MM 19: Poster Session

Time: Tuesday 18:00–20:00 Location: P5

MM 19.1 Tue 18:00 P5

RuNNer 2.0: A Fast Software Environment forHigh-Dimensional Neural Network Potentials — •Moritz R. Schäfer[1,2], Alexander L. M. Knoll[1,2], J. Richard Springborn[1,2], Henry Wang[1,2], K. Nikolas Lausch[1,2], Moritz Gubler[3], Jonas A. Finkler[4], Gunnar Schmitz[1,2], Alea Miako Tokita[1,2], Emir Kocer[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Paul Scherrer Institute PSI, Villigen, Switzerland — [4]Department of Chemistry and Bioscience, Aalborg University, Denmark

Machine learning potentials (MLPs) have emerged as a widely used approach for large-scale atomistic simulations in chemistry and materials science. They offer computationally efficient access to highly accurate potential energy surfaces (PES) derived from ab initio reference data. As techniques in this area continue to grow in complexity and reach greater maturity, the need for robust, efficient, and user-friendly tools becomes increasingly significant. Here, we introduce the second major release of RuNNer, an open-source, stand-alone software package designed for constructing and evaluating second-, third-, and fourth-generation high-dimensional neural network potentials (HDNNPs). RuNNer 2.0 integrates the complete workflow into a fully MPI-parallelized program – from generating atomistic descriptors and training machine learning models to deploying them in molecular dynamics simulations.

MM 19.2 Tue 18:00 P5

Coordination Corrected Enthalpies for the Thermodynamics of Ionic Materials — •Balaram Thakur[1,2] and Rico Friedrich[1,2] — [1]Technische Universität Dresden, 01062 Dresden. — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden.

Accurate formation enthalpies are essential for data-driven materials discovery. Density functional theory (DFT) predictions are accurate for compounds chemically similar to their elemental references (metallic systems like alloys). However, for ionic materials, it shows large deviations from the experimental values ($\geq$ 100 meV/atom), leading to incorrect stability predictions. The coordination-corrected enthalpies (CCE)[1] method addresses this issue by applying corrections based on oxidation state and cation coordination number. This reduces errors to about 25 meV/atom and resolves inconsistencies among polymorphs.

Here, we extend CCE beyond oxides to halides, focusing on fluorides and chlorides, chosen for their diverse bonding environments and technological relevance in the energy sector, electronics, and optics. Using AFLOW [2,3], these corrections broaden the applicability of CCE and improve thermodynamic predictions for halogen-based ionic compounds, thus enabling more reliable design and screening of functional materials.

[1] R. Friedrich, *et al.*, npj Comput. Mater. **5**, 59 (2019).
[2] R. Friedrich, *et al.*, Phys. Rev. Mater. **5**, 043803 (2021).
[3] S. Divilov, *et al.*, High Entropy Alloys and Mater. **3**, 178 (2025).

MM 19.3 Tue 18:00 P5

Experimentally supported machine-learning interaction potential for Pd-Si — •Przemyslaw Dziegielewski[1], Jerzy Antonowicz[1], Zuzanna Kostera[1], Oleksii Liubchenko[2], and Ryszard Sobierajski[2] — [1]Faculty of Physics, Warsaw University of Technology, Warsaw, Poland — [2]Institute of Physics Polish Academy of Sciences, Warsaw, Poland

Classical Molecular Dynamics (MD) simulations were utilised to reproduce the X-ray Free-Electron Laser (XFEL) experiment. Using the pump-probe technique, a Pd-Si alloy with various Si contents was melted and subsequently solidified with a high cooling rate. The EAM (Embedded Atom Method) potentials available for Classical MD allowed us to obtain simulation results showing high consistency with the experiment for pure Pd and the good glass-forming Pd83Si17 alloy.

However, at low Si contents, they become unreliable, generating a structure that is a combination of the hcp and fcc phases, whereas the experimental data clearly indicate the occurrence of the fcc phase only. The two phases differ only slightly in energy, and the occurrence of the hcp phase for alloys with nearly 100% Pd content takes place, for example, under high-pressure conditions. In our presentation, we introduce an alternative approach to simulating metallic alloys using a Machine Learning (ML)-generated potential within the VASP code. Our proposed procedure may constitute a universal approach for the effective and rapid creation of interaction potentials for the purpose of analysing experimental data.

MM 19.4 Tue 18:00 P5

Unveiling Anharmonicity in High-temperature Diffusion Through Transition State Thermodynamic Integration — •Wenchuan Liu[1], Xi Zhang[1], Xu Xiang[1], Sergiy Divinski[2], and Blazej Grabowski[1] — [1]Institute for Materials Science, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Institute of Materials Physics, University of Münster, 48149 Münster, Germany

Accurate modeling of high-temperature atomic diffusion requires a full treatment of thermal effects, particularly anharmonic lattice vibrations, which are often oversimplified in density functional theory (DFT)-based descriptions. We introduce a novel ab initio method, transition state thermodynamic integration (TSTI), that explicitly incorporates anharmonic contributions to vacancy migration Gibbs energies. TSTI combines DFT, molecular dynamics, and machine-learning interatomic potentials within a unified ab initio framework. Applied first to BCC tungsten, the method quantitatively captures non-Arrhenius diffusivities arising from anharmonicity. We further demonstrate its general applicability to metastable HCP aluminum, enabling high-fidelity input for CALPHAD-type mobility modeling. TSTI provides a general route to computing high-temperature diffusivities with DFT accuracy.

MM 19.5 Tue 18:00 P5

Every configuration counts: An Exact Approach to Doping Effects in AlN — •Oliver Heymer and Jens Kortus — Institute of Theoretical Physics, Freiberg, Germany

We present a new method to study doping effects within Kohn Sham density functional theory. Unlike Zungers Special quasirandom structures [1], our approach generates a complete and irreducible set of crystal structures, capturing all possible atomic configurations and making the description exact. Because we preserve full structural information, we can evaluate configurational entropies and identify the temperatures at which disordered doped AlN structures become energetically favored over the undoped material. Finally, we highlight how doping modifies the band structure and the density of states at the Fermi level.

[1] Zunger A, Wei S, Ferreira LG, Bernard JE. Special quasirandom structures. Phys Rev Lett. 1990 Jul 16;65(3):353-356. doi: 10.1103/PhysRevLett.65.353.

MM 19.6 Tue 18:00 P5

OpenCPMD: Plane-wave-based ab initio molecular dynamics code for large-scale HPC facilities — Tobias Klöffel[1,2], Christian L. Ritterhoff[1], Sagarmoy Mandal[1,2,3], Ritama Kar[3], Nisanth N. Nair[3], and •Bernd Meyer[1,2] — [1]ICMM/CCC, FAU Erlangen-Nürnberg — [2]National High Performance Computing Center, FAU Erlangen-Nürnberg — [3]Department of Chemistry, Indian Institute of Technology Kanpur (IITK), India

We present our recent advances in enabling fast and scalable *ab initio* molecular dynamics simulations on massively parallel HPC architectures with OpenCPMD (www.cpmd.org), an open source, plane-wave-based DFT code [1]. Code changes include new algorithms for hybrid functionals (localization of the orbitals, factorization of the Fock operator, multiple time-stepping [2]), revision of data distribution and communication patterns to reduce inter-node communication, introduction of overlapping computation and communication, partitioning the workload by auto-tuning algorithms, and porting to GPUs. The enhanced performance and scalability of the code is demonstrated on simulations of liquid water with up to 2048 molecules in the unit cell. We show that simulations with many hundred of water molecules for several 100 ps can be done now routinely within a few days, allowing systematic free energy calculations of chemical processes in liquids.

[1] T. Klöffel, G. Mathias, B. Meyer, Comput. Phys. Commun. **260** (2021) 107745
[2] R. Kar, S. Mandal, V. Thakkur, B. Meyer, N.N. Nair, J. Chem. Theory Comput. **19** (2023), 8351–8364

MM 19.7 Tue 18:00 P5

A Hartree-Fock Analysis of the Finite Jellium Model — •Michael Píro and Jaroslav Hamrle — Czech Technical University, Prague, Czech Republic

A Hartree-Fock analysis of the ground-state electronic structure of the finite spherical jellium model is carried out for systems containing up to 520 electrons in a positive background field with densities ranging from 10^{-3} to 1. The study focuses on resolving the energy-level ordering, accurately characterizing the total energy contributions, and evaluating the performance of local exchange and kinetic-energy approximations. All calculations are performed on a high-resolution real-space grid. Significant discrepancies are observed between the exchange energy obtained from the Hartree-Fock approximation and that predicted by the local density approximation (LDA) evaluated at the computed electron densities, both in the inner region and near the surface of the system. To reconcile these differences, a refined expression for the local one-electron exchange energy density is proposed. In addition, the breakdown of the Thomas-Fermi kinetic-energy model near the surface is addressed by introducing an improved expression for the one-electron kinetic-energy density.

MM 19.8 Tue 18:00 P5

Benchmarking Local Geometry Optimization Algorithms for Realistic Potential Energy Surfaces of Solids — •David Greten[1], Konstantin Jakob[1], Karsten Reuter[1], and Johannes T. Margraf[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universität Bayreuth

Efficient and robust local structure relaxations are central to computational materials discovery. We benchmark several widely used local optimizers (based on the BFGS, FIRE and conjugate gradient approaches) for relaxing inorganic crystal structures on complex many-body potential energy surfaces obtained from a universal machine-learned interatomic potential. From relaxations of over 170,000 trial structures generated via element substitution, we quantify convergence rates, relaxation efficiency, and the stability and diversity of obtained minima. Some algorithms (e.g. BFGS with line-search and SciPy's conjugate gradient) show substantially higher convergence rates and consistently yield low energy minima. Meanwhile, the computational effort of the tested algorithms is broadly comparable. Based on these insights we discuss how to optimally combine algorithms to obtain a good trade-off between robustness and diversity of explored minima.

MM 19.9 Tue 18:00 P5

Acquisition strategies in multi-objective Bayesian optimization — •Tatu Linnala[1,2], Matthias Stosiek[1], Joakim Löfgren[2], and Patrick Rinke[1,2] — [1]Department of Physics, Technical University of Munich, Garching, Germany — [2]Department of Applied Physics, Aalto University, Espoo, Finland

Bayesian optimization (BO) is a machine learning technique for optimizing expensive black-box functions, and it is increasingly used in computational and experimental materials optimization. Many BO applications involve multiple competing objectives, requiring multi-objective BO (MOBO) to approximate the Pareto front. We extended the Bayesian Optimization Structure Search (BOSS) code to support advanced MOBO methods, focusing on acquisition strategies. Specifically, we implemented three variants of the expected hypervolume improvement acquisition function: an exact form for bi-objective problems and Monte Carlo approximations for higher dimensions. Additionally, we included scalarization-based methods for greater computational efficiency. These methods were benchmarked on six test cases, including synthetic functions and a real-world lignin extraction problem. Results show that hypervolume-based methods yield the most accurate predictions at high computational cost, although scalarization methods may sometimes be sufficient. This highlights the trade-off between accuracy and computational cost, and the application specificity of the optimal strategy. We provide guidelines for selecting appropriate MOBO settings, and the extended BOSS code provides a flexible toolkit for multi-objective optimization.

MM 19.10 Tue 18:00 P5

Transfer Learning Pipeline for GRACE Foundation Models for Complex Materials — •Christian L. Ritterhoff[1], Yury Lysogorskiy[2], Anton Bochkarev[2], Bernd Meyer[1], and Ralf Drautz[2] — [1]Interdisciplinary Center for Molecular Materials (ICMM) and Computer Chemistry Center (CCC), FAU Erlangen-Nürnberg — [2]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum (RUB)

Foundation models of machine-learned interatomic potentials (MLIPs) offer overall good accuracy for a wide range of configurational and chemical spaces. However, achieving high fidelity and high efficiency for dedicated applications often requires further refinement of the model. This is commonly achieved by fine-tuning the foundation model on minimal specialized training data followed by distillation of the acquired knowledge into smaller models. We benchmark different strategies for the example of carbon with its demanding diverse chemistry and structure by fine-tuning the GRACE-1L-OMAT foundation model using the dataset by Qamar *et al.* [1]. Data efficiency is analyzed by training only on randomly chosen subsets of the complete dataset. Advantages of fine-tuning are demonstrated by comparing the obtained models against their randomly initialized counterparts. Finally, the resulting high-fidelity GRACE potential is used for knowledge distillation into a fast, local ACE model. This work validates the transfer learning and distillation paradigm as a robust and efficient pathway for creating deployable potentials for complex materials.

[1] M. Qamar, *et al.*, J. Chem. Theo. Comput. **19** (2023) 5151–5167

MM 19.11 Tue 18:00 P5

LLZO grain boundaries with doped amorphous domains by adaptively fine-tuned machine-learning interatomic potentials — •yuandong wang, yute chan, karsten reuter, and christoph scheurer — Fritz-Haber-Institut der MPG, Berlin, Germany

Garnet $Li_7La_3Zr_2O_{12}$ (LLZO) is a highly promising solid-state electrolyte (SSE) for lithium batteries. However, its application faces challenges, primarily arising from Li dendrite formation, the impact of grain boundaries (GBs) on Li transport and stability. Introducing amorphous intergranular domains can mitigate dendrite propagation while enhancing Li-ion mobility in GBs. Moreover, aliovalent cation doping (e.g., Al^{3+}, Ga^{3+}, Nb^{5+}, Ta^{5+}) in both cubic and amorphous LLZO offers additional levers to further enhance key properties. Rationally engineering the morphology of amorphous GBs offers an intriguing approach for tuning electrolyte performance.

In this study, we investigate strategies for generating structural motifs covering Li diffusion, GBs, and amorphous LLZO, which are diversified to include ion hopping transition states, large defects, amorphous motifs, etc. An adaptively fine-tuned MACE machine-learning interatomic potential (MLIP) is trained to accurately model large-scale and realistic nanoscale structures of LLZO with doped amorphous GBs. With the fine-tuned MLIP, the morphology, dopant effects and crystalline-amorphous interactions governing Li-ion diffusion pathways and activation barriers in LLZO can be studied in detail.

MM 19.12 Tue 18:00 P5

SEI-ntific Discoveries: A DFTB Journey with Constant Potential — •Anton Beiersdorfer[1], Tobias Melson[2], Felix Riccius[1], Chiara Panosetti[1], Christoph Scheurer[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Max Planck Computing and Data Facility, Garching

Lithium-ion batteries excel in short-term power grid balancing, yet their performance and longevity are strongly impacted by the solid electrolyte interphase (SEI) formed at the anode-electrolyte interface. Accurate SEI-formation modeling demands a simulation framework that can explore timescales inaccessible to *ab initio* molecular dynamics (MD) and is simultaneously capable of accounting for explicit electron transfer – a capability lacking in standard machine-learning interatomic potentials.

To this end, we introduce a novel approach that combines the thermopotentiostat [1] simulation scheme with density functional tight binding (DFTB) electronic structure calculations. This enables MD simulations of the anode-electrolyte interface at constant potential and up to the timescale of initial decomposition reactions on the anode surface. We assess the capabilities and limitations of this approach in providing valuable insights into SEI formation and its impact on battery performance and degradation.

[1] F. Deißenbeck *et al.*, Phys. Rev. Lett. **126**, 136803 (2021).

MM 19.13 Tue 18:00 P5

Separating light and heat effects in the electrochemical performance ofilluminated V_2O_5 lithium-ion battery cells — •Pavel Rozov[1], Tom Wickenhäuser[1], Luca Bischof[1], Ewa Mijowska[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Faculty of Chemical Technology and Engineering, West Pomeranian University of Tech-

nology, Szczecin, Poland

Recent studies have demonstrated that lithium-ion batteries can exhibit enhanced electrochemical performance under optical light illumination. However, light exposure also may cause local heating, making it challenging to separate bare photonic and photo-thermal effects. Here, the effects of light illumination on V_2O_5-based electrodes as photoactive cathode material are studied in lithium metal half-cells in which photo-thermal effects are monitored by means of an in-situ Pt1000 thermometer. Our studies allow us to disentangle photonic and temperature effects. We find slightly enhanced Li+ diffusion under illumination but do not confirm significant light-induced enhancement of the battery performance beyond temperature effects which is reported in the literature.

MM 19.14 Tue 18:00 P5

Shining a Light on Stored Charges: Linking Excitation Spectra to Polaron Dynamics in Solar Battery Materials — •Leon Müller, Matthias Kick, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Solar battery materials integrate light harvesting and charge storage within a single component, offering a pathway toward simplified systems that could serve as key elements in future nanoscale energy devices. First experimental findings suggest that charge storage involves the formation of long-lived polaronic states. However, the underlying processes of exciton generation, subsequent charge separation and trapping that enable stable charge storage remain elusive.

Experimentally, charging is accompanied by a reversible color change from white or yellow to blue, indicating a potentially more dynamic process in which charges can jump between multiple trapping sites. This photochromism has been observed in many of the solar battery materials discovered so far, hinting at a mechanism that may be universal to this class of systems.

To explore the processes of charge generation and trapping, we study $LiNbWO_6$ using time-dependent density-functional theory to model the optical response of polaronic states. By connecting the excitation spectra to the underlying dynamics of the stored charges, we aim to clarify the mechanisms that govern charge localization and stability, thereby establishing a microscopic framework for charge storage in solar battery materials.

MM 19.15 Tue 18:00 P5

Anisotropic Thermoelectric Energy Converters Based on Bi Microwires and Films. — •Leonid Konopko[1], Albina Nikolaeva[1], Tito Huber[2], and Denis Shiversky[1] — [1]Technical University of Moldova, Chisinau, Moldova — [2]Howard University, Washington, DC, USA

We demonstrate an innovative method for thermoelectric energy conversion utilizing a single-element device made from an anisotropic material. In such materials, heat flow generates a transverse thermoelectric electric field perpendicular to the direction of the heat transfer. For our experiments, we produced a sample using a 10-meter-long, glass-insulated, single-crystal tin-doped bismuth microwire (outer diameter - 20 μm; core diameter - 4 μm). A crucial aspect of this process was the successful growth of the microwire as a single crystal, achieved through laser-assisted recrystallization under a strong electric field. The microwire was coiled into a flat spiral and mounted onto a thin copper disk. This sample demonstrated high sensitivity to heat flow, reaching up to 10^{-2} V/W, with a time constant of approximately 0.2 seconds. Bismuth films with thicknesses ranging from 2 to 5 μm were deposited onto mica substrates. Experimental samples of heat flux sensors were then fabricated by recrystallizing these films under laser heating in a strong electric field. The observed voltage dynamics at the output of all sensors, in response to modulated heat fluxes, align well with theoretical predictions for anisotropic thermoelectric elements.

The study was supported by the State Project "ReBRAIN" #25.80013.5007.07RE, 2025-2026.

MM 19.16 Tue 18:00 P5

Structure and transport properties of Li-Zr-Cl-O oxychloride solid electrolytes — •Ziyan Zhang[1,2], Shuai Chen[3], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany — [3]TUM School of Natural Sciences, Chair for Physics of Energy Conversion and Storage, Garching, Germany

All-solid-state batteries using halide-based electrolytes have attracted attention due to their promising combination of room-temperature ionic transport, formability, and interfacial compatibility. Within this class, oxychloride compositions offer an additional degree of freedom via anion chemistry while retaining the beneficial processing of chlorides. The current study systematically characterizes mechanochemically prepared Li-Zr-Cl-O oxychlorides. A targeted Li2+yZrCl6-yOy series was established under standardized processing conditions. Laboratory powder X-ray diffraction was used to quantify the structural response to changes in oxygen content and processing conditions, using Rietveld analysis to determine lattice parameters. Electrochemical impedance spectroscopy yielded ionic conductivities and activation energies at ambient temperature. The resulting dataset provides a detailed composition-processing-structure- transport map for Li-Zr-Cl-O and delineates a practical recipe window for maximizing room-temperature conductivity under a purely mechanochemical synthesis route, thereby laying a robust laboratory baseline for subsequent interfacial and operando investigations.

MM 19.17 Tue 18:00 P5

Segregation of H in planar defects of BCC Fe — •Rohan Kumar, Mariano Forti, Rebecca Janisch, Thomas Hammerschmidt, and Ralf Drautz — Ruhr university Bochum, Universitatstr 150, 44801, Bochum Germany

The transition to a hydrogen-based economy in Europe is well underway, but challenges remain in the development of suitable infrastructure, as well as in migrating the existing facilities. Among other dificulties hydrogen embrittlement of steels hinders the applicability of known and new materials for hydrogen technologies.

This study focuses on the atomistic simulation assessment of hydrogen embrittlement in body-centered cubic (BCC) Fe using advanced computational methods. Density Functional Theory (DFT) is a standard tool for studying segregation phenomena, providing high accuracy but limited to small systems and short time ranges. In the other hand, the recent emergence of universal machine learning interatomic potentials (MLIPs) pose them as a powerful tool to study atomistic systems at larger scales with DFT precision.

In this work, we utilize GRACE MLIP to study tilt and twist grain boundaries (GBs) in ferritic Fe, finding GB energies in agreement with DFT results. The GBs were analyzed using DBSCAN and Voronoi analysis to identify hydrogen segregation sites. We study H segregating of in both tilt and twist GBs and analyze site preference trends.

MM 19.18 Tue 18:00 P5

Experimental Determination of Site Energy Spectrum of Hydrogen in Metal Thin Films — •Magdalena Seiler, Stefan Wagner, and Astrid Pundt — Karlsruhe Institute of Technology (KIT), Institute of Applied Materials (IAM-WK), Engelbert- Arnold-Straße 4, 76131 Karlsruhe, Germany

Metal-hydrogen interactions affect the mechanical properties of structural materials and the performance of solid-state hydrogen storage. Hydrogen occupies the metal lattices interstitial sites or different defects, whose site energy distribution characterizes the metal-hydrogen interaction. The site energy can be affected by the stress state, as suggested by theoretical calculations [1]. In this presentation, the constraints of a thin film adhered to a rigid substrate serve as a model 2D stress state. We experimentally determine the chemical potential of hydrogen in respective metal thin films during electrochemical hydrogen loading, and simultaneously measure the stress resulting in the hydrogen-absorbing, 1D expanding thin film. The result is compared to a Distribution of Site Energies (DOSE) model [2], in which Fermi-Dirac statistics are used to describe the hydrogen occupancy of the density of sites. Thereby, we obtain a site energy spectrum and quantify defect fractions.

[1] A. Dyck, T. Böhlke, A. Pundt, S. Wagner, Scripta Materialia 247 (2024) 116117.

[2] S. Wagner, A. Pundt, AIMS Materials Science 7 (2020) 399-419.

MM 19.19 Tue 18:00 P5

In-Situ Electrochemical Micromechanics of Hydrogen-Charged Palladium — •Hou Zhang[1], Henry Ovri[1], and Shan Shi[1,2] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany

The substantial lattice parameter mismatch between the hydrogen-diluted and hydrogen-rich phase, coupled with the embrittlement effect in metal hydrides, are critical factors limiting the long-term struc-

tural integrity and performance reliability of hydrogen-related functional materials used in actuation, sensing, transportation, and energy storage. Palladium, due to its high hydrogen solubility, rapid hydrogen diffusion at room temperature, and its ability to reversibly absorb and desorb hydrogen through electrochemical control, serves as a model material for studying the underlying chemo-mechanical coupling. However, the local mechanical response and microstructural evolution of Pd during electrochemical hydrogen absorption are not yet fully understood. In this study, we employ an in-situ electrochemical nanoindentation setup to conduct compression tests on Pd micropillars subjected to varying hydrogen concentrations. Electron backscatter diffraction (EBSD) analysis will be used to characterize grain orientation, enabling us to further investigate the influence of crystallographic orientation. The insights gained from this study will deepen the understanding of chemo-mechanical coupling in metal-hydrogen systems and contribute to the advancement of hydrogen-related technologies.

MM 19.20 Tue 18:00 P5

In-depth Study of Hydrogen Permeation through Zinc Coated Steel — •Tatjana Ott[1,2], Elahe Akbari[1], Christoph Cobet[2], Jiri Duchoslav[2], Heiko Groiss[2], Andreas Muhr[3], Reza Sharif[3], Thomas Steck[3], Laura Mears[1], and Markus Valtiner[1] — [1]Institute of Applied Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Johannes Kepler University Linz, Altenberger Straße 69, 4040 Linz, Austria — [3]voestalpine Stahl GmbH, 4020 Linz, Austria

Objectives: Hydrogen permeation measurements are used to obtain information such as diffusion coefficients and trap sites, as well as to investigate corrosion processes. Studying the hydrogen permeation through zinc coated steel sheets provides insights into the mechanisms of cathodic hydrogen generation and the protective capabilities of different zinc coatings. Utilizing samples prepared with an optimized sample preparation protocol, hydrogen permeation through zinc coated ultra-high-strength steel (UHSS) was investigated.

Results and Conclusions: The electrochemical process for the palladium deposition on steel was optimized, resulting in an increased sensitivity for hydrogen permeation. Different zinc coatings were compared to determine the protective abilities of the coating as well as different types of entry side reactions. Results showed that the zinc coatings provided significant protection against hydrogen permeation. Overall, hydrogen permeation measurements provided valuable insights regarding both the reactions taking place at different coating types and their protective abilities.

MM 19.21 Tue 18:00 P5

Hydrogen-induced resistance response in nanoporous Pd-Cu thin film — •Yushen Huang[1] and Shan Shi[2,1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany

The large-scale utilization of hydrogen energy requires high-performance sensing technologies for real-time hydrogen monitoring and leakage prevention. Pd-based hydrogen sensors are considered among the most promising candidates and are widely used in commercial devices due to palladium's strong affinity for hydrogen. However, during cyclic hydrogen absorption and desorption, Pd undergoes repeated phase transition, which can lead to accumulation of local misfit strains and defects. This results in signal hysteresis, prolonged response times, and poor reproducibility particularly in dense Pd films. Inspired by the excellent microstructural stability and actuation performance durability observed in nanoporous Pd bulk samples after over 1500 cycles of phase transition, this work investigates the potential of nanoporous Pd-Cu thin films for hydrogen sensing. In this work, a nanoporous Pd-Cu thin film (~100 nm thick) was prepared via electrochemical dealloying, and its electrical resistance response during electrochemical hydrogen charging was measured using a four-point probe method. Additionally, the pore size of nanoporous Pd-Cu will be tuned by adjusting the preparation conditions and post thermal treatment, enabling the sensors with enhanced stability, long-term reliability, and high-precision hydrogen monitoring.

MM 19.22 Tue 18:00 P5

Crystallization kinetics of supercooled liquid palladium — •Zuzanna Kostera[1], Przemyslaw Dziegielewski[1], Ryszard Sobierajski[2], and Jerzy Antonowicz[1] — [1]Warsaw University of Technology, Faculty of Physics, Warsaw, Poland — [2]Polish Academy of Science, Institute of Physics, Warsaw, Poland

In this work we use large-scale molecular dynamics to study crystallization kinetics of supercooled liquid palladium over 0.3-0.6 T_m (T_m = 1828K). The crystallization temperature strongly affects the final polycrystalline morphology, reflecting temperature-dependent nucleation and growth kinetics. From the evolving grain structure we extract homogeneous nucleation and growth rates and construct a time*temperature*transformation (TTT) diagram. The TTT diagram yields a critical cooling rate of 10^{13} K/s, consistent with Pd's poor glass-forming ability. Homogeneous nucleation peaks at 10^{35} $m^{-3}s^{-1}$ near 0.5 T_m and its temperature dependence agrees with classical nucleation theory.

MM 19.23 Tue 18:00 P5

DFT study of the optical and electronic properties of N-Acyl-N'-Aryl thiourea derivatives — •amani zaghdoudi — University of Carthage, Faculty of Sciences of Bizerte, Laboratory of Materials Physics: Structure and Properties (LR01ES15), Physics of Nanometric Components and Devices Group, Jarzouna 7021, Bizerte, Tunisia

We report a DFT-based theoretical study of novel N-acyl-N'-aryl thiourea derivatives as potential selective fluoride sensors. Molecular structures were optimized at the B3LYP/LANL2DZ level with GAUSSIAN 09.

IR, Raman, and UV-Vis spectra were simulated to probe their vibrational and electronic responses. UV-Vis analysis reveals π-π* and n-π* transitions influenced by aryl substituents and fluoride binding. IR and Raman results show characteristic C=O and C=S stretches, with frequency shifts upon complexation, indicating interaction at the thiourea core.

Mulliken and NBO analyses reveal charge redistribution and donor*acceptor interactions. Frontier molecular orbital analysis indicates a reduced HOMO-LUMO gap upon fluoride binding, suggesting enhanced reactivity. These findings support the application of these compounds as promising molecular fluoride sensors.

MM 19.24 Tue 18:00 P5

Electronic properties of Carbon nanoscrolls — •Tzu-Ching Hsu[1], Jhih-Shih You[1], Hsiu-Chuan Hsu[2], and Ion Cosma Fulga[3] — [1]Department of Physics, National Taiwan Normal University, Taipei, Taiwan, — [2]Graduate Institute of Applied Physics, National Chengchi University, Taipei, Taiwan — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany

Carbon nanoscrolls (CNS), rolled-up structures formed from single-layer graphene, have recently attracted significant attention owing to their distinctive geometry. In this work, we theoretically investigate the topological properties of a series of ABC-stacked CNS with various chiral vectors that break mirror symmetry, within the small-curvature approximation. As the chiral vector is varied, we find that the Dirac cones in the fictitious Brillouin zone shift away from half of the magnetic flux quantum. Furthermore, we show that the combined C_2T symmetry, the composition of a 180° rotation and spinless time-reversal symmetry, protects the Dirac cones even when chiral symmetry is broken. Our results provide a foundation for further studies of the fundamental physics and potential applications of CNS and other two-dimensional materials with similar geometries.

MM 19.25 Tue 18:00 P5

Correlating Atomic Structure and Grain Boundary Energy in the 5D Space of Degrees of Freedom — •Mahkam Madadi[1], Timo Schmalofski[1], Martin Kroll[2], Holger Dette[3], and Rebecca Janisch[1] — [1]ICAMS, Ruhr-University Bochum, Germany — [2]Chair of Stochastics and Machine Learning, University of Bayreuth, Germany — [3]Chair of Stochastics, Ruhr-University Bochum, Germany

In materials design, it is essential to develop grain boundary (GB) models that effectively relate the atomic structure to the macroscopic properties of grain boundaries. Grain boundaries are categorized by five degrees of freedom (DOF), which include grain boundary plane orientation, rotation axis, and the misorientation angles between adjacent grains. On the other hand, the energy associated with these boundaries is governed by microscopic state, including atomic positions and structural units . This study seeks to investigate the correlation between the microscopic structure and the energy of grain boundaries. Previous studies often explored only a subset of these DOFs, typically by varying one or two while keeping the others fixed. In contrast, this study employs molecular statics in combination with a statistical approach [1] to assess the complete 5D space of DOFs and to model and analyze the microstructure-energy relationship.

[1] T. Schmalofski, M. Kroll, H. Dette, and R. Janisch. Towards

active learning: A stopping criterion for the sequential sampling of grain boundary degrees of freedom. Materialia, 31:101865, 2023. https://doi.org/10.1016/j.mtla.2023.101865

MM 19.26 Tue 18:00 P5

Machine-learned interatomic potentials for hydrogen-affected fracture in silica minerals — •Valentína Berecová[1,2], Martin Friák[1], and Jana Pavlů[2] — [1]Inst. Phys. Mater., Czech Acad. Sci., Brno, Czech Republic — [2]Dept. Chem., Masaryk Uni., Brno, Czech Republic

Flint, a cryptocrystalline form of silica, is known for its ability to fracture into curved surfaces through conchoidal flaking. Although this behaviour has been used for millennia to produce cutting tools, the atomistic mechanisms that enable such edges remain poorly understood. To clarify these processes, we develop a machine-learned Si-O-H interatomic potential trained on high-accuracy quantum-mechanical data, providing near ab initio resolution at computational costs suitable for simulations. Particular attention is given to hydrogen-related interactions: natural flint contains hydration and hydroxylation that can influence fracture pathways and crack propagation. The training dataset includes hydrogen-containing species, surface terminations, strained configurations, amorphous structures and defect environments. The resulting potential is applied to atomistic simulations of fracture in defect-rich silica, offering new insight into conchoidal fracture at the atomic scale and supporting the design of brittle materials with controlled failure behaviour. Financial support from the Czech Academy of Sciences (Praemium Academiae of M.F. and the Strategy AV21 project "The power of objects: Materiality between past and future") is gratefully acknowledged. Computational resources were provided by e-INFRA CZ and IT4Innovations National Supercomputing Center.

MM 19.27 Tue 18:00 P5

Silica-Supported Nano Metal Complexes Derived from a Schiff Base Ligand: Structural, Theoretical, and Catalytic Investigations — •Tarek El-Dabea — Chemistry Department, Faculty of Science, King Salman International University, Ras Sudr, Sinai 46612, Egypt

Silica-based nanomaterials were prepared from natural silica sand and used as supports for nano metal complexes containing Ru(III), Fe(III), VO(II), and Ag(I) ions. The SiO2 support, obtained via a grinding and paste-based technique, provided a stable high-surface matrix for immobilization. Complexes derived from a bidentate Schiff base ligand were characterized by spectroscopic and analytical methods, confirming their geometry and stoichiometry. Solution studies showed stable metal-ligand coordination, while DFT and TD-DFT analyses gave insights into the optimized structures and electronic transitions consistent with experiment. Among the investigated systems, the Ru(III)/SiO2 composite exhibited distinctive electronic and catalytic properties, efficiently promoting multicomponent reactions under microwave irradiation. Optimized eco-friendly conditions (H2O/EtOH) gave high yields, and the catalyst

MM 19.28 Tue 18:00 P5

synchrotron XAFS Study of Fe3O4/Au core–shell nanoparticles for magnetic–plasmonic applications — •Mai EL-Masry[1], Giuliana Aquilanti[2], Messaoud Harfouche[3], Neama Imam[4], and Jan Ingo FLEGE[4] — [1]Thebes Higher Engineering Institute, Cairo, Egypt — [2]Elettra Sincrotrone Trieste, Italy — [3]SESAME Synchrotron, Aman, Jordan — [4]Brandenburg University of Technology Cottbus-Senftenberg, Germany

Magneto-plasmonic nanostructures enable multifunctional biomedical applications, including imaging, sensing, and targeted diagnostics. We synthesized Fe3O4/Au core–shell nanoparticles via a seed-mediated method and characterized them using synchrotron X-ray Absorption Fine Structure (XAFS) at the Fe K and Au L3 edges. XAFS analysis provided element-specific information on oxidation state, coordination, and local structure, confirming core–shell integrity and strong interfacial coupling. XRD and high-resolution TEM verified a crystalline Fe3O4 core and FCC Au shell, while VSM measurements demonstrated superparamagnetic behavior with high saturation magnetization. EXAFS and XANES results revealed metallic Au and Fe–O coordination consistent with magnetite, confirming successful shell formation. These results establish the structure-property relationship in magnetic–plasmonic nanostructures and demonstrate the importance of SESAME synchrotron techniques for advancing nanomaterials for sensing, imaging, and biomedical technologies.

MM 19.29 Tue 18:00 P5

Relaxation and crystallization behavior of the metallic glass former PdNiP near the glass transition temperature — •Noah Colell — Universität Münster, Institut für Materialphysik, Wihelm-Klemm Str. 10, 48149 Münster

Analysis of $Pd_{40}Ni_{40}P_{20}$ metallic glass is conducted with Flash DSC measurements, realizing high heating and cooling rates. Relaxation is realized through systematically varying temperatures and durations of annealing by cycling to investigate the effects on glass transition and crystallization. Different relaxation modes (α and β) are targeted and their response to the heat treatment is analyzed. Due to the high rates available in Chip calorimetry, the range of temperatures available for relaxation experiments avoiding crystallization can be extended. As one results, it is observed that the relaxation enthalpy does not show a linear trend even with logarithmic scaling. This might be due to the combining effects of α and β relaxation. Through different annealing times different relaxation modes seem to be activated. The so-called shadow glass transition (β) can be seen with smaller duration and converges into a stronger enthalpy recovery with larger ones. This indicates a connection between the two relaxation modes.

MM 19.30 Tue 18:00 P5

Molecular micro-heterogeneity: Structure formation and phase behavior in aqueous alkylamine mixtures — •Lena Friedrich[1], Martina Požar[2], Aurélien Perera[3], Michael Paulus[1], Nicola Thiering[1], Jaqueline Savelkouls[1], Eric Schneider[1], Bernada Lovrinčević[2], Dirk Lützenkirchen-Hecht[4], and Christian Sternemann[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]University of Split, Faculty of Science, 21000 Split, Croatia — [3]Sorbonne Université, Laboratoire de Physique Théorique de la Matière Condensée, F75252 Paris, France — [4]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany

Aqueous alkylamines exhibit an unusual phase behavior [1] and an intruiging form of self-assembly [2]. X-ray diffraction experiments at BL8 and BL9 (DELTA, TU Dortmund) reveal intense structur factor pre-peaks that vary with composition and chain length, indicating peculiar micro-heterogeneity. Diffraction intensities calculated from MD simulations resemble the measured intensities and show bilayer-like arrangements in which amine headgroups saturate and stabilize water domains, forming transient clusters that prevent macroscopic phase separation, explaining the remarkable miscibility of aqueous amines compared to other associating liquids such as alcohols [3]. Supported by BMBF via DAAD in PROCOPE (57704875 & 50951YA). [1] J. Glinski et al., J. Colloid. Interface Sci. 162, 129-134 (1994); [2] L. Almasy et al., PCCP 21, 9317 (2019); [3] A. Perera et al., arXiv:2510.02146

MM 19.31 Tue 18:00 P5

Effects of physical properties on the solidification kinetics of undercooled Zr-Cu-Ni alloy under reduced gravity — •Chu Yu, Yindong Fang, and Stephanie Lippmann — IAP, FSU Jena, Albert-Einstein-Straße 15, 07745, Jena, Germany

In our previous work, we investigated the solidification kinetics of glass forming alloy Zr50Cu35Ni15 using electromagnetic levitation facilities (EML) under different gravity conditions to compare with the electrostatic levitation facility (ESL). Using both methods, crystal growth velocities increased with increasing undercooling below 260 K. Within the undercooling range 260-320K, velocities plateaued. Compared to ESL, EML on the ground generated stronger convective flow in the undercooled melt. Slight differences in velocities were observed within the undercooling range 50-175K. However, the primary phase is not changed by the magnetic convection. To investigate the differences in the low undercooling region and the physical properties of the melt, we measured the conductivity and viscosity of the melt under reduced gravity during parabolic flight campaign 2023 and 2025. The relationship between viscosity and crystal growth velocities at the low undercooling region is discussed.

MM 19.32 Tue 18:00 P5

Exploring Molecular Fragmentation and Structure in PVP Thin Films via Atom Probe Tomography — •Parisha Diwan — University of stuttgart

In this work, spin coating was used to create thin films of polyvinylpyrrolidone (PVP), which were then analysed using atom probe tomography (APT). APT measurements were performed to in-

vestigate the polymer at the nanoscale after lift-outs were created and shaped into sharp edges. The mass spectrum identified the primary molecular fragments generated during analysis, and the 3D reconstruction demonstrated the arrangement of various PVP molecule components in the film. These findings show that APT can help us better understand the structure of polymer thin films by providing specific chemical information. This study supports the future application of APT in polymer research and thin-film characterisation by highlighting its potential as a helpful tool for organic material analysis.

MM 19.33 Tue 18:00 P5

Electronic property analysis of structure and bonding at oxidized aluminium surfaces — •Lütfi Çağlar Ege[1], Nebahat Bulut[1], Zhengqing Wei[1], Inna Plyushchay[2], and Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz, Germany — [2]Institute of Physics, National Taras Shevchenko University of Kyiv, Ukraine

The crystal structure has a large influence on material properties that are important for many applications, especially in the case of aluminium oxide (AlO_x), which forms a protective layer on aluminium. Understanding the structure and bonding during the oxidation mechanism of the low-energy aluminium surfaces Al(001), Al(110), and Al(111) is the main interest of this study, which highlights the surface reactivity. We attempted to analyse the interaction of the electronic states and forces of the oxygen and aluminum atoms to observe the relaxed bonding positions. First principles calculations were employed as the theoretical approach to investigate the electronic properties with respect to the position of oxygen within the irreducible wedge of the surfaces.

MM 19.34 Tue 18:00 P5

The vacancy effect to the mechanical properties of high entropy borides — •Nebahat Bulut[1], Inna Plyushchay[2], Anna Pliushchai[1], and Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz — [2]Institute of Physics, National Taras Shevchenko University of Kyiv, Ukraine

High entropy transition metal diborides ($HETMB_2$) present complex lattice distortions that strongly influence their mechanical properties. These distortions are the result of atomic mismatch, metal-boron site vacancies, and strong covalent/ionic bonding. The randomly disordered structures of $HETMB_2$ are constructed with equimolar metal atom ratios to obtain the elastic stiffness tensors. Small strains are applied to the equilibrium unit cell to calculate the elastic response by performing first principles calculations using Quantum Espresso. Understanding the influence of lattice distortion on mechanical properties, we introduce distortion parameters which show the vacancy effect of different transition metal atoms. The distortion parameters were quantified based on the interatomic distances of nearest neighbor bond lengths. Mechanical stability and elastic anisotropy of $HETMB_2$ were analyzed as function of configurational disorder. It is discussed how the lattice distortions modify the Peierls barrier for dislocation motion.

MM 19.35 Tue 18:00 P5

Band geometric transverse current driven by inhomogeneous AC electric field — •M Maneesh Kumar, Sanjay Sarkar, and Amit Agarwal — Indian Institute of Technology Kanpur, Kanpur, India

We develop a semiclassical theory for electron wavepacket dynamics in the presence of an inhomogeneous AC electric field. While static electric-field gradients are known to generate charge transport governed by the quantum metric, we show that AC field gradients induce an additional geometric current that vanishes in the DC limit. This response originates from a novel band-geometric quantity, the higher-order connection (HOC) tensor, constructed from cubic products of interband Berry connections. We derive explicit expressions for the AC field-limit and identify the symmetry conditions under which it arises. Remarkably, inhomogeneous AC fields can generate an anomalous Hall-like response even in nonmagnetic systems. Applying the theory to Bernal-stacked bilayer graphene, we demonstrate that the HOC-induced response produces a measurable Hall current peaking at band edges. These results establish inhomogeneous AC fields as a powerful probe of higher-order band geometric quantities beyond Berry curvature and the quantum metric.

MM 19.36 Tue 18:00 P5

Modelling heat transport in BTBT and its derivatives using non-equilibrium molecular dynamics (NEMD) simulations — •Simon Jamnik, Florian Lindner, Florian Unterkofler, and Egbert Zojer — Graz University of Technology

Benzothieno[3,2-b]benzothiophene (BTBT) is a high-performance organic semiconductor whose derivatives C8-BTBT (with an octyl side chain) and Ph-BTBT (with a phenyl side chain) are widely used in OFETs due to their high mobilities, environmental stability and solution processability. Side-chain engineering strongly influences their physicochemical and thermal properties: experiments show that alkyl chains improve solubility while suppressing heat transport, whereas phenyl chains enhance along-chain conductivity and reduce inter-chain transport.

To analyse these effects, we employ non-equilibrium molecular dynamics (NEMD), which provides a complementary real-space perspective through spatially resolved temperature profiles and enables the direct identification of thermal-transport bottlenecks. Accurate forces for large-scale NEMD were obtained using moment tensor potentials (MTPs) trained on ab initio data generated via VASPs on-the-fly machine-learning force-field (MLFF) framework, allowing near first-principles accuracy at greatly reduced computational cost.

MM 19.37 Tue 18:00 P5

Neural Network Potentials for Molecular Dynamics Simulations of NASICON Solid Electrolytes — •Insa F. de Vries and Nikos L. Doltsinis — Institute of Solid State Theory, University of Münster, Wilhelm-Klemm-Straße 10,48149 Münster

Solid-state electrolytes are by now well-established components for the development of safe and efficient batteries. Among them, the sodium superionic conductor (NASICON) family offers an appealing degree of tunability. Their open framework allows for the substitution of lattice sites and the adjustment of diffusing ion concentration, making them an attractive choice for material design. Accurately modeling and predicting ion and thermal transport properties in these systems by *ab initio* molecular dynamics (AIMD) simulations poses a challenge due to the large supercells and time scales required. In this study, we therefore train neural network (NN) potentials for various members of the $Na_{1+x}Zr_2Si_xP_{3-x}O_{12}$ ($x = 0, 1, 2, 3$) family using training data obtained by accelerated AIMD [1]. The NN potentials are then employed to calculate the sodium ion diffusion coefficient – a key transport property. The performance and results obtained with the NN potential are validated against those obtained from *ab initio* trajectories. In addition, both the NN potential and the *ab initio* results are then compared to corresponding data generated with a previously developed force field [2].

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MM 19.38 Tue 18:00 P5

An extended two-temperature model for copper — •Simon Kümmel and Johannes Roth — FMQ, University of Stuttgart, Germany

The two-temperature model (TTM) describes a set of coupled heat conduction equations of an electronic and lattice subsystem that allows the study of materials under strong electronic excitation following laser irradiation.

Here, we present recent advances in the development of an implementation coupled to a molecular dynamics code. In particular, this implementation allows the study of effects that emerge from the change of the bond strength at high degrees of excitation. For that, we recently developed an electron temperature-dependent interaction potential for copper [1] that is capable of reproducing bond-hardening at high degrees of excitation. We discuss the importance of energy conservation when using such interactions and propose an implementation strategy.

Furthermore, we discuss the importance of taking ballistic electron motion into account before the establishment of an electron temperature within such TTM simulations. We compare two approaches and discuss the differences.

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MM 19.39 Tue 18:00 P5

Ballistic transport effects on the thermal conduction in nanowires — Ralf Meyer[1], Graham W. Gibson[2], and •Alexander N. Robillard[1] — [1]Laurentian University, Sudbury, Ontario, Canada — [2]University of Alberta, Edmonton, Alberta, Canada

The effect of ballistic transport on the thermal conduction in nanowires is studied with molecular dynamics and phonon Monte Carlo simulations. Simulations of nanowires between a heat source and a heat sink show — in agreement with previous results by other groups — the occurrence of a non-linear temperature profile with steep temperature gradients near the source and the sink combined with a reduced temperature gradient in the middle of the wire. The reduced gradients in the centre are then compared to a simple radiator model. This model predicts linear temperature profiles with a reduced gradient and discreet jumps at the wire ends. The comparison shows that if the wires are longer than the typical mean free path of the phonons, the radiator model is able to describe the reduction of the temperature gradient in the middle of the wires as well as their thermal resistances. The steep gradients at the wire ends can then be seen as the realization of the radiator model's discreet jumps in the more complex computer simulations.

MM 19.40 Tue 18:00 P5

Many-body localization for fermions and bosons - similarities and differences — •Krystian Jablonowski — University of Warsaw, Poland

In this talk, I will present a study that employs energy-level statistics as a robust diagnostic of localization phenomena across different quantum statistics. Using energy-level statistics, I analyze how Hubbard-type interactions shape the transition between localized and delocalized regimes in disordered many-body systems. Particular attention is given to how the strength of interactions influences spectral properties and dynamical behavior. A central theme of the talk is the contrast between fermionic and bosonic systems. By examining how particle statistics modify level-spacing distributions and the stability of localized phases, the study highlights both shared mechanisms and fundamental differences in their localization dynamics. Beyond mapping out the transition, I discuss how disorder and interaction-induced correlations jointly determine the structure of the many-body spectrum, offering insight into when and why localization persists or breaks down. Overall, the talk aims to provide a unified yet discriminating perspective on how fermions and bosons experience many-body localization, clarifying the similarities and distinctions that arise from their quantum statistical nature.

MM 19.41 Tue 18:00 P5

Perturbation theory for light-induced frequency shifts of thin quartz acoustic resonators — •Marinus Lehmann, Marek Bekir, and Carsten Henkel — Universität Potsdam, Institut für Physik und Astronomie, Germany

Quartz microbalance devices (QCM) are widely used for high precision mass measurements and the characterisation of liquid overlayers. In addition, QCMs are sensitive to various environmental changes like heating due to light irradiation. A light-induced shift of the acoustic resonance frequency has been shown by various groups [1,2]. Its explanation requires a combination of acoustic theory [3] with calculations for heat conduction [4] to model the cross-coupling between static thermal strain and the acoustic resonance. We try to clarify the mechanism by focussing on the time constants of the frequency shift transients.

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MM 19.42 Tue 18:00 P5

Anomalous resistance behavior of NiTi alloys at high temperatures — •Tianyi Xu[1], Leo Pies[1], Oluwaseyi Oluwabi[2], Sven Graus[1], Andreas Kreyssig[1], Jan Frenzel[2], and Anna E. Böhmer[1] — [1]Experimental Physics IV, Ruhr-University Bochum, Bochum, Germany — [2]Institute for Materials, Ruhr-University Bochum, Bochum, Germany

NiTi-based shape-memory alloys, widely used in actuators, biomedical devices, and high-precision components, are well known for their thermally driven phase transformations and associated functional properties. While their structural behavior has been extensively characterized, the electrical transport properties—particularly at elevated temperatures—remain comparatively unexplored, despite their relevance for high-temperature functional applications. In this work, the electrical resistance of $Ni_{1+x}Ti_{1-x}$ was determined up to temperatures of more than 700 °C. The resistive signature of the established martensite-austenite transition was clearly detected. Remarkably, the resistance exhibits a reproducible exponential increase as the temperature exceeds 500 °C.

This high-temperature behavior has not been reported previously and suggests that additional mechanisms—beyond the known phase transitions—govern charge transport in NiTi at elevated temperatures. These findings highlight the need for deeper investigation of high-temperature electronic behavior in shape-memory alloys. We will discuss the possible mechanisms resulting in this behavior, including the formation of precipitate phases.

MM 19.43 Tue 18:00 P5

Correlated-electron metallic systems at extremely high temperature — •Zuzanna Helena Filipiak[1,2] and Andrew P. Mackenzie[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]School of Physics and Astronomy, University of St Andrews, Scotland, UK

Although the low-temperature regime is the most established experimental phase space to study correlated-electron systems, a unique physical insight can be won from study at much higher temperatures as well. In particular, the unresolved mystery of the Planckian dissipation - with its linear-in-temperature electrical resistivity sometimes persisting over a few orders of magnitude in temperature with an unchanged slope - is worth studying across wide ranges of temperature. We have developed two setups in which resistivity of a metallic sample is measured as a function of temperature (ranging from 2 to 1000 K), magnetic field (up to 14 T) and the chemical reactivity of the exchange gas (oxygen, argon, vacuum). In this contribution we report on our current understanding of the observed presence and lack of resistivity saturation in different compounds from the groups of the weakly-interacting delafossites ($PdCrO_2$ and $PdCoO_2$) and the more strongly-interacting ruthenates (Sr_2RuO_4, $Sr_3Ru_2O_7$ and $Ca_3Ru_2O_7$).

MM 19.44 Tue 18:00 P5

Thermal Conductivity Measurements Using Laser Flash Analysis in $Mg_3(Sb,Bi)_2$ and Related Compounds — •Thomas Terörde[1], Benjamin Bornmann[1], Christian Hess[1], Ran He[2], Vishak Sivasubramaniyan Sudandiradevi[2], and Kornelius Nielsch[2] — [1]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, Wuppertal, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany

This work presents temperature-dependent thermal conductivity measurements of $Mg_3(Sb,Bi)_2$-based thermoelectric compounds obtained using laser flash analysis down to 150 K. Maximizing thermoelectric performance requires high electrical conductivity while simultaneously minimizing thermal conductivity, which is achieved by reducing the lattice contribution and thereby weakening the Wiedemann-Franz relation. The Sb/Bi ratio of $Sb_{0.6}Bi_{1.4}$ yield favorable band convergence and minimal lattice thermal conductivity. Modification of the transport behavior is sought through additional codoping with Te and Nb. Our systematic measurements as a function of Mg, Te, and Nb contents yield intrinsically reduced thermal conductivity, where an increase in the Te and Nb contents leads to a rise in the thermal conductivity at elevated temperatures, consistent with previous reports.

MM 19.45 Tue 18:00 P5

Li transport in V2O5 quantified by optical microscopy — •Vidula Angane-Ambure, Monica Mead, and Guido Schmitz — Institute of Materials Science, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Vanadium pentoxide (V2O5) is an interesting cathode material due to its layered structure and high theoretical capacity; however, its electrochemical performance is strongly limited by lithium-ion transport and the evolution of phase boundaries during (de)intercalation. To measure lithium-ion transport in V2O5 and clarify transport mechanisms we apply a novel method that uses the optical response upon ion intercalation in in-situ optical microscopy. In this setup a clear diffusion geometry is established and therefore weaknesses of conventional electrochemical methods for quantification of diffusion in battery electrode materials can be circumvented. By evaluating the measured RGB values, the diffusion front is determined. Diffusional transport can then be separated from linear transport across a kinetic interface (such as phase boundaries) and the temperature dependence of the ion transport is quantified, yielding an activation energy for transport in V2O5. Additionally, the concentration-dependence of Li transport

in V2O5 is studied in lithiation and delithiation experiments, showing faster delithiation than lithiation.

MM 19.46 Tue 18:00 P5

Beyond arsenopyrite's monoclinic model: new insights on triclinic symmetry and local, chemically driven disorder in $FeAs_{1-x}S_{1+x}$ — •Esteban Zuñiga-Puelles[1,2], Ayberk Özden[2], Nebahat Bulut[2], Raul Cardoso-Gil[3], Christoph Hennig[4,5], Gerhard Heide[2], Cameliu Himcinschi[2], Jens Kortus[2], and Roman Gumeniuk[2] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Germany — [2]TU Bergakademie Freiberg, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [5]European Synchrotron Radiation Facility, Grenoble, France

In this work, we revisit the structural description of different natural $FeAs_{1-x}S_{1+x}$ specimens. High-resolution synchrotron PXRD reveals additional reflections incompatible with the commonly assumed monoclinic $P2_1/c$ model but fairly consistent with triclinic $P\bar{1}$ symmetry. Raman spectroscopy displays vibrational features deviating from monoclinic simulations, while Mössbauer spectra show multiple inequivalent Fe-sites linked to distinct local crystal electric fields. All samples show weak paramagnetism, and the magnetic moments decrease with increasing As-content, indicating that only a small portion of Fe-atoms resides in environments sufficiently distorted to cause deviations from the expected diamagnetism of low-spin Fe^{2+}. Altogether, the structural, vibrational, and magnetic responses support a revised view of arsenopyrite as a complex Fe-based semiconductor, where local As/S symmetry disruptions and chemically driven disorder govern its physical properties.

MM 19.47 Tue 18:00 P5

Heat-treatment dependent hydrogen embrittlement behaviour of additively manufactured 316L — •Kai Lagemann, Gabriele Palazzo, Stefan Wagner, and Astrid Pundt — Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany

This study investigates the mechanical behaviour of additively manufactured austenitic stainless steel 316L (AM316L) for different post-processing heat treatments and its susceptibility to hydrogen embrittlement. Specimens were produced in the as-built (AB) condition and after heat treatments at 400 °C, 650 °C, 900 °C, and 1050 °C. Comprehensive microstructural characterization and tensile testing were performed to evaluate the correlation between heat-treatment-induced microstructural changes and mechanical properties. Particular this study focuses on assessing the influence of hydrogen on the fracture behaviour and embrittlement sensitivity of the differently heat-treated AM316L conditions. The findings provide an improved understanding of the interplay between additive manufacturing, microstructural evolution during heat treatment, and diffusion-based hydrogen-induced degradation mechanisms in AM316L [1]. [1] Kai Stefan Lagemann, Gabriele Palazzo, Tim Lucas Haag, Svetlana Korneychuk, Stefan Wagner, Christian Kübel and Astrid Pundt. Influence of Microstructure and Heat Treatment on Hydrogen Diffusion in Additively Manufactured 316L Stainless Steel. manuscript submitted, 2026.

MM 19.48 Tue 18:00 P5

In Situ Investigation of Phase Evolution During Oxidation and Reduction of Powder Bed Fusion Copper Powders — •Eric Schneider[1], Lena Friedrich[1], Jaqueline Savelkouls[1], Fabienne Hellwig[2], Milli Suchita Kujur[2], Nick Hantke[3], Arne Röttger[2], Jan T. Sehrt[3], and Christian Sternemann[1] — [1]Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund — [2]Bergische Universität Wuppertal, Bahnhofstraße 15, D-42651Solingen — [3]Ruhr-Universität Bochum, Universitätsstraße 150, D-44801 Bochum

The additive manufacturing (AM) process of laser-based powder bed fusion of metals (PBF-LB/M) enables the efficient production of complex components with internal cavities. Fabricating dense structures from pure copper remains challenging due to copper's high thermal conductivity and its low absorption of infrared laser radiation. Targeted surface modification, such as oxidation or nickel coating, can enhance the processability and reusability of copper powders. This study examines the oxidation behavior of copper powder in air and its controlled reduction in an $Ar/2\%H_2$ atmosphere at temperatures up to 350 °C. X-ray diffraction measurements were conducted at the BL9 beamline of the DELTA synchrotron radiation source. The findings provide key insights into the evolution of copper powder surfaces under PBF-LB/M-relevant atmospheres and offer practical guidance for industrial copper powder processing. This research is funded by the DFG through projects 508745195, RO 4523/9-1, SE 2935/6-1, and STE 1079/9-1.

MM 19.49 Tue 18:00 P5

Transferable Hamiltonian-learning model for large-scale finite temperature electronic-structure calculations — •Kaiwen Chen, Martin Schwade, and David Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Exploring the optoelectronic properties of large-scale systems across various temperatures and structures using conventional density functional theory (DFT) often encounters significant computational challenges. Recent advancements in machine learning (ML) Hamiltonians and the wide availability of DFT-databases have made it possible to train models, capable of predicting accurate Hamiltonians and electronic structure across the chemical space. However, creating a model that can determine temperature-dependent electronic structure with such transferability remains a difficult task. Building on our earlier work involving a physics-informed temperature-transferable Hamiltonian-learning model [1], we introduce an extension of this method that enables it to be trained on a wider field of compositions and thus be able to predict accurate effective Hamiltonians for different chemical compositions.

[1] M. Schwade, S. Zhang, F. Vonhoff, F. P. Delgado, D. A. Egger, *Physics-informed Hamiltonian learning for large-scale optoelectronic property prediction,* arXiv:2508.20536 (2025).