# 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 Chryssos, 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 microbeam (50 $\mu$m 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 Su[1], Xu Chen[2], Huaping Zhao[1], Zhiyi Lu[2], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Key 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 AlO4 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 synthesize 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 coexist 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. Bauernfeind 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 Schreck[1], Gaetano Aiello[1], Pablo Estebanez[2], Andreas Meier[1], Theo Scherer[1], Dirk Strauss[1], Christoph Wild[3], and Eckhard Wörner[3] — [1]Karlsruhe Institute of Technology, Institute for Applied Materials, 76021 Karlsruhe, Germany — [2]Fusion for Energy, 08019 Barcelona, Spain — [3]Diamond 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 polycristalline 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 ($< 2*10$ E-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 distribution 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 $\Delta T$ 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 $\mu$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 $\Delta T$ even for $\mu$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 $LiNbO_3$ and $LiTaO_3$ 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 $LiNbO_3$ (LN) and $LiTaO_3$ (LT) is influenced, among other properties, by intrinsic defects. In particular, spectroscopic signatures of quasiparticles known as polarons are an hallmark of LN and LT, respectively. Unfortunately, very little is known about the intrinsic defects in $LiNb_{1-x}Ta_xO_3$ 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 $LiNbO_3$ from density-functional theory** — •Christa Fink and Simone Sanna — Institute for Theoretical Physics, Justus Liebig University Giessen, Germany

Hydrogen is always present in $LiNbO_3$ 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 invetigtions of diffusion path and energy barriers [3]. To fully understand the hydrogen diffusion in $LiNbO_3$ 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** — Mwanaidi Namisi[1], •Mohammad Moaddeli[2], Mansour Kanani[2], and Anna Grünebohm[1] — [1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany — [2]Department 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

[1] X. Ma and et. alPhys. Rev. B, vol. 107, p. 184105, 2023. [2] I. BergentiJ. Phys. D: Appl. Phys., vol. 55, p. 11, 2022. [3] M. Moaddeli and et. alPhys. Chem. Chem. Phys, vol. 25, p. 25511, 2023.

KFM 9.15 Mon 18:00 Poster E

**Synthesis of Aero-ZnS micro-nanoarchitectures on 3D networks of sacrificial ZnO microtetrapods** — •Tudor Braniste[1], Vladimir Ciobanu[1], Irina Jin[1], Veaceslav Ursaki[1,2], Victor Zalamai[1], Emil Rusu[3], Vadim Morari[3], Rainer Adelung[4], and Ion Tiginyanu[1,2] — [1]National Center for Materials Study and Testing, Technical University of Moldova, Stefan cel Mare Ave. 168, MD-2004 Chisinau, Republic of Moldova — [2]Academy of Sciences of Moldova, Stefan cel Mare Ave. 1, MD-2001 Chisinau, Republic of Moldova — [3]Institute of Electronic Engineering and Nanotechnology, Technical University of Moldova — [4]Institute 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 Schneider[1], Michael Paulus[1], Finn Ontrup[2], Nelson Filipe Lopes Dias[2], and Wolfgang Tillmann[2] — [1]Fakultät Physik/DELTA TU Dortmund University, 44221 Dortmund, Germany — [2]Institute of Materials Engineering, Dortmund, Germany

The aim of this project is to gain a fundamental understanding of the dependence between deposition parameters, layer structure and oxidation behavior of 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. Eng[3], Magnus Hegelund[2,7], Doru Lupascu[4], Bruno Correa[1], Levy Scalise[1], Boris Koppitz[3], Samuel Seddon[3], and Hans Hofsäss[2,6] — [1]University of Sao Paulo, Sao Paulo, Brazil — [2]European Organization for Nuclear Research (CERN) — [3]Technische Universität Dresden (TUD) — [4]University Duisburg-Essen — [5]KU Leuven — [6]University of Göttingen — [7]Aalborg 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 mbaris 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 Bräuninger[1], Damian Alexander Motz[1], Felix Seewald[2], Sebastian Praetz[3], Carla Vogt[4], Birgit Kannengiesser[3], Hans-Henning Klauss[2], and Hermann Seifert[1] — [1]Institute for General Radiology and Medical Physics, University of Veterinary Medicine Hannover Foundation, Bischofsholer Damm 15, Hanover, 30173, Lower Saxony, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden,Haeckelstraße 3, Dresden, 01069, Saxony, Germany — [3]Institute of Optics and Atomic Physics, TU Berlin, Hardenbergstraße 36, Berlin, 10623, Berlin, Germany — [4]Institute of Analytical Chemistry, TU Bergakademie Freiberg, Leipziger Straße 29, Freiberg, 09599, Saxony, Germany

Prussian Blue compounds (PBC) have shown a huge potantial of applications in physics, chemistry, medicine and radioecology, e.g., selected PBC are acting as efficient ion exchanger extracting the radioistope $^{137}Cs$ in solutions. In this study, the focus is the PBC ammonium iron(III) hexacyanoferrate(II) ($NH_4\{Fe(III)[Fe(II)(CN)_6]\}$), 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 $^{57}Fe$-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 Thiessenhusen[1], Ritz Aguilar[1], Michal

Smid[1], Thomas Kluge[1], Michael Bussmann[1,2], Thomas Cowan[1], Nico Hoffmann[1], Lingen Huang[1], and Jeffrey Kelling[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Center for Advanced Sytem 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 $KNbO_3$ single crystal: investigation of phase transitions, ferroelastic domains and dislocations** — •Felix Drechsler[1], Cameliu Himcinschi[1], Oliver Preuss[2], Xufei Fang[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg, Germany — [2]TU Darmstadt, Department of Materials and Earth Sciences, Division Nonmetallic-Inorganic Materials, D-64287 Darmstadt, Germany

We investigated a $KNbO_3$ 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 $KNbO_3$. 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-Selinger[3], Maik Butterling[5], Eric Hirschmann[5], Emma Huntley[1], Adrian Langrehr[1], Maciej Oskar Liedke[5], Lucian Mathes[2,1], Christoph Springl[1], Monia Vadrucci[4], Andreas Wagner[5], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum, TU München — [2]TU München, School of Natural Sciences, Physics Department — [3]MPI für Plasmaphysik, Garching bei München — [4]ENEA Frascati, Development of Particle Accelerators and Medical Applications — [5]Helmholtz-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 evolution 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. Tokle[1], Leonie Richarz[1], Edith Bourret[2], Zewu Yan[2,3], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [3]ETH 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 $Er(Mn,Ti)O_3$, 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 Lehninger[1], Michael Paulus[1], Christian Sternemann[1], and Patrick Degen[2] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Carl 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 c ell 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 Meessen[1], Jan Köttgen[1], Michael Feuerbacher[3], Christian Stenz[1], Thomas Schmidt[1], Jonathan Frank[1], Yuan Yu[1], and Wuttig Matthias[1,2,4] — [1]1. Institute of Physics (IA), RWTH Aachen University, 52074 Aachen, Germany — [2]JARA Institute "Energy-efficient information technology (PGI-10)", RWTH Aachen University, Germany — [3]Ernst Ruska-Centrum für Mikroskopie und Spektroskopie mit Elektronen (ER-C), Forschungszentrum Jülich GMBH, 52428 Jülich, Germany — [4]JARA-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 critical 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 metavalent 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 $^{60}$Co and $^{207}$Bi 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** — •Alexius 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 cotrolled 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 Hofsäss — 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-Li(p,alpha) 4-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 $SrTiO_3$** — •Pavlína Kružíková[1,3] and David R. Bowler[2,3] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany — [2]London Centre for Nanotechnology, London, UK — [3]Department of Physics and Astronomy, UCL, London, UK

A typical property of $SrTiO_3$ 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 Σ13 (510) grain boundary in $SrTiO_3$ 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 $SrTiO_3$ grain boundary and further insights about the AFD mechanism. Several related systems were also studied to compare the findings, e.g., the Σ13 (210) grain boundary, SrTiO3 bulk with AFD rotations and $SrTiO_3$ 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 $CaMnO_3$** — •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. $CaMnO_3$ 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 $CaMnO_3$, 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 Ho[1], Rouven Maier[2], Vadim Vorobyov[2], Andrej Denisenko[2], Anke Krueger[1], and Jörg Wrachtrup[2] — [1]Institute of Organic Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart — [2]3rd 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 Dömer[1], Julian Koelmann[1], Anton Pfannstil[1], Mirco Imlau[1], and Steffen Ganschow[2] — [1]Inst. Physics, Barbarastr. 7, Osnabrück Univ., Germany — [2]Leibniz-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, $LiNb_xTa_{1-x}O_3$ with $0 \leq x \leq 1$) 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 Koelmann[1], Sören Domke[1], Anton Pfannstiel[1], Steffen Ganschow[2], and Mirco Imlau[1] — [1]School of Mathematics/Informatics/Physics, Barbarastr. 7, Osnabrüuck University, Osnabrüuck, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, Berlin, Germany

Optical damage is reported for the mixed crystal system $LiNb_{1-x}Ta_x$ ($0 \leq x \leq 1$) 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 $Fe_{Li}^{3+/4+}$, that may be interpreted by a more pronounced landscape of intrinsic defects in LNT including the photo-excitation of small bound $Nb_{Li}^{4+}$ 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-incuded, 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 Pfannstiel[1], Tobias Hehemann[1], Simone Sanna[2], Nils Schäfer[2], Yuriy Suhak[3], Holger Fritze[3], and Mirco Imlau[1] — [1]Inst. Physics, Barbarastr. 7, Osnabrück Univ., Osnabrück — [2]Dept. of Physics, Heinrich-Buff-Ring 16, Justus Liebig University , Giessen — [3]Inst. 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 ($\sim 1.0\,eV$) band at $\sim 2.1\,eV$ and are likely assigned to $Ta_{Li}^{4+/5+}$ antisites. Also, the presence of interstitial $Ta_i^{3+}$ defect centers is discussed in literature, but experimental evidence for respective small polaron formation is missing in literature, so far. We have adressed this question by polarized absorption spectroscopy of optically gated small polarons in thermally reduced $LiTaO_3$ (congruently melting composition). Upon exposure to gating light ($\lambda = 488\,nm$) and polarized detection of the absorption change at T=80 K, we discovered that the NIR absorption feature is due to a superposition of two individual bands peaking at 1.6 eV and 2.1 eV, respectively. These findings are found in agreement with the energies estimated for $Ta_{Li}^{4+}$ 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 Shelyug[1], Chukwudalu Okafor[2], Oliver Preuss[2], Judith Jung[1], Christoph Gebert[1], Christoph Kirchlechner[1], Hans-Jürgen Seifert[1], and Xufei Fang[1,2] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department 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.