is crucial for maintaining array uniformity. A short nucleation period fails to anchor particles, resulting in undesired diffusion. To resolve this, pre-annealing nucleation is extended to initiate III-V growth of a pedestal structure that secures the array's highly ordered geometry. A detailed analysis of MOVPE sub-processes supports the development of a refined growth model.

KFM 14.5 Wed 17:00 P1

Synthesis, Properties, and Phase Transitions analysis of ferroelectric TMCM-MnCl3 hybrid halide — •Chithra Kandappanthodi, Sobhan Fathabad, Doru C.Lupascu, and Vladimir V.Shvartsman — Institute for material science, Essen, Germany

Organic-inorganic hybrid halides have gained significant attention in material science due to their environmentally friendly, cost-effective fabrication and exceptional piezoelectric or optoelectronic properties. In this study, we synthesized trimethyl chloromethyl ammonium manganese trichloride (TMCM-MnCl3) and Fe-doped TMCM-MnCl3 crystals. We demonstrate that TMCM-MnCl3 exhibits a monoclinic crystal structure at room temperature, which transforms into a hexagonal structure upon heating, as confirmed by temperature-dependent x-ray diffraction. The phase transitions at 408 K for TMCM-MnCl3 and 404 K for TMCM-Mn0.95Fe0.05Cl3 were further corroborated by differential scanning calorimetry. The step-like anomaly in the temperature dependence of dielectric permittivity observed in TMCM-MnCl3 indicates an improper ferroelectric transition. Piezoresponse force microscopy revealed regular ferroelectric domains. Additionally, Raman spectroscopy identify the vibrational modes of the crystal. Through UV-vis spectroscopy, we observed that the bandgap is tunable through moderate Fe doping. This comprehensive characterization highlights the potential of TMCM-MnCl3 for advanced applications.

KFM 14.6 Wed 17:00 P1

Investigation of hydrogen diffusion in $LiNbO_3$ and $LiTaO_3$ from density-functional theory — •Christa Fink and Simone Sanna — Institute for Theoretical Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Hydrogen is always present in $LiNbO_3$ and $LiTaO_3$ crystals. Therefore, the lattice locations 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, there exist less investigations of diffusion paths and energy barriers. To fully understand the diffusion of hydrogen in LiNbO$_3$, LiTaO$_3$ and their solid solutions, 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 [1, 2]. Starting from the energetically most favorable position, we calculate minimum energy paths through the crystal towards the next equivalent position. We extend our calculations from the stoichiometric material to crystals with Lithium vacancies, which are the most common defects in LN and LT, for a better comparison to experimental results [3, 4].

[1] G. Kresse, J. Furthmüller, Computational Materials Science 6, 15 (1996). [2] G. Kresse, J. Furthmüller, Phys. Rev. B 54, 11169 (1996). [3] Kofahl, C. et al., Defect and Diffusion Forum, 429, 136-143 (2023). [4] Kofahl, C. et al., Solid State Ionics 403, 116383 (2023).

KFM 14.7 Wed 17:00 P1

Epitaxial Growth of Phase-Pure LiNbO3 Thin Films on LiTaO3 by Pulsed Laser Deposition (PLD) — •Hyeyeon Cho, Steffen Ganschow, René Bararugurika, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany

Lithium niobate (LiNbO3) is a widely used material in electro-optical and electroacoustic devices due to its outstanding ferroelectric, piezoelectric, electro-optical, and nonlinear optical properties. Thin-film LiNbO3 offers significant advantages, including component miniaturization, broader bandwidths at higher frequencies, and reduced operational voltages. However, achieving these benefits requires the growth of phase-pure films with excellent crystalline quality, stoichiometric composition, and low surface roughness. Pulsed Laser Deposition (PLD) is a reliable method for growing LiNbO3 thin films, providing precise control over stoichiometry and the ability to produce high-quality epitaxial layers. However, high volatility of Li2O at enhanced temperatures during deposition often leads to Li-poor secondary phase formation. In this study, we investigated the effects of various deposition parameters to optimize the growth of phase-pure LiNbO3 films on LiTaO3. Key parameters, including substrate temperature, oxygen partial pressure, laser fluence, laser frequency, and target-substrate distance, were systematically varied. We also explored the use of lithium-rich targets to address lithium loss at high temperatures. X-ray diffraction (XRD) and atomic force microscopy (AFM) analyses confirmed the epitaxial growth of high-quality films with smooth surfaces.

KFM 14.8 Wed 17:00 P1

PALS of Hot-Rolled and Subsequently T4-Treated AlCuMgAg — •Lucian Mathes[1], Leon Heinl[2], Andreas Wagner[3], Maik Butterling[3], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum, TU München — [2]Institute of Casting Research, Montanuniversität Leoben, Austria — [3]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics

Positron annihilation lifetime spectroscopy (PALS) is a unique tool for studying the concentration and types of open-volume defects. We performed depth-resolved PALS to investigate such defects and the properties of precipitates in differently (heat) treated AlCuMgAg samples. Alloying AlCu with Ag has been shown to leverage the formation of the so-called Ω(Al$_2$Cu) phase, known for its high strength and thermal stability. We present PALS measurements of Al-4Cu-0.3Mg-0.7Ag containing Ω phase precipitation after hot-rolling and subsequent T4-treatment. Our findings showcase the high thermal stability of the Ω phase and that positron annihilation studies help in understading and optimizing the process of strength hardening AlCuMgAg alloys.

KFM 14.9 Wed 17:00 P1

Polycrystalline FeS as ultra-fast charging sodium-ion battery anode — •Zidong Wang and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Fast charging is considered a key development trend and a competitive advantage for sodium-ion battery (SIB) technology. Achieving fast-charging SIBs relies on developing electrode materials that combine high rate performance with excellent capacity retention. While iron sulfide, known for its high theoretical capacity, has shown potential, its fast-charging performance is hindered by poor rate performance due to volume expansion. Conventional approaches, such as compositing with carbon materials or adjusting the cut-off voltage, come with drawbacks*carbon composites reduce volumetric energy density, while cut-off voltage adjustments compromise capacity. Neither approach aligns well with practical applications. To address these challenges, we capitalized on the crystalline structural diversity of iron sulfides and successfully synthesized carbon-free polymorphic FeS. This material achieves high rate performance without relying on carbon additives or cut-off voltage adjustments, marking a significant step forward in SIB development. Impressively, anode demonstrates the best rate performance reported to date at an exceptionally high current density, achieving 236 mAh/g at 50 A/g.

KFM 14.10 Wed 17:00 P1

Nanoscale Thermal Expansion in Crystals Probed by Echo-Resolved Terahertz Spectroscopy — •Nicolas Sylvester Beermann, Andreas Gebauer, Wentao Zhang, Tomoki Hiraoka, Savio Fabretti, Hassan Hafez, and Dmitry Turchinovich — Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

Thermal expansion of solids is a ubiquitous phenomenon in condensed matter physics [1]. However, its observation was out of limits for terahertz time-domain spectroscopy (THz-TDS) due to the relatively long sub-millimeter wavelength of THz radiation. To address this, we introduce echo-resolved THz spectroscopy (ERTS) that utilizes THz main and echo pulses in time-domain measurements to simultaneously determine frequency-dependent complex optical constants and material thickness [2]. By numerically solving complex transcendental transmission equations, ERTS allows for sample thickness measurements with deep-subwavelength precision on the order of $\lambda/1000$. We used the ERTS to analyze the THz-TDS data of magnesium oxide, sapphire, and gallium arsenide crystals measured in the temperature range of 10-300 K. The thermal expansion of the crystals on a sub-micrometer scale was measured, and the simple phonon model was applied to determine the material-specific Grüneisen parameters.

[1] K. Takenaka, Sci. Technol. Adv. Mater. 13, 13001 (2012)

[2] N. S. Beermann et al., Terahertz Time-Domain Spectroscopy for Simultaneous Measurement of Optical Constants, and Material Thickness with Deep-Subwavelength Precision, submitted manuscript

KFM 14.11 Wed 17:00 P1

Two Photon Absorption in Lithium niobate tantalate inspected via *z*-scan technique — •Niklas Dömer[1], Anton Pfannstiel[1], Steffen Ganschow[2], Mike Pionteck[2], Simone Sanna[3], and Mirco Imlau[1] — [1]Inst. Physics, Barbarastr. 7, Osnabrück Univ., Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, Berlin, Germany — [3]Center for Materials Research J.L.-Univ. Giessen, Heinrich-Buff-Ring 16 , Giessen, Germany

The knowledge of the nonlinear optical properties of polar oxide crystals, such as the two-photon absorption (TPA) coefficient β in lithium niobate (LN), is of significant importance for tailoring technological applications in (integrated) photonics. Here, we present the results of our studies on the dispersion properties $\beta(\lambda)$, i.e. the imaginary part of the third-order susceptibility $\chi^{(3)}_{\mathrm{Im}}$, in the model system lithium niobate tantalate (LNT, LiNb$_x$Ta$_{1-x}$O$_3$ with 0≤x≤1). Experimentally, an open-aperture z-scan experiment pumped by fs-pulses in the spectral range of 330 - 600 nm from an optical parametric amplifier (OPA) is used. The obtained results are compared with literature data for LN ($x = 0$) and LT ($x = 1$) and the non-vegard-like behavior of the band gap. In extension, the study is applied for the determination of the density of states with LN as an example. We discuss our findings with ab-initio calculations for LN and in the framework of transient absorption phenomena induced by TPA in LNT [N. Dömer, J. Koelmann *et al.*, New J. Phys. **26** (2024) 083027]. This work is financially supported by the DFG (projects IM37/13-1, GA 2403/7-1 and SA1948/3-1 within the research unit FOR 5044, ID: 426703838).

KFM 14.12 Wed 17:00 P1

Refractive Indices and Birefringence Behavior of Lithium Niobate Tantalate Solid Solutions — •Tobias Hehemann[1], Anton Pfannstiel[1], Steffen Ganschow[2], and Mirco Imlau[1] — [1]Institute of Physics, Osnabrueck University — [2]Leibniz-Institut für Kristallzüchtung, IKZ, Berlin

Lithium niobate tantalate solid solutions (LNT, LiNb$_{1-x}$Ta$_x$O$_3$ with $0 \leq x \leq 1$) exhibit a wide range of linear and nonlinear optical properties, that can be tuned by composition x. A unique feature is the disappearance of the birefringence Δn for x between $0.93 \leq x \leq 0.96$ [Wood *et al.*, J. Phys.: Condens. Matter **20** 235237 (2008)] enabling customized applications in photonics. While the dispersive behavior of the ordinary $n_o(\lambda)$ and extra-ordinary $n_e(\lambda)$ indices are well documented for the edge compositions LiNbO$_3$ (LN, x=0) and LiTaO$_3$

(LT, x=1), there remains a lack for LNT along x. In particular, nearly nothing is known about the structural relation between the index of refraction and composition. We here present our results for the dispersion behavior of n_o and n_e of LNT for several x, measured using an interferometric technique at specific wavelengths in the visible spectrum. Our data allow for a more detailed inspection of the birefringence $\Delta n = n_o - n_e$ of LNT at room temperature. The obtained data are analyzed and discussed in the context of existing literature, providing deeper insights into the relation between structure and optical properties of LNT. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 426703838 (IM 37/13-1, GA 2403/7-1 of the FOR 5044).

KFM 14.13 Wed 17:00 P1

Surface and near-surface positron annihilation spectroscopy at very low positron energy — •Maximilian Suhr[1], Lucian Mathes[1,2], Vassily V. Burwitz[2], Danny R. Russell[1], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum, TU München — [2]School of Natural Sciences, Physics Department, TU München

Positron annihilation spectroscopy is a highly sensitive tool for defect characterization in solids. We present the Setup for Low-Energy Positron Experiments (SLOPE) at TUM. This monoenergetic positron beam is realized via a high-activity ^{22}Na source, a W moderator, a sophisticated electromagnetic beam guidance system and two high purity Ge detectors. Our instrument features a state-of-the-art range of implantation energy, namely 3 eV to 40 keV, enabling bulk measurements as well as investigations of surfaces. With three different measurements we showcase the versatile applications of SLOPE: a full range depth profile of a W monocrystal, coincidence ratio curves of H-loaded Ni, and a valley-to-peak (positronium formation) scan of Cu and Kapton at very low implantation energies.

KFM 14.14 Wed 17:00 P1

Microscopic view into non-volatile resistive switching in Au/Prussian blue/Ag layer stacks — •Mohammed Fayis Kalady[1], Daniel Wolf[1], Michael Pohlitz[2], Christian Mueller[2], and Axel Lubk[1,3] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Helmholtzstraße 20, 01069 Dresden — [2]University of Applied Sciences Zwickau, 08056 Zwickau, Germany — [3]Institute of Solid State and Materials Physics, TU Dresden, Haeckelstraße 3, 01069 Dresden, Germany

Due to their distinct electrochemical properties, Prussian blue (PB) and its analogs (PBA) are emerging materials for memristor applications. This study uses transmission electron microscopy (TEM) techniques to explore resistive switching in PB-based memristors. Our work will utilize in-situ TEM to apply electrical bias, correlating nanoscale structural changes with electronic properties and employing methods like high-resolution TEM, electron energy-loss spectroscopy, and energy-filtered TEM. By changing the polarity of the external voltage, the Au/PB(A)/Ag is switched between two stable resistance states, the high resistance state and the low resistance state. The experimental technique seeks to elucidate the resistive switching mechanism, contributing to designing efficient and reliable memristor devices for advanced memory applications.

KFM 14.15 Wed 17:00 P1

Phonon Properties of perovskite oxides and halides — •Mwanaidi Mauwa Namisi and Benyao Sun — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany

Perovskite materials, which have proven useful in many areas including photovoltaics and ferroelectrics [1], are highly structurally unstable due to the dynamic nature of the metal-halide octahedra and cation off-centering. It is therefore evident that understanding the vibrational properties of these materials is crucial in their modelling and applications. Meanwhile, there is considerable research value in developing high-performance, environmentally friendly, and health-conscious lead-free ferroelectric materials [2, 3]. Particularly, BaTiO3- based lead-free perovskites have become a major research focus. However, systematic studies on BaTiO3-based superlattices combined with BaSnO3 remain scarce. Here, we investigate the phonon properties of perovskite oxides (BaSnO3) and halides (CsPbX3, (X=I, Br, Cl) and discuss the distortions, do- main structures by the anharmonicity. We also investigate how these instabilities couple with an external field and discuss the differences in the ferroelectric nature between perovskite oxides and halides. Additionally, structural optimization was performed on BaTiO3/BaSnO3 superlattices with varying Sn concentration gradients. References (1) Bergenti, I. Appl. Phys. 2022, 55, 033001. (2) Grunebohm, A., Madhura, M., Claude, E. Appl. Phys. Lett. 2015, 107,102901. (3) Grunebohm, A.; Marathe, M. Phys. Rev. Mat. 2020, 4,4417.

KFM 14.16 Wed 17:00 P1

Thermodynamics of Barium Boranate using DFT — •Markus Mehlhorn[1], Konrad Burkmann[2], Angus Demmer[2], Jakob Kraus[1], Franziska Habermann[2], Jürgen Seidel[2], Klaus Bohmhammel[2], Jens Kortus[1], and Florian Mertens[2] — [1]Institut für Theoretische Physik, TU Bergakademie Freiberg — [2]Institut für Physikalische Chemie, TU Bergakademie Freiberg

Materials containing high hydrogen content are interesting candidates for solid hydrogen storage. However, there are well-known fundamental challenges to address like the reversibility of the (de)-hydrogenation and sufficiently fast kinetics for these processes before possible applications. Here we present results on thermodynamic properties of $Ba(BH_4)_2$. Unfortunately, the isobaric heat capacity function of this material is not accessible experimentally. $Ba(BH_4)_2$ could not be synthesized in sufficient purity. Therefore we attempt to fill this gap by means of computations based on density functional theory using the PBEsol functional. The quasi harmonic approximation is used to describe volume expansion due to thermal effects assuming that for each fixed volume the harmonic approximation can be employed. For each volume the phonon density of states has been calculated via density functional perturbation theory. This procedure allows to calculate the Gibbs free energy and therefore gives access to thermodynamic properties like entropy and isobaric heat capacity. Comparing the heat capacity to other metal boranates, which have been synthesized and measured, one finds very similar behavior.

KFM 14.17 Wed 17:00 P1

3D nanoscale chemical analysis of WO_3 using Atom Probe Tomography — •Katharina Wolk[1], Jack T. Eckstein[2], Kasper A. Hunnestad[1], Constantinos A. Hatzoglou[1], Gustau Catalán[3], Ekhard K. H. Salje[2], Julia Glaum[1], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Department of Earth Sciences, University of Cambridge, Cambridge, UK — [3]Institut Català de Nanociència i Nanotecnologia, Campus Universitat Autònoma de Barcelona, Bellaterra, Catalonia

The functional properties of oxides are closely linked to their chemical composition. The transition metal oxide WO_3 is notable for its structural versatility and unusual physical properties, such as the formation of superconducting ferroelastic domain walls. To understand the relation between local variations in chemical composition and material properties, we apply atom probe tomography (APT). APT offers compositional mapping in 3D with sub-nanometer spatial resolution and chemical sensitivity of 100 ppm. Using scanning electron microscopy, we image the ferroelastic domain structure in WO_3 single crystals and extract specimens from different regions of interest with a focused ion beam for the APT analysis. Based on 3D reconstructions, we investigate site-specific variations in chemical composition, exploring the oxidation state and potential formation of oxygen defects. Varying experimental APT parameters, such as laser energy, enables insights into optimizing compositional accuracy.

KFM 14.18 Wed 17:00 P1

Isovalent exchange of Al, Mg and Zr in strontium hexagallate (SrGa12O19) — •Finn. H. Bietz[1], Ch. Rhode[2], and S. Sanna[1,3] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Gießen 35392, Germany — [2]Leibniz Institut für Kristallzüchtung, Max Born Straße 2, 12489 Berlin — [3]Center for Materials Research (ZfM), Justus Liebig University Gießen, Gießen 35392, Germany

$SrGa_{12}O_{19}$ can be used as a substrate for the growth of barium hexaferrite, a ferrimagnetic and quantum paraelectric material. The lattice parameters of $SrGa_{12}O_{19}$ can be adjusted by substitution of Ga by Al or Mg and Zr respectively for lattice-matched growth and strain engineering of barium hexaferrite. A microscopic picture of the doping mechanisms and their effect on the lattice parameters is missing.

In this contribution, we report on first-principles calculations performed to determine the lattice site of Al, Mg and Zr atoms in the $SrGa_{12}O_{19}$ structure, and support corresponding experiments performed at the IKZ in Berlin. Thereby the defect formation energies of Al, Mg and Zr atoms incorporated in the dilute limit at different lattice sites were calculated within density functional theory.

The atomistic models reveal that Mg populates the so called Ga$^{(3)}$ position, Al prefers the Ga$^{(1)}$ site, but also populates the Ga$^{(4)}$ and Ga$^{(5)}$ sites, and that the Zr is incorporated the Ga$^{(4)}$ site. While the results are in very good agreement with the experimental results in the case of Mg and Al doping, the experimentally determined lattice site of Zr differs from the theoretical predictions, suggesting the formation of defect complexes or co-doping related effects.

KFM 14.19 Wed 17:00 P1

Tailoring ferroelectric and magnetic properties in polycrystalline hexagonal manganites — Jonas Åmli Ingdal[1], •Ruben Skjelstad Dragland[1], Catalina Salazar[2], Ellinor Benedikte Anjali Lindström[1], Katharina Wolk[1], Tino Gottschall[2], Jiali He[1], Jan Schultheiss[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology (NTNU), Trondheim, Norway — [2]Dresden High Magnetic Field Laboratory, Dresden, Germany

Rare-earth hexagonal manganites are extensively studied for their diverse physical phenomena, including tunable electronic behavior at ferroelectric domain walls, pronounced magnetocaloric effects, and significant thermal Hall conductivity, which make them highly interesting as advanced multi-functional materials. The intriguing effects arise from the unique combination of improper ferroelectricity and antiferromagnetic ordering, which are intimately linked to the rare-earth ions.

In this study, we systematically investigate the role of the rare-earth atom on the ferroelectric and magnetic properties of h-RMnO3. Polycrystalline samples with R = Tm, Er, Y, Ho, and Dy are synthesized using a solid-state approach. Ferroelectric order is verified across all compositions using piezoresponse force microscopy. Direct adiabatic temperature change measurements in the cryogenic regime reveal a strong correlation between rare-earth magnetism and the caloric response. Our results highlight the possibility to tune both the ferroelectric order and magnetic responses, offering new opportunities for optimizing the system for envisioned applications.

KFM 14.20 Wed 17:00 P1

Characterizing Domains in GeTe using Atom Probe Tomography — •Jan Köttgen[1], Maria Häser[1], Lina Jäckering[1], Julian Pries[1], Carl-Friedrich Schön[1], Pengfei Cao[3], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons ER-C, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The thermoelectric GeTe undergoes a solid-state phase transition from its cubic to its rhombohedral crystal structure when cooled from the melt to room temperature. This phase transformation results in domains. In this study a polycrystalline GeTe bulk sample was investigated using atom probe tomography (APT), which enables the determination of the sample*s stoichiometry with atomic resolution. The APT analysis revealed that different domains evaporate with different probabilities of multiple events (PME). Metavalent solids such as GeTe are known generally to exhibit a high PME in APT. Our experiments additionally show an anisotropy between different grains as observed in the PME. Using a correlative approach involving TEM, EBSD, AFM, SNOM, and DFT calculations, this effect can be attributed to an expansion of the unit cell and a concomitant change of the dielectric function. Our experiments open new avenues for atom probe tomography as a tool to investigate domains and the atomic distribution simultaneously crucial to improve the performance of thermoelectrics.

KFM 14.21 Wed 17:00 P1

Long-lived, pulse-induced transient absorption in LiNb$_{1-x}$Ta$_x$O$_3$ ($0 \leq x \leq 1$) solid solutions — •Julian Koelmann[1], Niklas Dömer[1], Mira Hesselink[1], Tobias Hehemann[1], Anton Pfannstiel[1], Felix Sauerwein[1,2], Laura Vittadello[1,2], Steffen Ganschow[3], and Mirco Imlau[1] — [1]Institute of Physics, Barbarastr. 7, Osnabrück University, Osnabrück, Germany — [2]Research Center for Cellular Nanoanalytics, Osnabrueck (CellNanOs), Osnabrueck University, Barbarastr. 11, Osnabrueck, 49076, Germany — [3]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, Berlin, Germany

Femto-/nanosecond pulse-induced, red and near-infrared absorption is studied in LiNb$_{1-x}$Ta$_x$O$_3$ (LNT) solid solutions with the aim of studying transient optical nonlinearities associated with optically generated small bound electron polarons. As a result, a long-lived transient absorption is uncovered for LNT which exceeds lifetimes and starting amplitudes of LiNbO$_3$ (LN) and LiTaO$_3$ (LT) by a significant factor. The transients provide strong evidence for an underlying hopping transport mechanism of small bound polarons. All findings are discussed in comparison to the model systems LN and LT within the framework of appropriate band models and optical generation of polarons via two-photon excitation. To explain the significant differences, the simultaneous presence of Nb$_{\mathrm{Li}}^{5+}$, Ta$_{\mathrm{Li}}^{5+}$ antisites, and Ta$_{\mathrm{V}}^{5+}$ interstitial defects is assumed for LNT. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) * Project-ID 426703838 (IM 37/13-1, GA 2403/7-1 of the FOR 5044).

KFM 14.22 Wed 17:00 P1

Investigation of Pressure-Induced Dimerization in a Pyrene-based Dyad Crystal: Associated with Auxiliary exhibition of thermally Induced Intramolecular Charge Transfer — •Argha Barman[1], Agniezska Huć[2], and Krishnayan Basuroy[1] — [1]DESY, Hamburg, Germany — [2]University of Warsaw, Poland

We present the design and photophysical properties of a D-B-A dyad with N, N-dimethylaniline (DMA) as the electron donor and pyrene (Py) as the acceptor, linked by a -CH=CH- chain. The molecule crystallizes in the triclinic space group P-1, undergoing a reversible phase transition with solvent-dependent transition temperatures (e.g., 200K in cyclohexane, 198K in toluene, 209K in dichloromethane). Structural changes include variations in bond lengths and pyramidalization at the tertiary nitrogen atom, with persistent strong π***π stacking. Photophysical analysis reveals a small HOMO-LUMO gap (3.06 eV) and temperature-dependent dual fluorescence from locally excited (LE) and intramolecular charge transfer/excimer (ICT) states, with ICT emission diminishing above 220K. Under hydrostatic pressure (0.5*2.0 GPa), the crystals exhibit piezochromic behavior with emission redshift and quenching. These multifunctional properties make Py-CH=CH-DMA crystals promising for optoelectronics and pressure sensors.

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Multiscale modeling of intergranular corrosion in iron — •Vahid Jamebozorgi[1], Karsten Rasim[2], and Christian Schröder[1] — [1]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences and Arts, Interaktion 1, 33619 Bielefeld, Germany — [2]Faculty of Physics, Bielefeld University, Universitätsstraße 4, 33615 Bielefeld, Germany

Localized corrosion, particularly intergranular corrosion, causes a significant economical and structural challenge across various industries. An accurate predictive intergranular corrosion modeling should incorporate atomic scale details, including crystallographic aspects of grain boundaries, and their evolution by time increment. However, the size and scale limitations imposed by atomistic methods hinder the development of realistic models. To overcome these limitations, we propose a novel multiscale modeling approach that combines the detailed atomistic insights provided by reactive molecular dynamics with the computationally tractable finite element method. This multiscale strategy not only ensures the preservation of crucial atomistic details but also enables the simulation of larger spatial and temporal scales, thereby offering a comprehensive view on the microstructure*s evolution during the intergranular corrosion process.

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Theoretical Investigation of [100] Edge Dislocations in Ferroelectric Perovskites — •Himal Wijekoon[1], Pierre Hirel[2], and Anna Grünebohm[1] — [1]Interdisciplinary Center for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High-performance Materials (ZGH), Ruhr Universität Bochum, Germany — [2]Université de Lille, CNRS, INRAE, Centrale Lille, UMET, F-59000 Lille, France

Ferroelectric switching is critically influenced by nucleation and pinning at defects within the material. Despite their significance particularly at strained interfaces, the role of dislocations on switching is however largely unexplored. We employ atomistic core-shell potentials [1] to demonstrate that edge dislocations can facilitate domain nucleation and reduce the coercive field. These findings suggest that a more comprehensive understanding of these defects could lead to improved material performance.

[1] M. Sepliarsky, A. Asthagiri, S.R. Phillpot, M.G. Stachiotti, and R.L. Migoni, Atomic-level simulation of ferroelectricity in oxide materials, Current Opinion in Solid State and Materials Science, 9(3):107-113, June 2005.

KFM 14.25 Wed 17:00 P1

Interaction of $NaYF_4$:Yb:Er Upconversion Nanoparticles with ultrashort laser pulses — •Leon Siemon[1], Felix Sauerwein[1], Thibault Mengis[1], Leonie Birk[2], Eike Wienbeuker[2], Markus Haase[2], Jacob Piehler[2], and Mirco Imlau[1] — [1]Institute of Physics, Osnabrück University, Germany — [2]Dept. of Biology/Chemistry, Osnabrück University

Lanthanide-doped upconversion nanoparticles (ucNP), such as $NaYF_4$:Yb:Er, play a significant role for future all-optical interrogation techniques of cellular systems due to their ability to convert infrared excitation light (980 nm/Yb-absorption) into green/red luminescence (520, 540, 660 nm/Er-emission). The corresponding conversion characteristics and energy transfer mechanisms have been studied extensively under continuous-wave illumination - however, so far, the interaction of ucNPs with ultrashort laser pulses has not been studied. We have adressed this question via diffuse fs-pulse reflectometry [C. Kijatkin *et al.*, Photonics **4** (2017) 11] of $NaYF_4$:Yb:Er nanoparticles ($d \approx 18\,nm$) exposed to 980 nm sub-ps-pulses ($\tau_{\mathrm{pulse}} > 40\,\mathrm{fs}$) at peak intensities up to $10^{14}\mathrm{W/m^2}$ and repetition rates down to 50 Hz. We observe severe differences in the intensity dependence, quantum yield and average power density that are attributed to modified population pathways in the energy diagram if the pulse duration falls below the resonant energy transfer time between Yb and Er ions. The impact of our findings for ucNP applications in cellular environments, particularly to reduce laser-induced cell damages, is discussed. Financial support DFG/RTG2900, 'nanomaterials@biomembranes'.

KFM 14.26 Wed 17:00 P1

Harmonic Nanoparticles: State-of-the-knowledge and future applications — •Moritz Domack[1], Jan Klenen[1], Mirco Imlau[1], and Laura Vittadello[2] — [1]Inst. Physics, Barbarastr. 7, Osnabrück Univ., Germany — [2]Laboratoire SYMME, 7 Chemin de Bellevue, Université Savoie Mont Blanc, France

Harmonic nanoparticles (HNPs) are receiving growing attention in anorganic chemistry, nanophotonics and life sciences due to their potential for upcoming imaging techniques. For instance, HNPs are successfully used as nanophotonics markers in the near-infrared (NIR) bio-optical windows (III) and (IV), so-called NIR-to-NIR imaging [L. Vittadello *et al.*, Nanomaterials **11** (2021) 3193], as well as for destruction free in-vivo imaging [L. Vittadello *et al.*, Opt. Mater. Express **11.7** (2021) 1953-1969]. HNPs are based on polar oxide nanocrystals with pronounced nonlinear optical response, such as sodium niobate ($NaNbO_3$) or potassium niobate ($KNbO_3$) and can already be synthesized at the nanometer scale (<100 nm), e.g. via hydrothermal synthesis [N. Kohlenbach *et al.*, Nanoscale **12** (2020) 19223], but also surface-functionalized. Nonlinear Diffuse femtosecond-pulse reflectometry of powder-pressed-HNP-samples has been established as major tool for characterization of the nonlinear optical properties [C. Kijatkin *et al.*, Photonics **4.1** (2017) 11]. We here give insight to the state-of-the-art processing routine of HNPs from synthesis, via characterization to applications and highlight upcoming fields, particularly in the framework of all-optical interrogation of cellular environments. Financial support by the DFG/RTG2900, 'nanomaterials@biomembranes'.