Metal and Material Physics Division
Fachverband Metall- und Materialphysik (MM)

Rebecca Janisch
ICAMS, Ruhr-Universität Bochum
Universitätsstr. 150
44801 Bochum
rebecca.janisch@rub.de

Overview of Invited Talks and Sessions

(Lecture halls SCH/A215, SCH/A216, SCH/A251, and SCH/A315; Poster P5)

Invited Talks

MM 2.1	Mon	9:30–10:00	SCH/A251	**Deep-Learning and Generative AI for the Discovery of Electron-Phonon Superconductors** — •Richard Hennig
MM 6.1	Mon	15:00–15:30	SCH/A251	**Transformation-induced plasticity in zirconia ceramics: simulations and experiments** — •David Rodney
MM 10.1	Tue	9:30–10:00	SCH/A251	**Chemically graded materials for accelerated exploration of the TRIP-TWIP Ti-alloy family** — •Lola Lilensten
MM 24.1	Wed	15:00–15:30	SCH/A251	**Recent advances in processing of rare-earth free MnBi magnets by severe plastic deformation** — •Andrea Bachmaier, Lukas Weissitsch-Reiner, Martin Kraus, Michael Meindlhumer, Stefan Wurster
MM 29.1	Thu	9:30–10:00	SCH/A251	**Three dimensional sub-Ångström resolution imaging from 4D-STEM experiments** — •Philipp Pelz
MM 33.1	Thu	15:00–15:30	SCH/A251	**LPBF with Ultrashort Laser Pulses - Additive Manufacturing Beyond Current Limits** — •Stefan Nolte, Hagen P. Kohl, Lisa Matthäus, Tobias Ullsperger, Dongmei Liu, Stephanie Lippmann
MM 38.1	Fri	9:30–10:00	SCH/A251	**Alloy design and deformation behaviour of Mo-based silicide materials** — •Manja Krueger

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky

SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the joint Symposium AI and Data Challenges behind Emerging Self-Driving Laboratories (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	HSZ/AUDI	**Data and Experimental Foundations for Reliable Self-Driving Laboratories** — •Dr. Marcus Tze-Kiat Ng
SYAI 1.2	Thu	10:00–10:30	HSZ/AUDI	**Digital Catalysis - AI for Experiment Planning and Control** — •Christoph Scheurer
SYAI 1.3	Thu	10:30–11:00	HSZ/AUDI	**Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron** — •Jan Janssen, Joerg Neugebauer
SYAI 1.4	Thu	11:15–11:45	HSZ/AUDI	**Machine Learning for Autonomous Optimization and Discovery of Materials** — •Pascal Friederich
SYAI 1.5	Thu	11:45–12:15	HSZ/AUDI	**Transforming Our View on Transformers in the Sciences** — •Kevin Maik Jablonka

Sessions

MM 1.1–1.1	Sun	16:00–18:15	TRE/MATH	**Hands on tutorial: Linking Large Language Models with Digital Workflows for Materials Science Simulations (joint session MM/TUT)**
MM 2.1–2.1	Mon	9:30–10:00	SCH/A251	**Invited Talk: Richard Hennig**
MM 3.1–3.9	Mon	10:15–12:45	SCH/A215	**Mechanical Properties and Alloy Design I**
MM 4.1–4.9	Mon	10:15–13:00	SCH/A216	**Materials for the Storage and Conversion of Energy I**
MM 5.1–5.7	Mon	10:15–12:45	SCH/A251	**Topical Session: Physics-driven Artificial Intelligence for Materials I**
MM 6.1–6.1	Mon	15:00–15:30	SCH/A251	**Invited Talk: David Rodney**
MM 7.1–7.10	Mon	15:45–18:30	SCH/A215	**Mechanical Properties and Alloy Design II**
MM 8.1–8.10	Mon	15:45–18:30	SCH/A216	**Materials for the Storage and Conversion of Energy II**
MM 9.1–9.9	Mon	15:45–18:30	SCH/A251	**Topical Session: Physics-driven Artificial Intelligence for Materials II**
MM 10.1–10.1	Tue	9:30–10:00	SCH/A251	**Invited Talk: Lola Lilensten**
MM 11.1–11.6	Tue	10:15–11:45	SCH/A215	**Structurally and Chemically Complex Alloys**
MM 12.1–12.9	Tue	10:15–12:45	SCH/A216	**Materials for the Storage and Conversion of Energy III / Functional Materials I**
MM 13.1–13.9	Tue	10:15–12:45	SCH/A251	**Data-driven Materials Science: Big Data and Workflows I**
MM 14.1–14.5	Tue	11:30–12:45	SCH/A315	**Liquid and Amorphous Materials I**
MM 15.1–15.7	Tue	14:00–15:45	SCH/A215	**Phase Transformations I**
MM 16.1–16.7	Tue	14:00–15:45	SCH/A216	**Functional Materials II**
MM 17.1–17.7	Tue	14:00–15:45	SCH/A251	**Data-driven Materials Science: Big Data and Workflows II**
MM 18.1–18.6	Tue	14:00–15:30	SCH/A315	**Liquid and Amorphous Materials II**
MM 19.1–19.49	Tue	18:00–20:00	P5	**Poster Session**
MM 20.1–20.1	Wed	9:30–10:00	SCH/A251	**Topical Talk: Shigenobu Ogata**
MM 21.1–21.10	Wed	10:15–13:00	SCH/A215	**Phase Transformations II**
MM 22.1–22.9	Wed	10:15–12:45	SCH/A216	**Data-driven Materials Science: Big Data and Workflows III**
MM 23.1–23.5	Wed	10:15–11:30	SCH/A251	**Topical Session: Dislocations in Functional Materials I (joint session MM/FM)**
MM 24.1–24.1	Wed	15:00–15:30	SCH/A251	**Invited Talk: Andrea Bachmaier**
MM 25.1–25.5	Wed	15:45–17:00	SCH/A215	**Interface Controlled Properties, Nanomaterials, and Microstructure Design I**
MM 26.1–26.5	Wed	15:45–17:00	SCH/A216	**Transport in Materials: Diffusion, Charge, or Heat Conduction I**

MM 27.1–27.5	Wed	15:45–17:15	SCH/A251	**Topical Session: Dislocations in Functional Materials II (joint session MM/FM)**
MM 28	Wed	17:15–18:45	SCH/A251	**Members' Assembly**
MM 29.1–29.1	Thu	9:30–10:00	SCH/A251	**Invited Talk: Philipp Pelz**
MM 30.1–30.6	Thu	10:15–11:45	SCH/A215	**Interface Controlled Properties, Nanomaterials, and Microstructure Design II**
MM 31.1–31.10	Thu	10:15–13:00	SCH/A216	**Transport in Materials: Diffusion, Charge, or Heat Conduction II**
MM 32.1–32.6	Thu	10:15–12:45	SCH/A251	**Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom I**
MM 33.1–33.1	Thu	15:00–15:30	SCH/A251	**Invited Talk: Stefan Nolte**
MM 34.1–34.7	Thu	15:45–17:30	SCH/A215	**Hydrogen in Materials I**
MM 35.1–35.7	Thu	15:45–17:30	SCH/A216	**Additive Manufacturing / Transport in Materials III**
MM 36.1–36.5	Thu	15:45–17:15	SCH/A251	**Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom II**
MM 37.1–37.5	Thu	15:45–17:00	SCH/A315	**Development of Calculation Methods I**
MM 38.1–38.1	Fri	9:30–10:00	SCH/A251	**Invited Talk: Manja Krüger**
MM 39.1–39.9	Fri	10:15–12:45	SCH/A215	**Hydrogen in Materials II**
MM 40.1–40.8	Fri	10:15–12:30	SCH/A216	**Transport in Materials: Diffusion, Charge, or Heat Conduction IV**
MM 41.1–41.9	Fri	10:15–12:45	SCH/A251	**Development of Calculation Methods II**

Members' Assembly of the Metal and Material Physics Division

Wednesday 17:15–18:45 SCH/A251

- discussion of MM activities
- announcement of the poster awards
- exchange of ideas for the next DPG meeting

MM 1: Hands on tutorial: Linking Large Language Models with Digital Workflows for Materials Science Simulations (joint session MM/TUT)

Advanced computational simulations often require chaining several models and software packages together, a process that demands careful workflow management. In this tutorial you can gain hands-on experience with the Python based workflow environment pyiron (www.pyiron.org). Participants in the tutorial will be able to run all the examples shown in the presentation interactively on their own laptops. There is no need to install any code, just a standard web browser to explore the applications interactively.

Time: Sunday 16:00–18:15 Location: TRE/MATH

Tutorial MM 1.1 Sun 16:00 TRE/MATH

Hands on tutorial: Linking large language models with digital workflows for materials science simulations — •Jörg Neugebauer[1], Tilmann Hickel[1,2], and Ralf Drautz[3] — [1]Max Planck Institute for Sustainable Materials — [2]Bundesanstalt für Materialforschung und -prüfung — [3]ICAMS, Ruhr Universität Bochum

Advanced computational simulations now reliably predict material properties, but they often require chaining several models and software packages together, a process that demands expert knowledge and careful workflow management. Efficient, reproducible research therefore hinges on automated workflow tools that can handle this complexity. In this tutorial we introduce pyiron (www.pyiron.org), a Python based workflow environment for building and executing fully automated simulation pipelines. We show how complex simulations workflows can be constructed programmatically via Python code as well as via a flow-based graphical user interface. We further introduce how large language models (LLMs) can be embedded to streamline the "human in the loop" tasks. After a brief overview of pyiron's core concepts, we construct workflows for computing ab initio thermodynamic bulk phase diagrams. The necessary steps, such as density functional theory calculations, training ACE-based machine learning potentials, and exploring phase stability using foundational models like GRACE, are all performed within pyiron workflows. Participants will learn how to develop and integrate such workflows into their own materials science simulations, thereby enabling faster, more transparent, and more reproducible research.

MM 2: Invited Talk: Richard Hennig

Time: Monday 9:30–10:00 Location: SCH/A251

Invited Talk MM 2.1 Mon 9:30 SCH/A251

Deep-Learning and Generative AI for the Discovery of Electron-Phonon Superconductors — •Richard Hennig — University of Florida, Gainesville, Florida, USA

The search for new superconductors with higher critical temperatures, T_c, and critical fields, H_c, is limited by the cost of electron-phonon calculations and the vastness of compositional and structural space. To overcome both obstacles, we develop an integrated deep-learning workflow for conventional, electron-phonon-mediated superconductors.

First, we introduce BEE-NET, an ensemble of equivariant graph neural networks trained to predict the Eliashberg spectral function $\alpha^2F(\omega)$ and T_c directly from crystal structures, optionally augmented by the phonon density of states. Unlike traditional approaches that learn T_c directly, predicting $\alpha^2F(\omega)$ treats superconductors and non-superconductors on equal footing and, together with explicit phonon-spectrum information, leverages electron-phonon physics to improve predictions for rare superconducting materials. Embedded in a multistage screening pipeline that combines elemental substitution strategies with machine-learned interatomic potentials, BEE-NET scans over 1.3×10^6 candidate structures and down-selects to 741 dynamically and thermodynamically stable compounds with DFT-confirmed $T_c > 5$ K, including two experimentally realized new superconductors.

Finally, I will briefly show how guided diffusion models for crystal structures and our Open Materials Generation (OMatG) framework based on stochastic interpolants extend this physics-informed, data-driven approach to the generative design of new superconductors.

MM 3: Mechanical Properties and Alloy Design I

Time: Monday 10:15–12:45 Location: SCH/A215

MM 3.1 Mon 10:15 SCH/A215

Mechanical Properties of Disordered Fe-Co Nanoparticles — •Yarden Nathan — Technion, Haifa, Israel

We synthesized Fe- 50 at.% Co nanoparticles (NPs) via solid-state dewetting of Fe-Co bilayers deposited on a sapphire substrate at the temperature of 900 *C followed by slow cooling. By employing X-ray diffraction and electron diffraction in transmission electron microscope (TEM) we demonstrated that the NPs are fully disordered α-FeCo body centered cubic (BCC) phase. We demonstrated that the size and orientations of the disordered BCC NPs can be controlled by varying their fabrication parameters. Most of the NPs were faceted single crystals with their top (110) facet oriented parallel to the substrate. The mechanical properties of the NPs were measured by employing in-situ micro compression tests in the scanning electron microscope (SEM). The near-theoretical strength of α-FeCo NPs was demonstrated. We propose that the fully disordered NPs behave similarly to the defect-free NPs of pure metals. The plasticity of these NPs is controlled by the dislocation nucleation requiring near-theoretical stress. This mechanism explains the near-theoretical strength and the distinct "smaller is stronger" size effect observed in this metastable phase.

MM 3.2 Mon 10:30 SCH/A215

Role of Structural Hierarchy on Tensile Properties of Nanoporous Metals — •Wei-Che Chang[1], Yong Li[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

Nanoporous gold (NPG) is drawing significant attention as functional, lightweight material due to its low density, high surface area, and tunable structures. Despite the inherent ductility of bulk gold, NPG often exhibits brittleness under tension [1]. Recently, hierarchical nanoporous gold (HNPG) with multiple levels of well-defined porosities has attracted significant interest for its enhanced functional performance and improved compressive properties at reduced solid fraction [2]. However, whether these mechanical enhancements under compression also extend to tension, particularly whether structural hierarchy can mitigate the intrinsic brittleness of nanoporous networks under tension, remains an important open question. In this work, we introduce an in-situ micro-tensile setup for real-time observation of deformation and fracture behaviors in a scanning electron microscope (SEM). Our results show that the hierarchical structure improves ductility by a factor of five. The mechanism of tensile deformation is further revealed by molecular dynamics simulations.

[1] N. Badwe, X. Chen, K. Sieradzki, Acta Mater. 129 (2017) 251-258
[2] S. Shi, Y. Li, B. Ngo-Dinh, J. Markmann, J. Weissmüller, Science 371 (2021) 1026-1033

MM 3.3 Mon 10:45 SCH/A215

Mechanical shielding of holes in elastic solids — •Kanka Ghosh and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Holes inside an elastic solid reduce its overall mechanical stiffness. We examine whether a stiff shell around the hole can act as a shield under external loading, maintaining overall mechanical properties of the solid as if the hole were absent. For this purpose, an isotropic, homogeneous, linearly elastic material, loaded uniformly under plane strain with low concentrations of holes is considered. Instead of changing the materials to conceal a hole, we suggest to adjust the thickness of the shell for given elasticity parameters. A corresponding analytical expression for the thickness of the shell is derived. We extend this idea to the atomistic level using molecular dynamics simulations of model Lennard-Jones solids. Consistency of the resulting shell thickness for mechanical shielding at the atomistic scale attests the robustness of our continuum elasticity predictions. The concept is crucial for lightweight construction without compromising elastic materials properties.

We acknowledge support of this work through the European Union (EFRE) and the State Saxony Anhalt through project no. ZS/2024/02/184030.

Reference: K. Ghosh and A. M. Menzel, Mechanically concealed holes, arXiv:2511.00135

MM 3.4 Mon 11:00 SCH/A215

Synthesis and mechanical properties of multi-scale hierarchical Ni and Cu foams — •Ulrike Dette[1,2] and Shan Shi[1,3] — [1]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

As functionalized materials gain importance and component miniaturisation advances, there is an increasing demand for optimized structured materials. This talk presents a novel and straightforward alloying-dealloying approach to fabricate metals such as Ni and Cu with two- and three-level hierarchical network structures. Due to the significant difference in vapour pressures between the target metals, vapor phase alloying (VPA) of a metal foam with Zn resulted in Zn-based intermetallic alloy foams. This is then followed by vapor phase dealloying (VPD) which removes Zn and creates a finer porosity, resulting in a second level. A subsequent VPA-VPD cycle produces a third hierarchical level. Compression tests on these hierarchical foams with varying solid fractions were performed to determine Young's modulus and strength. The experimental results align well with the predictions of our new scaling law.

15 min. break

MM 3.5 Mon 11:30 SCH/A215

Formation and properties of crystalline and amorphous high-entropy ZrTiTaMoWNi thin films using magnetron sputtering of a segmented target — •Anna Kornyushchenko[1,2], Vyacheslav Perekrestov[2], Marilena Tomut[1,3], Harald Rösner[1], Martin Peterlechner[4], and Gerhard Wilde[1,5] — [1]Institute of Materials Physics, University of Muenster, Muenster, Germany — [2]Laboratory of Vacuum Nanotechnologies, Sumy State University, Sumy, Ukraine — [3]GSI Helmholtz Center for Heavy Ion Research, 64291 Darmstadt, Germany — [4]Karlsruhe Institute of Technology, Laboratory for Electron Microscopy, 76131 Karlsruhe, Germany — [5]Herbert Gleiter International Institute, Liaoning Academy of Materials, Shenyang, China

Using direct current magnetron sputtering of a segmented target under conditions of thermodynamical equilibrium, single-phase bcc or amorphous ZrTiTaMoWNi high entropy alloy layers have been formed. The crystalline layers have been obtained in the form of nano-patterns, with crystal growth occurring preferentially on the basis of (310) crystallographic plane, which aligns parallel to the substrate surface. The amorphous layers have smooth surface, featureless morphology and demonstrate structural stability. TEM studies have shown that their crystallization into a single bcc phase occurs at the annealing temperature of 800 C. The microhardness of the amorph and the crystalline films has measured to be 10 GPa and 4.6 GPa, correspondingly. Resistance to impact of swift heavy Au ions irradiation with energies 4.8 MeV/u have been compared for amorph and crystalline layers.

MM 3.6 Mon 11:45 SCH/A215

Microstructural and Chemical Analysis on MoSiTi samples with PDC coating for High Temperature Application — •Ingrit Nurak[1], Daniela Camacho[2], Lukas Korell[3], Giorgia Guardi[1], Heike Störmer[1], Svetlana Korneychuk[1], Yolita M. Eggeler[1], Astrid Pundt[1], and Samuel A. Kredel[2] — [1]Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Technische Universität Darmstadt, Darmstadt, Germany — [3]Dechema Forschungszentrum, Frankfurt, Germany

MoSiTi material is of high interest for high temperature applications, such as Mo-20Si-52.8Ti [Schliephake et. al., 2019]. In this presentation, we investigate the combination of this material with a Cr-bond coat and a Si(Hf, Ta)BCN(O)-polymer derived ceramic (PDC) upper layer. The structural and chemical evolution of the layered material, depending on the specific synthetic routes used and additional thermal treatments will be addressed by using different scanning and transmission electron microscopy (SEM, TEM) techniques. TEM will be applied to the (i) polymer-derived ceramic nanocomposites coating, to the development of (ii) ultra-high temperature silicides and to the (iii) Cr bond coat layer. Heat treatments will be addressed at 1200°C and 1400°C both in air and in argon atmosphere. The experimental outcomes demonstrate that the Materialsystem exhibits the capacity to withstand temperatures of 1200°C for an hour without delamination. Notwithstanding the application of heat treatment at 1400°C, there is no oxygen penetration into the MoSiTi substrate occurred. Moreover, the PDC coating was found to remain partially amorphous.

MM 3.7 Mon 12:00 SCH/A215

Understanding Alloying Effects on Grain Boundary Adhesion in Nickel Alloys by Atomistic Simulation — •Aljoscha F. Baumann[1], Reyhaneh Ghassemizadeh[1], and Daniel F. Urban[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]Freiburger Materialforschungszentrum, Freiburg, Germany

When increasing the in-service performance of engineering metallic materials, interfaces such as phase or grain boundaries (GB) may act as the weakest links. For the nickel-base superalloy Alloy 718 intergranular cracking can be a relevant damage mechanism as a result of high-temperature fatigue in an oxygen-rich environment. The reliable prediction of adhesion and mechanical stability at grain boundary interfaces from atomistic calculations remains a challenge due to the high-dimensional parameter space of chemical compositions and GB structures. Recently developed machine learning interatomic potentials (MLIPs) such as GRACE offer a promising solution to explore this parameter space by combining high accuracy with computational efficiency. Here we use a MLIP to perform cleavage simulations on grain boundaries in fcc Ni with Cr and Fe as alloying elements at varying concentrations and statistical distributions. This approach provides a pathway for atomistic simulations towards a more comprehensive modelling of alloys and their interface mechanical properties, thereby providing insights into intergranular failure mechanisms. Our results can be used to parametrize traction separation laws used in finite element modelling, allowing for microstructure-sensitive modelling of fatigue crack formation and growth.

MM 3.8 Mon 12:15 SCH/A215

Phase stability and surface segregation in multinary noble-metal alloys: an atomistic study with universal models — •Quentin Bizot, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, 44780 Bochum, Germany

Multinary alloys are complex solid solutions composed of several elements. They rarely behave like ideal solid solutions due to differences in phase stability, atomic size, and crystalline preferences. In bulk, short-range order can therefore be significant, leading to the formation of specific phases or distortions across the lattice. In addition to the effects in the volume, surface segregation affects the order and composition of the few first layers at the surface. A detailed understanding of these effects at the atomic scale is essential to predict and control the distribution and ordering of surface atoms, as well as their influence on material properties.

In this work, we investigate complex solid solutions based on noble metals with atomistic simulations demonstrating the formation of stable phases in the bulk as well as the segregation of specific elements at the surface. For this purpose, we used tailored GRACE model capable of describing interactions for 25 transition metals as well as universal GRACE models trained on diverse datasets.

MM 3.9 Mon 12:30 SCH/A215

First-principles study of aluminum alloy - polymer interfaces: From surface structures to adsorbate interactions — •Zhengqing Wei[1], Inna Plyushchay[2], Nebahat Bulut[1], Florian Lehmann[4], Philip Grimm[5,6], Maik Gude[4], Julia Hufenbach[5,6], and Sibylle Gemming[1,3] — [1]Inst. Physics, TU Chemnitz, Germany — [2]Natl. Taras Shevchenko University of Kyiv, Ukraine — [3]MAIN Center, TU Chemnitz, Germany — [4]ILK, TU Dresden, Germany — [5]IFW Dresden, Germany — [6]Inst. Materials Science, TU-BA Freiberg, Germany

Aluminum alloy surfaces face strict demands regarding extreme environmental conditions. The joining of aluminum alloy materials with engineering plastics enhances the overall resilience of composite. This study employs density functional theory (DFT) to model aluminum alloy surfaces while including electronic structure considerations. The surface stability was investigated as functions of alloying composition particularly on surfaces doped with Mg, Zr, and Si. The study includes the alloy's diffusion tendency, which shows that differential electron density variations occur simply at the outermost surface layer in contact with vacuum. Surface vacancy and migration barriers, and when the surface is bonded to the polymers, the interactions between atomic species of polymer side chains and aluminum alloy surfaces as well as surface vacancy sites were also analyzed. The modeled adsorbates on aluminum alloy surfaces provides modified local potential parameters for classical modeling of large-scale aluminum alloy–polymer surface and interfacial regions.

MM 4: Materials for the Storage and Conversion of Energy I

Time: Monday 10:15–13:00 Location: SCH/A216

Topical Talk MM 4.1 Mon 10:15 SCH/A216

Photoelectric properties of dislocations in SrTiO3 single crystals — •Marin Alexe — University of Warwick

Dislocations are one-dimensional crystallographic line defects traditionally regarded as detrimental to the functional properties of conventional semiconductors. However, it has been recently shown on Fe-doped SrTiO3 single crystals containing well-ordered, high-density dislocation structures that dislocations can significantly enhance photoconductivity. Local photoconductivity measurements using atomic force microscopy (AFM) revealed that regions surrounding dislocation cores exhibit up to a fourfold increase in photoconductivity compared with dislocation-free areas of the crystal. Furthermore, macroscopic in-plane surface measurements using microcontacts aligned along dislocation slip bands showed orders-of-magnitude enhancement in photoconductivity. This might be due a significant increase of the carrier density at the core of dislocation due to a to a non-chemical local doping induced by the strain or strain gradient.

These results provide unambiguous evidence that dislocations in oxide semiconductors can be beneficial for specific functional properties. The anisotropic enhancement of photoconductivity along dislocation cores highlights their potential as active elements in future one-dimensional oxide electronic and optoelectronic devices.

MM 4.2 Mon 10:45 SCH/A216

Defect-driven carrier dynamics in tantalum nitride photoelectrodes — •Lukas M. Wolz[1], Johannes Dittloff[1,2], Laura I. Wagner[1,2], Julius Kühne[1,2], Luc-Fabrice Tremel[1], Lina M. Todenhagen[1,2], Lissa Eyre[1,2], Felix Deschler[1,2,3], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Walter Schottky Institute, Technische Universität München, Germany — [3]Institute for Physical Chemistry, Heidelberg University, Germany

Tantalum nitride (Ta_3N_5) is a widely studied semiconductor for solar-driven water splitting. Yet, experimentally realized efficiencies often remain below theoretical limits largely because native and impurity-related defect states alter charge carrier dynamics by promoting trapping and recombination. Here, we investigate how distinct defect properties in Ta_3N_5 thin films govern ultrafast photocarrier behavior using femtosecond transient absorption spectroscopy, complemented by photoluminescence (PL) and PL excitation measurements. Ta_3N_5 photoelectrodes were synthesized by annealing TaO_x, TaN_x, and Ta precursor films in NH_3, enabling systematic control over shallow and deep defect state concentrations. The controlled defect properties allow us to disentangle the roles of nitrogen vacancies and oxygen-related defects in shaping carrier dynamics. Our results reveal that deep defects function as efficient trapping and recombination centers for free carriers. Here, we correlate ultrafast spectroscopy with complementary optical and photoelectrochemical data.

MM 4.3 Mon 11:00 SCH/A216

Probing Defect-State Photoionization in Ta_3N_5 Thin Films via Photocurrent Excitation Spectroscopy — •Luc-Fabrice Tremel[1], Lukas M. Wolz[1], Johannes Dittloff[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Walter Schottky Institute, Technische Universität München, Germany

Transition-metal nitrides are a highly interesting material space for solar-energy conversion due to their suitable bandgap for visible light absorption and high theoretical solar-to-hydrogen efficiencies. A prominent example is Ta_3N_5, which combines a bandgap of 2.2 eV with favorable band alignment for solar water splitting. In practice, however, its photoelectrochemical performance is strongly constrained by shallow and deep defects. Here, we use photocurrent excitation spectroscopy, complemented by power-dependent photocurrent measurements, to determine how these defect states shape the spectral photocurrent response of Ta_3N_5. By tracking photocurrent as a function of photon energy, light intensity, and applied potential, we distinguish the sharp band-edge transition from a broadened onset dominated by defect-assisted photoionization into the conduction band. These insights into the defect-controlled photoresponse of Ta_3N_5 provide guidance for improved fabrication strategies and the development of higher-performing nitride-based solar-fuel devices.

MM 4.4 Mon 11:15 SCH/A216

Piezoresponse force microscopy on substituted BaTiO3-relaxors — •Markus Kratzer[1], Philipp Fahler-Muenzer[2], Christian Maier[4], Klaus Reichmann[3], Marco Deluca[5], and Christian Teichert[1] — [1]Chair of Physics, Department of Physics, Mechanics and Electrical Engineering, TU Leoben, Leoben, Austria — [2]University of Warwick - Department of Physics, Coventry, United Kingdom — [3]Institute for Chemistry and Technology of Materials, Graz, Austria — [4]Materials Center Leoben GmbH, Leoben, Austria — [5]Silicon Austria Labs GmbH, Sandgasse 34, 8010 Graz, Austria

Relaxor ferroelectrics are key materials in electrostatic capacitors for energy storage but also for high-performance actuators and transducers. Classical relaxor ferroelectric systems often contain lead, which is environmentally unsound. Thus, lead free relaxors are highly desired. A promising route is via substituted barium titanate (BaTiO3). In this study we focus on B-site-substituted polycrystalline BaTiO3, where the central Ti ion in the perovskite lattice is partially substituted by Zr or Nb. In such systems, information on the microscopic ferroelectric domain structure is still lacking, even though detailed macroscopic characterization using a variety of techniques has been undertaken. We use piezoresponse force microscopy to investigate domain structure and local polarization switching at different temperatures and compositions. We find that temporal stabilization of domains with limited volume is still possible, even though long-range ferroelectric order is strongly supressed with increasing levels of substitution. This suggests the presence of residual highly unstable polar nanoregions.

15 min. break

MM 4.5 Mon 11:45 SCH/A216

Tunable TiO_xN_y Photoelectrodes for Efficient Solar Energy

Conversion — •Sebastian Trautschold and Johanna Eichhorn — TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Oxynitrides have recently emerged as a versatile material class for photoelectrochemical energy conversion, offering a pathway to combine the stability of oxides with the visible-light absorption and favorable charge transport of nitrides. Their key advantage lies in the continuous tunability of optical and electronic properties via adjusting the O/N ratio. TiO_xN_y provides a particularly illustrative platform: while TiO_2 is limited by a wide bandgap and TiN is metallic, TiO_xN_y can be tuned into an intermediate semiconducting regime, enabling improved utilization of the solar spectrum without sacrificing transport.

Here, we deposit TiO_xN_y thin films by pulsed gas reactive sputtering, enabling precise stoichiometric control over a broad composition range. Post-annealing in ammonia and nitrogen is then used as an additional handle to tailor crystallinity, phase evolution, and defect chemistry. By correlating deposition and annealing parameters with structural, chemical, and optoelectronic characteristics - particularly bandgap and defect properties - we identify processing windows that optimize qualities relevant for solar harvesting. Our results demonstrate the strong sensitivity of TiO_xN_y to both growth kinetics and thermal treatment, and establish practical guidelines for engineering oxynitride photoelectrodes toward efficient and durable solar energy conversion systems.

MM 4.6 Mon 12:00 SCH/A216

In Situ Scanning Transmission Electron Microscopy Investigation of Solid-State Batteries Under Realistic Processing Conditions

— •Thomas Demuth, Shamail Ahmed, and Kerstin Volz — Philipps Universität Marburg, Department of Physics and mar.quest, Marburg, Germany

Solid-state batteries promise safer energy storage with higher energy density compared to conventional lithium-ion batteries with liquid electrolytes. To ensure good ionic conductivity between the cathode active material (CAM) and solid electrolyte (SE), the interface area must be maximized. This can be achieved by co-sintering the materials at elevated temperatures. However, high-temperature treatment can induce secondary phase formation at the SE - CAM interface. To optimize material stability, a fundamental understanding of the materials' structure and the processes occurring at the interface are required. Here, in situ (scanning) transmission electron microscopy ((S)TEM) offers insights into nanoscale reaction processes. In our study, we have heated the CAM LiNiO2 (LNO) as a model system in an oxygen atmosphere, utilizing a closed gas cell heating holder, which enables heating the sample in a gaseous atmosphere of 1 bar to temperatures of up to 1000 °C. Using a scanning nanobeam mode allows rapid switching between live imaging for the observation of morphological changes and recording of 4D diffraction pattern datasets for structural analysis. Our findings indicate that the onset temperature for phase degradation is significantly higher in an oxygen atmosphere compared to vacuum, highlighting the importance of replicating realistic processing conditions.

MM 4.7 Mon 12:15 SCH/A216

Voltage-Dependent CEI Development on LMO Cathodes in-situ monitored via Langasite Microgravimetry

— •Robert Löser and Guido Schmitz — University of Stuttgart, Stuttgart, Germany

Understanding the formation and evolution of the cathode-electrolyte interphase (CEI) is essential for improving the stability of high-voltage lithium-ion battery materials such as LiMn2O4 (LMO). In this work, we investigate the CEI formation and composition in-situ on sputtered LMO thin films using an electrochemical microbalance based on a Langasite (La3Ga5SiO14) resonator. Unlike conventional quartz crystal microbalances, Langasite substrates enable high-temperature annealing of sputtered oxide films while keeping their piezoelectric properties, making them uniquely suited for preparing crystalline cathode layers directly on the resonator surface. LMO films were cycled to different upper voltage cutoffs to investigate how oxidative potentials influence CEI formation. The coupled electrochemical-gravimetric data reveal clear voltage-dependent mass changes associated with electrolyte decomposition, surface reconstruction, and dissolution processes. By correlating frequency shifts with electrochemical signatures, we quantify the onset, magnitude, and reversibility of CEI species formation dependent of the upper voltage boundary. This study demonstrates that Langasite-based microgravimetry enables powerful, in-situ investigation of CEI evolution and interphase dynamics on annealed cathode films such as LMO, opening the way for systematic studies across a broader range of high-temperature processed electrodes.

MM 4.8 Mon 12:30 SCH/A216

Tuning electronic structure of CoNi LDHs via surface Fe doping for achieving effective oxygen evolution reaction

— •Yunli Shi[1,2], Huaping Zhao[1], Junqi Li[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]School of Materials Science and Engineering, Shaanxi University of Science and Technology, Xian 710021, China

Cobalt and nickel based layered double hydroxides (LDHs) are promising oxygen evolution reaction (OER) catalysts, but their performance is limited by poor conductivity and low intrinsic catalytic activity. In this study, CoNi LDHs were used as a matrix, with iron sites introduced onto the surface via cation replacement (Fe-CoNi LDHs). Unlike ternary Fe-CoNi LDHs synthesized through conventional one-step methods, the iron sites in Fe-CoNi LDHs are primarily located on the surface and edges of nanosheets, ensuring abundant exposure of reactive sites. Surface doping was found to optimize the coordination environment and electronic structure, reducing the binding energy between reactants and active sites. As a result, Fe-CoNi LDHs exhibit an overpotential of only 260 mV at 10 mA cm**, demonstrating superior OER performance. This study elucidates the electronic structure and mechanism of enhanced activity, highlighting the potential of surface doping to advance electrocatalytic applications.

MM 4.9 Mon 12:45 SCH/A216

NiCo2O4/Fe3O4 Nanocomposite with a Sea Urchin-like Morphology as a High-Performance Dual-Functional Material for Advanced Lithium-Ion Batteries and Supercapacitors

— •Amina Zafar, Amjad Nisar, and Mashkoor Ahmad — Pakistan Institute of Nuclear Science and Technology (PINSTECH), Islamabad, Pakistan

The development of advanced electrode materials with multifunctional electrochemical properties is critical for next-generation energy storage systems. In this study, mesoporous sea urchin-like nickel cobaltite/magnetite (NiCo2O4/Fe3O4) composite was synthesized and systematically investigated for lithium-ion batteries and supercapacitors. The resulting composite offers high specific surface area, improved conductivity, abundant active sites and favorable structural characteristics. DFT calculations reveal that the composite exhibits enhanced redox kinetics and improved charge transfer compared to pristine NiCo2O4, leading to superior electrochemical performance. As an anode for lithium-ion batteries, the NiCo2O4/Fe3O4 electrode delivers a high reversible capacity of around 730 mAh/g at 0.3 A/g with excellent cycling stability, retaining 87.1 % of its capacity after 1000 cycles. For supercapacitor, the electrode exhibits an enhanced specific capacitance of 1330 F/g at 1 A/g, outperforming both NiCo2O4 and Fe3O4. The assembled (NiCo2O4/Fe3O4//activated carbon) device achieved a specific capacitance of 221 F/g and an energy density of 69.6 Wh/kg, along with excellent cycling stability, retaining around 94 % capacitance after 8000 cycles.

MM 5: Topical Session: Physics-driven Artificial Intelligence for Materials I

Time: Monday 10:15–12:45 Location: SCH/A251

Topical Talk MM 5.1 Mon 10:15 SCH/A251

Machine Learning for Materials Discovery: from Big Data to Predictive Insights — •Silvana Botti — Research Center Future Energy Materials and Systems and Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Universitätsstraße 150, D-44801 Bochum, Germany

Machine learning (ML) models for materials science are rapidly evolving, driven by large-scale, high-quality datasets and innovative neural network architectures. This talk explores critical challenges in improving the accuracy and reliability of complex ML models, examining the interplay between the quality and quantity of training data and model performance across material properties. Recent advances have been marked by the creation of extensive FAIR databases, such as Alexandria (https://alexandria.icams.rub.de/), which provides over 7 million density-functional theory calculations spanning periodic compounds of various dimensionalities. These comprehensive datasets enable systematic investigation of the relationship between training data volume/quality and model accuracy.

J. Schmidt, T.F.T. Cerqueira, A.H. Romero, A. Loew, F. Jäger, H.-C. Wang, S. Botti, M.A.L. Marques, Improving machine-learning models in materials science through large datasets, Mater. Today Phys. 48, 101560 (2024).

MM 5.2 Mon 10:45 SCH/A251

Screening of high-entropy oxides as oxygen conductors for fuel cells — •Jesper R. Pedersen, Ciku Parida, Benjamin H. Sjølin, and Ivano E. Castelli — Department of Energy Conversion and Storage, Technical University of Denmark, Kgs. Lyngby 2800, Denmark

High-entropy materials are at the cutting edge of materials design and this work investigates their suitability for use in fuel cells. However, screening high-entropy materials is computationally demanding, especially for properties such as oxygen migration barriers which are critical for components used in fuel cell cathodes. We aim to address this challenge by fine-tuning the MACE foundation model to a generated database containing more than 400 nudged elastic band (NEB) calculations spanning the chemical space of double perovskites. We show this new model achieves accuracy similar to the DFT calculations not only on structural relaxations, but also for the more complex task of saddle-point discovery. This enables the continued rapid exploration of the chemical space beyond the initial screening, leading to new insights into factors governing oxygen migration in fuel cell cathodes.

MM 5.3 Mon 11:00 SCH/A251

Interpretable Bayesian Optimization for Autonomous Materials Discovery — •Akhil S. Nair[1,2], Lucas Foppa[1], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max Planck Society, Berlin, Germany — [2]Institut für Chemie und Biochemie, Freie Universität Berlin, Germany

Bayesian Optimization (BO) can accelerate materials discovery by exploring complex design spaces using surrogate models and acquisition functions [1]. Its efficiency, however, relies on identifying a small set of key parameters or features that are potentially correlated with the target property. Existing feature-selection methods often fall short, as they struggle to capture nonlinearities and interactions among features [2], limiting BO's performance in high-dimensional spaces. To overcome this challenge, we introduce the Sparse Adaptive Representation-based Bayesian Optimization (SARBO) framework, which integrates BO with the Sure-Independence Screening and Sparsifying Operator (SISSO) method [3]. By capturing the non-linear interactions, SARBO identifies the most relevant features and adaptively updates their selection during the BO cycles, ensuring the optimization is continuously guided by the features that matter most. We demonstrate SARBO's effectiveness through the simulated discovery of single-atom alloy catalysts for CO_2 activation.

[1] Y. Tian, et al., npj Comput. Mater. 11, 209 (2025)

[2] M. R-. Kochi et al., Chem. Sci. 16, 5464 (2025)

[3] R. Ouyang et al., Physical Review. M 2, 8 (2018)

MM 5.4 Mon 11:15 SCH/A251

Fantastic Polaronic Peaks and Where to Find Them: Learning Vibrational Spectra of a Disordered Energy Material — •Christoph Dähn[1], Yang Wang[2], Risov Das[2], Bettina V. Lotsch[2], Karsten Reuter[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]MPI für Festkörperforschung, Stuttgart

Vibrational Raman and infrared spectroscopy offers unique opportunities for characterizing microscopic structural and dynamical properties. For energy materials and in particular for solar batteries [1], a straightforward interpretation of such spectra is however hindered by the intrinsic structural and occupational disorder, which includes defects and polarons. At the same time, this also prevents their accurate *ab initio* simulation, which would require extensive calculations at a hybrid level of density-functional theory (DFT) in a multitude of disordered supercells. In this work, we discuss how machine-learning interatomic potentials trained on high-level DFT data can be used to capture the otherwise inaccessible vibrational dynamics. We demonstrate this approach for a two-dimensional titanium niobate featuring partially occupied metal sites and polarons. By Monte Carlo sampling its configurational disorder, we are able to disentangle polaronic signatures and disorder induced contributions in the spectra. This reveals how local atomic environments control polaron stability and offers insights on how doping can be used to control charge retention in such compounds.

[1] M. Rinaldi *et al.*, J. Phys.: Mater. **8**, 031003 (2025).

15 min. break

Topical Talk MM 5.5 Mon 11:45 SCH/A251

Leveraging data science technologies to enable AI-driven materials design — •Tilmann Hickel[1,2], Han Mai[2], Shankha Nag[1], Sarath Menon[3], Osamu Waseda[2], Liam Huber[1,2], Jan Janssen[2], and Jörg Neugebauer[2] — [1]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — [2]MPI für Nachhaltige Materialien, Düsseldorf, Germany — [3]Ruhr University Bochum, Germany

The handling of materials data is of key importance in designing and producing engineering systems. Therefore, consortia such as NFDI MatWerk aim to develop a sustainable infrastructure for the digital representation of materials science and engineering. The goal is to seamlessly integrate decentralized data and metadata, experimental and computational workflows, and a materials ontology to maximize interoperability and reproducibility of materials data processing. Many AI techniques particularly benefit from structured workflows for data generation and exploitation. For example, the generation and application of machine-learning interatomic potentials becomes accessible for many materials scientists via workflow-management systems such as pyiron. In conjunction with semantic technologies and large-language models they allow to design and validate novel, complex workflows solutions in materials science. We will demonstrate these advantages in the context of atomistic approaches to chemo-structural couplings in metallic alloys. To this end, a high-throughput analysis of the segregation behaviour to grain boundaries will be introduced. Further, hydrogen solubility trends in alloys will be discussed. We will conclude future perspectives in materials informatics.

MM 5.6 Mon 12:15 SCH/A251

Unveiling the Core of Materials Properties via SISSO and Sensitivity Analysis: Use-case Demonstration for Perovskites — •Lucas Foppa and Matthias Scheffler — The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Berlin, Germany.

Interpretable AI can help reveal the physical principles governing intricate material properties and functions. In particular, the sure-independence screening and sparsifying operator (SISSO) symbolic-regression approach identifies analytical expressions correlating a target materials performance to a small set of physical descriptive parameters, termed materials genes, selected from a vast pool of primary features. However, the identified genes influence the SISSO models to different degrees. Here, we use the gradient-based partial-effect sensitivity analysis to pinpoint the most influential genes, thus enhancing SISSO's interpretability and enabling deeper physical insights. This analysis also highlights that different combinations of genes can yield equally accurate descriptions of the correlation. The approach is demonstrated for the bulk properties of perovskites.

MM 5.7 Mon 12:30 SCH/A251

Towards automated calculation of phase diagrams with machine learning interatomic potentials — •Sarath Menon and Ralf Drautz — ICAMS, Ruhr University Bochum, Germany

Calculation of thermodynamic properties and phase diagrams through atomistic simulations provides valuable insights for the design and assessment of new materials. Accurate phase diagram prediction requires determining the Helmholtz and Gibbs free energies for relevant phases and understanding their dependence on thermodynamic state variables, yet conventional approaches remain technically complex and computationally demanding.

In this work, we introduce algorithms that streamline the computation of multicomponent phase diagrams. Relevant phases are identified using a combination of materials databases and machine learning interatomic potentials, and their free energies are computed with atomic cluster expansion potentials. Temperature and composition effects are assessed through non-equilibrium thermodynamic integration and alchemical sampling, including both vibrational and configurational entropy contributions.

We demonstrate the methodology by computing unary pressure-temperature and several binary temperature-composition phase diagrams as well as phase equilibria in ternary materials. We provide all corresponding computational tools. The workflows are designed to be independent of the interatomic potential and material system, supporting broader use and advancing the accessibility of thermodynamic phase diagram computation in atomistic simulations.

MM 6: Invited Talk: David Rodney

Time: Monday 15:00–15:30 Location: SCH/A251

Invited Talk MM 6.1 Mon 15:00 SCH/A251

Transformation-induced plasticity in zirconia ceramics: simulations and experiments — •David Rodney — Insitut Lumière Matière, University of Lyon, France

Similar to steels, zirconia ceramics display transformation-induced plasticity (TRIP) through an stress-induced tetragonal-to-monoclinic phase transformation. However, the conditions under which TRIP occurs remain unclear, owing to the intrinsic complexity of the transformation, which involves multiple variants and intermediate phases, and to experimental and computational limitations. Experimentally, the transformation is difficult to track in situ and classical interatomic potentials do not capture zirconia's polymorphism.

We present a combined experimental and numerical study addressing these challenges. Experimentally, we perform in situ Laue microdiffraction on ceria-doped zirconia micropillars compressed along different crystallographic directions. We replicate the same loading conditions in atomistic simulations using a neural-network interatomic potential (NNIP) trained on extensive DFT data and capable of describing the phase behavior of pure and ceria-stabilized zirconia.

Comparison between experiments, NNIP simulations, and DFT calculations provides new insights into the transformation mechanisms. The results clarify the origin of tetragonal stabilization by ceria and show that TRIP proceeds through a complex sequence of stable and metastable phases, including multiple monoclinic and orthorhombic structures, revealing a richer transformation landscape than previously recognized.

MM 7: Mechanical Properties and Alloy Design II

Time: Monday 15:45–18:30 Location: SCH/A215

MM 7.1 Mon 15:45 SCH/A215

On-the-Fly Machine Learning of Interatomic Potentials for Elastic Property Modeling in Al-Mg-Zr Solid Solutions — •Lukas Volkmer[1], Leonardo Medrano Sandonas[1], Philip Grimm[2,3], Julia Kristin Hufenbach[2,3], and Gianaurelio Cuniberti[1,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials,TUD Dresden University of Technology — [2]Institute of Materials Science, Technische Universität Bergakademie Freiberg — [3]Leibniz Institute for Solid State and Materials Research Dresden — [4]Dresden Center for Computational Materials Science, TUD Dresden University of Technology

Aluminum-based alloys offer exceptional mechanical performance due to their low density, high specific strength, and strong resistance to oxidation and corrosion. In this work, we develop a scalable and transferable machine-learning interatomic potential (MLIP) capable of accurately predicting thermodynamic, mechanical, and microstructural properties across a broad concentration space of Al-Mg-Zr alloys. The MLIP is trained using an active-learning workflow that combines ab initio molecular dynamics, Bayesian uncertainty quantification, and kernel ridge regression, enabling efficient exploration of diverse atomic environments. Additionally, we model an Al/Al3Zr grain-boundary system using experimentally observed orientation relationships and calculate the stress-strain behavior. This framework provides a computationally efficient strategy for exploring the phase space of Al-based alloys and guiding the design of materials with optimized mechanical properties.

MM 7.2 Mon 16:00 SCH/A215

Atomistic modelling of Ni-based superalloys at real chemical complexity — •Aditya Vishwakarma, Sarath Menon, Thomas Hammerschmidt, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Germany

Ni-based superalloys are critical high-temperature high-load materials for jet-engine turbine blades. While *ab-initio* computation has been essential for fundamental understanding (e.g., in binary NiAl), simulating the full chemical complexity of commercial superalloys has remained computationally infeasible. In this work, we demonstrate how Graph Atomic Cluster Expansion (GRACE) foundational models overcome this limitation to investigate the complex phase stability of the γ and γ' phases in industrially relevant Ni-based superalloys. We compute the binary NiAl phase diagram, successfully reproducing the critical γ-γ' phase coexistence. We then extend these phase stability calculations to a CMSX-4 type multi-component composition using hybrid Molecular Dynamics/Monte Carlo simulations. Our results reveal the short-range order (SRO) in the γ phase and quantify long-range order (LRO) in the γ' phase. We specifically find that refractory alloying elements (Ta, W, Ti) exhibit strong LRO alongside Al across the operational temperature range. These findings validate that foundational machine learning interatomic potentials are now capable of calculating complex phase diagrams and capturing subtle ordering and clustering phenomena in multi-component alloys. This capability marks a crucial step toward realizing faster, computationally-driven design of next-generation, single-crystal Ni-based superalloys.

MM 7.3 Mon 16:15 SCH/A215

A machine-learning approach to investigate deformation mechanisms in Mo-Si-based alloys — •Julie Hammoud and Karsten Albe — Technische Universität Darmstadt, Darmstadt, Germany

Mo-Si-X alloys have gained significant attention for high-temperature applications such as turbine blades, due to their outstanding creep resistance, thermal stability and corrosion resistance. In general, Mo-Si-X alloys include three phases: two intermetallic phases (Mo_3Si and Mo_5SiX_2) and a Mo solid solution phase Mo_{ss}. Despite its limited oxidation resistance, the solid solution phase enhances the room temperature fracture toughness of the system. However, the Mo solid solution also incorporates Si-rich subphases with a complex microstructure that leads to an unconventional and still insufficiently understood solid solution strengthening behaviour. Previous studies indicate that small additions of Si (0.1 wt.%) soften Mo, motivating a closer examination of this effect. In this study, we employ a machine-learning interatomic potential (MLIP) based on the Atomic Cluster Expansion (ACE) formalism for the Mo-Si binary system. MLIPs have demonstrated their capability to combine first principles calculations accuracy with the scalability characteristic of empirical potentials. To investigate how Si affects the mechanical response of Mo, we examine two aspects: (i) the concentration dependence of Si on the elastic moduli, analyzed within the framework of the Fleischer model, and (ii) the influence of Si on the behaviour of screw dislocations activity under external loading.

MM 7.4 Mon 16:30 SCH/A215

Jog-Pair Formation and Climb Mechanisms of Dissociated Dislocations in FCC Metals — •Erik Bitzek[1], Sergei Starikov[2], and Daria Smirnova[1,2] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]ICAMS, Ruhr-Universität Bochum, Germany

Jogs on dislocations are preferred sites for vacancy segregation and thus play a critical role in dislocation climb. Under conditions of high point-defect supersaturation – such as after quenching or irradiation – the availability of jogs along the dislocation line can become the rate-limiting factor for climb. Understanding jog-pair nucleation is therefore essential for modeling the kinetics of dislocation creep. Jog pair formation on split edge dislocations in fcc metals was first investigated by Thomson and Balluffi [J. Appl. Phys. 1962] and atomistic simulations [Sarkar et al., PRB 2012] confirmed the suggested mechanism. However, both studies assumed a certain vacancy configuration at the dislocation as the initial nucleus.

Using high-temperature molecular dynamics simulations of dislocations in vacancy supersaturated nickel, we identify an alternative pathway that takes place without predefined nuclei. We demonstrate the role of $\langle 110 \rangle$-oriented vacancy tubes in the climb of edge and 60° dislocations and propose a new climb mechanism for 30° dislocations involving double cross-slip of the screw partial dislocation. These findings highlight how atomistic simulations can inform mesoscale models of creep and annealing.

MM 7.5 Mon 16:45 SCH/A215

Seeking descriptors for predicting mechanical properties of transition-metal light-element compounds — •Rui Zhang[1,2], Xinlei Gu[1], Kan Zhang[1], Chang Liu[3], and David Holec[2] — [1]Department of Materials Science, Jilin University, Changchun 130012, China — [2]Department of Materials Science, Montanuniversity Leoben, Franz Josef-Straße 18, 8700 Leoben, Austria — [3]College of Physics, Jilin University, Changchun 130012, China

Mechanical strength and durability are key properties that dictate service life. To meet requirements of modern technological and industrial applications, it is essential to screen, sort and predict targeted mechanical properties via finding descriptors that can effectively identify materials with specific application needs. Transition-metal light-element (TMLE) compounds show superb mechanical, chemical and thermal properties. We focus on the analysis of the intrinsic physical/chemical parameters of the component elements and structure factors to identify the key factors affecting the mechanical properties of TMLE. In this presentation, we will introduce two research works: (1) Core electron count as a versatile and accurate new descriptor for sorting mechanical properties of diverse transition metal compounds; and (2) Nitrogen vacancy regulated lattice distortion improvement of mechanical properties and wear resistance of (NbMoTaW)Nx thin films. Ultimately, our work yielded a universal descriptor incorporating core electron count and established nitrogen-vacancy-driven lattice distortion as a key structural factor, offering two distinct pathways to guide the design of high-performance materials.

15 min. break

MM 7.6 Mon 17:15 SCH/A215

Atomistic-to-Mesoscale Computational and Experimental Analysis of the Interactions between Dislocations, Precipitates, Grain and Phase Boundaries in Complex Alloys — •Liming Xiong — NC State University, Raleigh, NC, USA

In this talk, we will present multiscale computational and experimental analysis on the deformation behavior of complex alloys. In experiments, polycrystalline nickel, alloy 709, and Ni3Al-NiCr (γ/γ') alloys are deformed in a transmission electron microscope (TEM). Microstructure evolution is imaged through in-situ TEM. Local stress build up at the slip-GB/PBs are measured by electron backscattering diffraction (EBSD). Meanwhile, concurrent atomistic-continuum (CAC) simulations are performed to understand how a queue of dislocations interacts with the atomically structured precipitates, coherent twin boundaries (CTBs), GB, and γ/γ' PB. One unique feature of CAC is to accommodate the microscale slip containing a large population of dislocations together with the atomistic structure nearby the precipitates/GB/PBs all within one model. Our several findings are: (i) the sequential dislocation-precipitates differs from the single dislocation-precipitates. It is history dependent and has a mechanism cross-over from Orowan bowing out to cross-slip; (ii) the CTBs don't block dislocations. They can accommodate incoming dislocations by allowing them to migrate and form a pileup on the CTB; (iii) dislocation motion is smooth in γ phase but jerky in γ' phase. Such insight will support the design of high-performance alloys by configuring the precipitates, CTBs, GBs, and PBs in them appropriately.

MM 7.7 Mon 17:30 SCH/A215

The Effect of Rhenium on Irradiation Induced Defects in Tungsten-Rhenium Alloys Studied by Positron Annihilation Spectroscopy — •Lisa-Marie Krug[1], Danny R. Russell[1], Maximilian Suhr[1], Leon Chryssos[1], Lucian Mathes[1], Mikhail Zibrov[2], Thomas Schwarz-Selinger[2], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Garching, Germany — [2]Max Planck Institute for Plasma Physics, Garching, Germany

The plasma-facing components in a nuclear fusion reactor have to withstand irradiation by 14 MeV neutrons. Tungsten is considered to be the most suitable plasma-facing material, due to its high melting point, high thermal conductivity and low erosion under fusion reactor operating conditions. In addition to radiation damage, neutron irradiation of tungsten induces nuclear transmutation reactions, resulting in the formation of rhenium. We investigated the effect of Re on the defects produced during the irradiation of W. We provide bench-marking data at extremely high damage doses using ion-irradiation. Transmutation to Re is substituted by Re-ion irradiation or the use of W-Re alloys. Positrons provide a non-destructive, atomic scale resolution of defect analysis of the irradiation damage. Positron Annihilation Spectroscopy (PAS) is a suitable method to determine the defect type, concentration and chemical surrounding. We observe a positive effect of Re on the radiation damage after irradiation at both room temperature and 1350 K. We have found evidence that fewer vacancy clusters are present after irradiation of W-3%Re alloys.

MM 7.8 Mon 17:45 SCH/A215

Understanding the influence of residual elements on the toughness of martensitic steels towards recycled steels — •Eloho Okotete, Subin Lee, and Christoph Kirchlechner — Karlsruhe Institute of Technology, Karlsruhe, Germany

Martensitic steels are critical for many load-bearing applications due to their inherent microstructure, giving rise to unique mechanical properties. However, traditional steelmaking routes produce high greenhouse gas emissions, posing a long-term threat to our environment. Cleaner steel production alternatives aim to use recycled iron scrap as input to electric arc furnaces used in steelmaking. A significant concern for key stakeholders in the steel industry and academia is the presence of residual elements, including Cu, Sn, Sb, As, and P, in iron scrap. Hence, an in-depth analysis of the role of the residual elements on the local and global mechanical properties of martensitic steel would provide relevant insights for the development of environmentally friendly steelmaking alternatives. Small-scale mechanics using indentation-based techniques can help locally probe how the critical microstructural features of lath martensite, such as prior austenite grain boundaries, packets, blocks, and laths, are affected by residual elements.

In this talk, we use nanoindentation, micro-pillar compression, and micro-cantilever bending experiments to identify the residual element that has the most detrimental effect on the microstructure and properties of our lath martensite. Then, proceed to determine the most impacted microstructural feature of our microstructure as well as the predominant damage mechanism in the steel samples.

MM 7.9 Mon 18:00 SCH/A215

Martensitic phase transformation and anomalous hardening of CrMnFeCoNi high-entropy alloy deformed by high pressure torsion — Robert Chulist[1], Aurimas Pukenas[2], Anton Hohenwarter[3], Reinhard Pippan[3], and •Werner Skrotzki[2] — [1]AGH University of Science and Technology, Krakow, Poland — [2]Technische Universität, Dresden, Germany — [3]Montanuniversität, Leoben, Austria

Under hydrostatic pressure, the CrMnFeCoNi high-entropy alloy

(HEA) undergoes a phase transformation from face-centered cubic to hexagonal close-packed. The onset pressure is strongly reduced by high pressure torsion (HPT): shear stress promotes partial dislocation slip. HPT of the low stacking fault energy HEA leads to a nanocrystalline microstructure. The hardness anomaly is due to the extreme nanostructuring, with grain boundary/interphase boundary sliding acting as predominant deformation mechanism: inverse Hall-Petch regime, in which hardness increases with increasing grain size. In submicrocrystalline materials, conventional Hall-Petch hardening dominates, i.e., hardness decreases with increasing grain size.

MM 7.10 Mon 18:15 SCH/A215

Insights into loading condition and microstructural evolution under tribological load — •Antje Dollmann, Robin Freville, Patric Gruber, Christoph Kirchlechner, and Christian Greiner — IAM, KIT, Karlsruhe, Germany

Tribological loading changes the microstructure of materials in contact, e.g. in coarse-grained metals, grain refinement occurs, followed by cracks formation and wear particles removal leading to component failure. This requires an adequate description of the stress field to understand the ongoing microstructural evolution. Due to the complexity of tribological loading, two approaches were explored, both on single-crystalline face-centred cubic metallic materials:

(1) The experiments on CoCrFeMnNi were designed in such a fashion that in some crystal orientations deformation twins were formed. These served as probes to validate various stress field models. General trends regarding the influence of different materials parameters can be identified. The most significant mismatch is between the experimentally observed deformation layer depth and the calculated depth by the stress field. (2) In copper, one deformation layer was analysed by *Laue. Based on its higher sensibility towards small deformations, the deformation layer thickness was greater than what had been detected previously. The combination of those approaches gives deep insight into the so far hidden stress field, which will support future efforts in designing materials to withstand tribological loading.

MM 8: Materials for the Storage and Conversion of Energy II

Time: Monday 15:45–18:30 Location: SCH/A216

MM 8.1 Mon 15:45 SCH/A216

Self-Consistent Hubbard Corrections for Accurate Modelling of Li- and Na-Ion Cathodes — •Valentina Sanella[1,2], Stefan Schären[1,3], Cristiano Malica[4], Livia Giordano[5], Nicola Marzari[1,3,4], Claude Ederer[2], and Iurii Timrov[1] — [1]PSI, Switzerland — [2]ETHZ, Switzerland — [3]EPFL, Switzerland — [4]U Bremen, Germany — [5]UniMiB, Italy

Accurate first-principles modelling of layered transition-metal oxides is essential for understanding and optimizing cathode materials for Li- and Na-ion batteries.

In this work, we investigate two widely studied systems: $LiCoO_2$ and P2-Na_xMnO_2, using density-functional theory (DFT) with self-consistent Hubbard corrections (DFT+U+V). We apply onsite U parameters to both transition-metal $3d$ orbitals and oxygen $2p$ states, together with intersite V derived from density-functional perturbation theory (DFPT), enabling a consistent treatment of electron localization and metal-oxygen hybridization.

For $LiCoO_2$, we show that including a U correction on oxygen significantly improves predictions of the intercalation voltages, resolving known inaccuracies associated with standard DFT approaches. In Na_xMnO_2, the extended Hubbard formalism provides a more realistic description across varying sodium concentrations, leading to reliable predictions of structural stability and electrochemical trends.

Our results demonstrate that self-consistent U and V parameters provide significant improvements over empirical or fixed values, enabling reliable predictions of structural and electronic properties.

MM 8.2 Mon 16:00 SCH/A216

Voltage Profile Predictions for Na-Ion Cathodes: A Hybrid MLIP / PBEsol+U+V approach — •Stefan Schären[1,2], Valentina Sanella[1,3], Manuel Dillenz[4], Nicola Marzari[2], and Iurii Timrov[1] — [1]PSI, Villigen, Switzerland — [2]EPFL, Lausanne, Switzerland — [3]ETHZ, Zürich, Switzerland — [4]DTU, Copenhagen, Denmark

Sodium-ion batteries are emerging as a sustainable alternative to lithium-ion batteries, but are limited by the lack of a cathode that offers high voltage, energy density and long-term stability. Here, we present a computational approach that accelerates the prediction of voltage profiles during cathode discharge, using a combination of self-consistent Hubbard-corrected DFT (PBEsol+U+V), and foundational machine-learning interatomic potentials (MLIPs). Using $Na_xV_2(PO_4)_3$ (NVP) as a test case, we show that MLIP-based prescreening reduces the number of required DFT calculations to a fraction of those needed for a traditional cluster expansion, while retaining comparable accuracy. Furthermore, the self-consistent Hubbard U and V corrections yield electronic occupations that closely match the chemical intuition for oxidation states, enabling a direct analysis of vanadium redox activity and associated volume changes during desodiation. Altogether, the approach delivers a useful and predictive toolkit for identifying high-performance Na-ion cathodes in the future.

MM 8.3 Mon 16:15 SCH/A216

Electronic structure of perovskite oxides calculated with dynamical mean field theory — •Daniel Mutter[1], Jannis Ehrlich[1], Frank Lechermann[2], Daniel F. Urban[1], and Christian Elsässer[1] — [1]Fraunhofer IWM, Freiburg — [2]Institut für Theoretische Physik III, Ruhr-Universität Bochum

Perovskite oxide materials containing first-row transition-metal (TM) elements are regarded as promising alternatives to platinum-based electrodes for high-temperature solid-oxide fuel and electrolyser cells. This is due to the strong electronic correlation effects of the localized 3d electrons of the TM, which directly influence the mechanism and activity of the oxygen reduction reaction. We analyze the electronic structure of perovskite oxides by means of a combined approach of density functional theory and the dynamical mean field theory (DFT+DMFT) to account for the correlation of the electrons in the TM-3d orbitals. We exemplarily demonstrate the influences of static versus dynamic correlation. In addition, we consider correction methods to treat the correlation in the O-2p orbitals, namely the self-interaction correction (SIC) or the DFT-1/2 method. A systematic study of different A- and B-site occupations of the ABO_3 perovskite phases will be presented.

MM 8.4 Mon 16:30 SCH/A216

Unraveling the connection between Jahn-Teller dynamics and charge transport in $LiMn_2O_4$ — •Manuel Dillenz, José Maria Castillo Robles, Mikkel Agerbo Essendrop, Ivano Eligio Castelli, and Juan Maria García Lastra — Department of Energy Storage and Conversion, Technical University of Denmark, Kgs. Lyngby, DK-2800, Denmark

Future energy storage solutions demand batteries that are energy-dense, fast-charging, and based on abundant materials. However, ultrafast dynamics in battery electrodes remain insufficiently characterized despite their crucial role in energy storage performance. Moreover, charge transport in Mn- or Ni-based cathodes is strongly influenced by local structural distortions originating from Jahn-Teller active centers. $LiMn_2O_4$ (LMO) exemplifies this behavior, featuring a ferrodistortive tetragonal ground state that undergoes an order-disorder transition at 290K, where pseudorotations continuously reorient the Jahn-Teller axis. These processes occur on timescales relevant for to polaron and ion transport in the electrode. By combining ab initio molecular dynamics (AIMD) simulations with nudged elastic band (NEB) calculations, we reveal that the interplay of JT and polaron dynamics governs the kinetics of charge transfer in LMO. Our work provides essential mechanistic understanding for enhancing charge transport in Jahn-Teller active electrode materials.

MM 8.5 Mon 16:45 SCH/A216

Defect Landscape of $Ba_2In_2O_5$: The Role of Oxygen Interstitials — •Rachele Sciotto and Karsten Albe — achgebiet Materialmodellierung, Institut für Materialwissenschaft, Technische Universität Darmstadt, Otto-Berndt-Str. 3, D-64287 Darmstadt, Germany

$Ba_2In_2O_5$ (BIO) is a promising n-type mixed ionic and electronic conductor (MIEC) for oxygen permeation membranes and solid oxide fuel cells (SOFCs). At ambient conditions, BIO adopts an orthorhombic brownmillerite structure with alternating InO_6 octahedral and InO_4 tetrahedral layers that can host interstitial oxygen atoms at sites of structural vacancies. Existing defect thermodynamics models consider only this type of oxygen interstitial; however, oxygen interstitials forming O-O dumbbells, found in oxides like ZnO and In_2O_3, are also possible. In this work, we investigate the potential existence of O-O dumbbells in BIO using density functional theory (DFT). By calculating formation enthalpies as a function of Fermi level and concentrations as a function of oxygen chemical potential, we identify two distinct classes of interstitial configurations. Neutral O-O dumbbells are stabilized over a wide Fermi-level range, while negatively charged interstitials at the structural oxygen vacancy site become favorable under *n*-type conditions. Although the neutral dumbbells do not contribute to charge compensation, they form in high concentrations. They could therefore serve as intermediate positions for oxygen diffusion pathways, thereby influencing the material's ionic and electronic conductivity.

15 min. break

MM 8.6 Mon 17:15 SCH/A216

Interplay of Dynamic Defects and Ultrafast Carrier Dynamics in Lead-Free Double Oxide Perovskites Toward Stable, High- Performance Photovoltaics — •Manasa Gattavadi Basavarajappa, Arijeet Sarangi, and Sudip Chakraborty — Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Prayagraj - 211019, India

Oxide-based double perovskites are gaining increasing attention as stable and environmentally benign alternatives to halide perovskites in photovoltaic and optoelectronic devices. Their structural versatility and chemical flexibility open pathways for fine-tuning both electronic and lattice properties, yet their carrier dynamics and defect behavior remain less understood. In this work, we investigate these aspects using a combination of first principles calculations and advanced simulation techniques. Non-adiabatic molecular dynamics is employed to capture ultrafast carrier relaxation and to quantify the role of electron*phonon coupling in determining charge transport and recombination lifetimes. The results highlight efficient charge separation and suppressed nonradiative recombination channels, which are essential for high photovoltaic efficiency. To establish the dynamical stability of the materials, we carry out a phonon-based symmetry analysis that confirms the absence of imaginary modes and reveals the interplay between structural distortions and vibrational spectra. In parallel, we explore the formation and dynamic evolution of intrinsic point defects through defect-mediated molecular dynamics simulations.

MM 8.7 Mon 17:30 SCH/A216

Morphological study of $LiNi_{0.5}Mn_{1.5}O_4$ synthesized with alkali molybdates by density functional theory — •Liang-Yin Kuo[1], Tavinder Singh[1], Rio Akbar Yuwono[2], Fu-Ming Wang[2], and Harald Oberhofer[1] — [1]Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth — [2]Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology

High-voltage spinel $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) has emerged as a promising cathode active material for next-generation lithium-ion batteries due to its high operating voltage ($\sim$ 4.7 V vs. Li/Li^+), manganese abundance, and potential for high energy density. Single-crystal (SC) LNMO has attracted particular interest because it offers enhanced structural integrity, reduced surface area for electrolyte interaction, and improved cycling stability. Among the synthesis methods, molten-salt synthesis has shown promise for producing SC LNMO. However, the role of the precursor salts remains unclear. In this study, the effects of alkali molybdates, specifically Li_2MoO_4 and Na_2MoO_4, on the SC LNMO formation mechanism are investigated by density functional theory (DFT). Surface energies of various facets are calculated to analyze the resulting Wulff shapes. Our results indicate that LNMO synthesized with Li_2MoO_4 tends to form a truncated octahedron shape, whereas Na_2MoO_4 leads to an octahedron morphology with aggregation into polycrystalline structures. Furthermore, the influence of surface energy on nucleation is discussed, providing insight into morphology control in SC LNMO synthesis.

MM 8.8 Mon 17:45 SCH/A216

Thermodynamic Stability of $MgSc_2Se_4$ Surfaces — •Sebastian Utz[1] and Axel Gross[1,2] — [1]University Ulm, Ulm, Germany — [2]Helmholtz Institute Ulm, Ulm, Germany

$MgSc_2Se_4$ represents a promising candidate for post-lithium battery technologies as a solid-state magnesium ion conductor. With magnesium being significantly more abundant and cheaper than lithium, magnesium-based materials could offer sustainable alternatives for next-generation energy storage systems. While the bulk properties and ion diffusion of $MgSc_2Se_4$ have already been studied extensively, its surface structure and properties remain largely unexplored. However, understanding its surface behaviour is crucial as surfaces and interfaces can behave substantially differently from the bulk. In real applications, like batteries, the properties of surfaces and their interfaces may be limiting factors for stability and mass transfer. This work addresses this gap in the literature by investigating the low-index surfaces of $MgSc_2Se_4$ using grand-canonical density functional theory. Our computational approach enables the characterisation of thermodynamic surface stability and structure under varying chemical potentials. The results provide fundamental insights into surface terminations and their stability in different chemical environments. Combined with experimental validation, these findings could enable detailed atomistic studies of mass transfer at and through $MgSc_2Se_4$ surfaces, supporting the rational assesment of $MgSc_2Se_4$ as a battery material.

MM 8.9 Mon 18:00 SCH/A216

LDH Under Stress: Assessing Degradation Pathways of Ni-Fe-V Catalysts Under Technical Operating Conditions — •Juan Manuel Lombardi, Charles Pare, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

The transition to a sustainable energy landscape relies on electrocatalysts that are not only active and affordable but also structurally robust under operating conditions. Ni-based layered double hydroxides (LDHs) doped with Fe and V are among the most promising OER candidates for anion-exchange membrane water electrolyzers (AEMWE), owing to their tunable lattice chemistry and rich redox behavior. However, the mechanistic influence of these dopants and how they reshape catalytic performance and structural stability remains insufficiently understood due to the immense configurational complexity.

In this contribution, we present an integrated strategy tailored to address this complexity directly. Our evolutionary exploration framework EZGA provides a systematic route through the high-dimensional composition-structure landscape, employing chemically informed operators and explicit diversity control to generate physically meaningful structural candidates. Machine-learning interatomic potentials (MLIPs) enable high-throughput sampling of thermally accessible configurations with near first-principles fidelity, revealing how dopants modulate stability and reactivity. Together, these elements deliver a predictive workflow that reveals how dopants reshape the accessible configurational landscape and provides a mechanistic picture of their influence on stability and reactivity.

MM 8.10 Mon 18:15 SCH/A216

Quantum-mechanical study of miscibility of Sn in $LaNi_5$ — •Martin Friák[1], Petr Čípek[2,1], Anna Huňařová[2,1], Kateřina Dočkalová[2,1], Jana Pavlů[2,1], and Ondřej Zobač[1] — [1]Institute of Physics of Materials, v. v. i., Czech Academy of Sciences, Žižkova 22, Brno, 61600, Czech Republic — [2]Institute of Chemistry, Masaryk University in Brno, Kotlářská 2, Brno, 61137, Czech Republic

The $LaNi_5$ compound is a prototypical hydrogen-storage material intended for future energy applications. Some of its properties have not been sufficiently studied so far, and some critically important data are missing. In particular, there are conflicting literature reports related to the substitution of Ni atoms with Sn atoms in $LaNi_5$. We have employed quantum-mechanical calculations implementing the density functional theory (DFT) within the generalised gradient approximation (GGA) to determine the ground-state structural, electronic, thermodynamic, and vibrational properties of several substituted $La(Ni,Sn)_5$ phases. Our computational cell containing 48 atoms allowed for simulating different Sn/Ni ratios as well as different configurations of substituting Sn atoms. Our results indicate that the free energy of formation is concave and there is a miscibility gap and a decomposition into two phases, one with a low and one with a high Sn concentration. Our theoretical study was complemented by experiments which found a similar miscibility gap, too.

MM 9: Topical Session: Physics-driven Artificial Intelligence for Materials II

Time: Monday 15:45–18:30 Location: SCH/A251

Topical Talk MM 9.1 Mon 15:45 SCH/A251

Atomistic simulations in the ternary Fe-O-H system: interatomic potential development and applications — •Baptiste Bienvenu[1], Mira Todorova[1], Matous Mrovec[2], Ralf Drautz[2], Dierk Raabe[1], and Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr Universität Bochum, Germany

Atomistic modeling of iron oxides is challenging, requiring accurate electronic structure calculations and extensive length and time scales to simulate elementary mechanisms such as the extraction of metallic iron from its oxides through hydrogen-based reduction. To enable atomic scale modeling of these and other technologically relevant processes within the ternary Fe-O-H system (e.g., hydrogen embrittlement, water splitting), an accurate yet efficient interatomic potential is needed, something that is currently lacking in the literature. First, we focus on the binary Fe-O system, for which we previously developed a robust and transferable Atomic Cluster Expansion (ACE) machine-learning potential with an explicit account of magnetism, to study bulk diffusion and the structure and stability of various surfaces of iron oxides. We then extend the model to include hydrogen and show that the resulting ACE potential can faithfully reproduce key mechanisms of the Fe-O-H system: (i) surface reactions and microstructure evolution during hydrogen reduction of iron oxides, (ii) surface reactions of iron and its oxides with water and (iii) hydrogen trapping, interaction with extended defects and permeation in metallic iron.

MM 9.2 Mon 16:15 SCH/A251

Learning long-range interactions with equivariant charges — •Marcel F. Langer, Egor Rumiantsev, Tulga-Erdene Sodjargal, Michele Ceriotti, and Philip Loche — Laboratory of Computational Science and Modeling, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Machine-learning interatomic potentials trained on first-principles data have become key tools across computational physics, chemistry, and biology. Equivariant message-passing neural networks, including transformer variants, now deliver state-of-the-art accuracy, but their cutoff-based graphs restrict the treatment of long-range physics such as electrostatics, dispersion, and electron delocalisation. Existing long-range corrections based on inverse-power laws of distances capture only scalar interactions and cannot convey higher-order geometric information, limiting their applicability. To address this, we propose the use of equivariant (rather than scalar) charges to mediate long-range interactions and build a graph neural-network architecture, LOREM [1], around this equivariant message-passing scheme. The talk will outline the architecture, present results on several benchmark datasets, and discuss our work on universal long-range interatomic potentials.

[1] Egor Rumiantsev, Marcel F. Langer, Tulga-Erdene Sodjargal, Michele Ceriotti & Philip Loche, arXiv:2507.19382 (2025).

MM 9.3 Mon 16:30 SCH/A251

Physics-informed Hamiltonian-learning for large-scale electronic-structure calculations — •Martin Schwade, Shaoming Zhang, Frederik Vonhoff, Frederico P. Delgado, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Exploring the optoelectronic properties of large-scale materials systems across a wide temperature range using conventional density functional theory (DFT) is often prohibitively computationally expensive. Recent advances in deep neural network approaches offer a promising route to efficiently predict accurate effective Hamiltonians, yet incorporating temperature dependence remains challenging, largely due to the substantial volume of training data typically required. In this work, we introduce HAMSTER [1], a physics-informed Hamiltonian-learning framework that achieves high accuracy with exceptional data efficiency, requiring only a small fraction of the training data demanded by alternative machine-learning models. We demonstrate the capabilities of Hamster on several halide perovskite systems, known for their soft lattices and strong electron-phonon coupling, and show that it reliably reproduces their optoelectronic properties across a broad range of temperatures.

[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)

MM 9.4 Mon 16:45 SCH/A251

Making equivariant graph neural network prediction of electronic structure properties fast and accurate — •Chen Qian[1], Valdas Vitartas[1], James Kermode[1], and Reinhard J. Maurer[1,2] — [1]University of Warwick, UK — [2]University of Vienna, AT

Machine learning predictions of band structures and equivariant electronic properties, such as real-space density functional theory (DFT) operator matrices and response properties, have the potential to accelerate electronic structure prediction while avoiding expensive ab initio calculations. However, most current models struggle to strike a balance between prediction accuracy and inference speed. Following our previous work on the equivariant graph neural network MACE-H [arXiv:2508.15108], we assess the model's performance on DFT operator matrices and, subsequently, on a property based on electron-phonon response, the electronic friction tensor. We compare its applications across various datasets. Furthermore, we analyze several existing algorithm- and hardware-based acceleration methods for the computationally intensive Clebsch-Gordan tensor product in terms of accuracy and computational efficiency, and discuss their respective suitable application scenarios. To this end, we present the MACE-H2 framework, which features an O(3) equivariant graph neural network with many-body expansion and suitable acceleration approaches and provides separate routines for DFT operator matrices and electron-phonon response prediction. The model achieves high accuracy and inference speed and is suitable for high-throughput band-structure calculations and material discovery.

15 min. break

MM 9.5 Mon 17:15 SCH/A251

Predicting the Thermal Properties of Semiconductor Defects with Equivariant Neural Networks — •Jonas A. Oldenstaedt, Manuel Grumet, Xiangzhou Zhu, Patrick Rinke, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Predicting temperature-dependent properties of defects in semiconductors remains computationally challenging, even with density functional theory (DFT), due to the large supercells and long simulation times required for the calculations. In our recent work [1], we developed an active-learning workflow to accelerate defect calculations by combining two equivariant graph neural networks, trained using DFT calculations: MACE for predicting energies and forces needed in molecular dynamics, and DeepH-E3 for predicting electronic Hamiltonians needed for computing electronic properties across many thermally-excited configurations. We discuss the performance of our approach for predicting structural and electronic properties of intrinsic defects in the prototypical semiconductor GaAs, and demonstrate calculation accuracy comparable to DFT at much reduced computational cost. Furthermore, we discuss extensions of our approach to predict the thermal behavior of defects in more complex semiconductors such as halide perovskites.

[1] X Zhu, P. Rinke and D. A. Egger, arXiv:2511.18398 (2025).

MM 9.6 Mon 17:30 SCH/A251

Learning exact exchange with symbolic regression — •Noah Hoffmann, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin, Berlin, Deutschland

Density functional theory (DFT) is the most widely used method for the ab-initio prediction of material properties. It is used for computing structural, vibrational, and electronic properties and more. One important factor influencing the accuracy of the predictions is the choice of the exchange-correlation functional. PBE is the de-facto standard functional because of its good results for ground-state properties at comparatively low computational cost. The most prominent downside of this functional, however, is the underestimation of electronic band gaps. Hybrid functionals like PBE0 compensate this by mixing PBE with the non-local exact-exchange (EXX) energy. This improves band-gaps but comes with a drastic increase in computational cost. We apply symbolic regression (SR), a machine-learning technique, to find inexpensive yet accurate exchange potentials as a surrogate for the

EXX potential. This enables computationally efficient DFT calculations with an accuracy close to that of hybrid functionals. To generate the training data for the SR models, we used the optimized effective potential (OEP) method, in which a local approximation to the EXX potential is constructed. The OEP method provides rather accurate electron densities. The SR models are then validated with respect to their numerical stability and their ability to predict band gaps. Compared to PBE, the SR models show improved band gap predictions on OEP band gaps with comparable computational cost.

MM 9.7 Mon 17:45 SCH/A251

Development of a GRACE Machine-Learning Potential for Modeling SiC Epitaxial Growth — •Anders Vesti, Thomas Hammerschmidt, and Ralf Drautz — Ruhr Universtät Bochum, Bochum, Germany

Silicon carbide (SiC) is a highly attractive wide band-gap semiconductor for power electronics due to its high breakdown field and low on-state resistance. However, the widespread adoption of SiC-based devices is hindered by challenges in epitaxial growth, including uncontrolled polytype switching and defect formation, which ultimately increase production costs.

In this work, we present the development and benchmarking of a physics-driven machine-learning interatomic potential for SiC based on the GRACE formalism. Starting from a general-purpose foundational model, we refit the potential using comprehensive C, Si, and SiC datasets to construct a specialized model tailored for simulating SiC epitaxy.

We validate the resulting GRACE potential against density functional theory (DFT) calculations and available experimental data for Si, C, and SiC. The developed model provides a basis for testing proposed growth mechanisms in SiC epitaxy.

MM 9.8 Mon 18:00 SCH/A251

Integrating FlashMD into LAMMPS for Efficient Long-Timestep Molecular Dynamics — •Johannes Spies, Filippo Bigi, and Michele Ceriotti — Laboratory of Computational Science and Modeling, Institut des Matériaux, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

FlashMD [1] is a machine-learning model that predicts future molecular configurations from the current state, reducing the need to call machine-learning interatomic potentials at every timestep and enabling larger effective integration steps.

I present its integration into LAMMPS. The implementation acts as a drop-in replacement for standard integrators and makes FlashMD directly available to the molecular simulation community. The interface is modular and extensible through the metatomic ecosystem, allowing new predictor models to be added with minimal effort.

The contribution outlines the integration strategy and initial performance results, focusing on usability, extensibility, and compatibility with existing MLIP workflows. The approach provides a practical route to accelerating large-scale atomistic simulations by reducing the frequency of expensive potential evaluations while maintaining physical reliability.

[1] Filippo Bigi, Sanggyu Chong, Agustinus Kristiadi & Michele Ceriotti, arXiv:2505.19350 (2025).

MM 9.9 Mon 18:15 SCH/A251

Learning to Converge: ML-based Initialization for Fast DFTB Simulations — •Maximilian L. Ach, Karsten Reuter, and Chiara Panosetti — Fritz-Haber-Institut der MPG, Berlin

Density Functional Tight-Binding (DFTB) [1], a class of semiempirical electronic structure methods, captures the electronic structure of a material, unlike conventional machine-learned (ML) interatomic potentials, at a significantly lower computational cost compared to *ab initio* methods. Despite this gain in efficiency, for many processes, DFTB does not scale favorably with the number of atoms, and simulations of realistic material systems often represent a significant challenge due to the associated computational overhead. A large portion of this cost can be attributed to the difficulty of converging these calculations efficiently. To address this, we introduce an ML-enhanced scheme, which significantly accelerates and improves the DFTB self-consistent charge convergence. Our approach leverages state-of-the-art ML methods to provide improved initializations for DFTB calculations, hence reducing the overall cost. We demonstrate the effectiveness of this method on small molecules and a range of materials.

[1] B. Hourahine *et al.*, J. Phys. Chem. A **129**, 5373 (2025).

MM 10: Invited Talk: Lola Lilensten

Time: Tuesday 9:30–10:00 Location: SCH/A251

Invited Talk MM 10.1 Tue 9:30 SCH/A251

Chemically graded materials for accelerated exploration of the TRIP-TWIP Ti-alloy family — •Lola Lilensten — IRCP - CNRS, Paris, France

Twinning induced plasticity (TWIP) and transformation induced plasticity (TRIP) in β-metastable titanium alloys provide remarkable work hardening, enhancing ductility and strength, opening up new possibilities for titanium alloys. These mechanisms depend on the metastability of the retained β phase and thus on the alloy composition.

However, the development of these alloys is still limited. Current design approaches are mostly empirical, relying on datasets that focus on composition and deformation mechanisms, neglecting factors like processing conditions, grain size, and oxygen content. This leads to inconsistencies and overlooks optimization opportunities through microstructure engineering.

The chemically graded materials approach is proposed to tackle this problem, enabling quick identification of compositional ranges where specific deformation mechanisms occur, and consistent results since all compositions share the same processing. This method accelerates the study and development of TRIP/TWIP Ti-alloys.

MM 11: Structurally and Chemically Complex Alloys

Time: Tuesday 10:15–11:45 Location: SCH/A215

MM 11.1 Tue 10:15 SCH/A215

Quantifying chemical short-range order in Ti–Zr–Nb alloys — Yujun Zhao[1,2], Andrea Fantin[3], Yue Li[1], Tong Li[2], and •Yilun Gong[4] — [1]Max-Planck-Institut für Nachhaltige Materialien, Düsseldorf, Germany — [2]Ruhr Universität Bochum (RUB), Bochum, Germany — [3]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany — [4]University of Oxford, Oxford, UK

Chemical short-range order (CSRO) is expected to influence phase stability and defect interactions in Ti–Zr–Nb alloys, yet its direct quantification in equiatomic TiZrNb has remained unresolved. Here, we apply X-ray absorption spectroscopy (XAS) and X-ray pair-distribution-function (PDF) analysis to experimentally probe local chemical environments in single-phase bcc TiZrNb. Nanometre-scale compositional fluctuations and elemental pair distributions are further explored using orientation-specified atom-probe tomography (APT). XAS and PDF measurements reveal small but systematic local distortions in element-specific partial coordination shells (from XAS), consistent with emerging CSRO, and ensemble-averaged structural distortions in the atomic network (from PDF). To interpret these findings, we develop density functional theory-trained interatomic potentials and perform on-lattice Monte Carlo simulations to obtain the temperature-dependent equilibrium CSRO pair correlations. Together, these results provide the first quantitative CSRO map for TiZrNb, capturing its temperature and crystallographic dependence. This establishes TiZrNb as a reference system for understanding how CSRO influences phase stability, interstitial accommodation, and mechanical behaviour in refractory alloys.

MM 11.2 Tue 10:30 SCH/A215

Radiation Tolerance in High Entropy Alloys — •Jyoti Verma[1], Paul Chekhonin[2], Andreas Worbs[1], Cornelia Kaden[2], Maciej Oskar Liedke[3], and Gregor Hlawacek[1] — [1]Institute of Ion Beam Physics and Material Research,Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstrasse 400 — [2]Institute of Resource Ecology,Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstrasse 400 — [3]Institute of Radiation Physics,Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstrasse 400

High-entropy alloys (HEAs), or compositionally complex alloys (CCAs), are near-equiatomic multicomponent materials forming single-phase solid solutions with exceptional mechanical strength, thermal stability, and radiation resistance, making them strong candidates for structural use in advanced nuclear systems. In Generation IV fission and future fusion reactors, materials must endure 500*600 °C, high neutron fluxes, and helium and hydrogen generated by 14 MeV neutrons, which significantly influence irradiation-induced defect evolution. We are investigating the irradiation response of Co-free (CrFeMnNi) CCAs using Fe-ion irradiation at 300°C to 1, 3, and 10 dpa. Transmission electron microscopy revealed typical dislocation loops, while positron annihilation spectroscopy identified vacancy-type defects and vacancy-dislocation complexes, whose concentration decreased with dose, suggesting progressive interaction and annihilation between vacancies and dislocations at higher irradiation levels. These results demonstrate the promising irradiation tolerance of Co-free CCAs for structural use in next-generation reactors.

MM 11.3 Tue 10:45 SCH/A215

Preparation of an impurity-free quinary alloy surface without significant changes in composition — •Yong-He Pan[1], Niklas Osterloh[1], Wun-Chang Pan[1], Natalia Pukhareva[2], Alfred Ludwig[2], and Karina Morgenstern[1] — [1]Physical Chemistry I, Ruhr University Bochum, Universitätsstr. 150, 44780 Bochum, Germany — [2]Centre for Interface-Dominated High-Performance Materials (ZGH), Ruhr University Bochum, Universitätsstr. 150, 44780 Bochum, Germany

Compositionally Complex Solid Solutions (CCSSs) are a promising new pathway to electrochemical catalysts [1,2]. Their complex surface offers multiple adsorption sites for different reaction steps simultaneously [3]. We investigated the composition of the surface elements and impurities using X-ray photoelectron spectroscopy. The quinary alloy sample Ag-Au-Ir-Pd-Pt was prepared in ultra-high vacuum by argon sputtering and annealing. Surface impurities were removed by sputtering, and the alloy composition remained stable even during prolonged thermal treatment. Optimal sputtering and annealing parameters for achieving a clean surface were established. This study clarifies the effects of these processes on the surface composition ratio of Ag-Au-Ir-Pd-Pt alloys.

[1] H. J. Qiu et al., J. Mater. Chem. A, 2019, 7, 6499 [2] T. Löffler et al., Angew. Chem. Int. Ed. 2021, 60, 26894 [3] J. K. Pedersen et al., ACS Catal. 2020, 10, 2169

MM 11.4 Tue 11:00 SCH/A215

Effect of partial occupancy on the properties of FeCr σ-phase — •Mariano Forti[1], Guillaume Laplanche[1], Wenhao Zhang[2], Ralf Drautz[1], and Thomas Hammerschmidt[1] — [1]Ruhr Universität Bochum, Germany — [2]LINK, CNRS-Saint-Gobain- NIMS

The σ-phase forms in Fe-Cr alloys over 870K at about 50 at.% Cr, strongly affecting their performance. Atomistic studies usually assume a sublattice model, but experiments show fractional occupancy of the Whyckoff sites, creating many possible local atomic configurations. This complexity limits direct sampling with DFT and opens questions about the effect of partial occupancy on properties of the σ-phase.

We address the problem using a combination of DFT and MLIPs for a Fe$_{16}$Cr$_{14}$ σ-phase with experimentally observed site occupancy. We use a GRACE potential to screen all possible configurations of the intermetallic and validate the predictions with DFT calculations of a representative selection of configurations.

This approach enables a direct comparison between the traditional sublattice models and explicit disorder. Our results show that partial occupancy stabilizes the σ-phase, while mechanical properties differ roughly 10% from those predicted by sublattice models.

These findings provide a clearer picture of the local chemical disorder effects on the mechanical response of the σ-phase.

MM 11.5 Tue 11:15 SCH/A215

Accurate temperature-dependent Gibbs free energies of point defects in B2 MoTa — •Xiang Xu[1], Xi Zhang[1], Sergiy V Divinski[2], and Blazej Grabowski[1] — [1]University of Stuttgart, Stuttgart, Germany — [2]Universität Münster, Münster, Germany

Controlling order-disorder motifs is proven to be a key strategy for tuning performance in complex concentrated alloys. To this end, understanding ordered configurations is particularly important, as they represent the theoretical boundary of atomic diffusion, phase stability, and order-disorder phenomena. Since point defects like vacancies and antisites control diffusion and thereby affect ordering and phase evolution, their thermodynamic properties provide critical insight into the fundamental mechanisms behind property tuning. However, difficulties in stabilizing highly ordered refractory phases and the computational complexity of finite-temperature free energy calculations have limited quantitative understanding of their defect thermodynamics. To address this gap, we employ first-principles methods to investigate vacancy thermodynamics in the prototype B2-ordered MoTa alloy systematically. By explicitly accounting for electronic excitations and thermal vibrational contributions, particularly the explicit anharmonicity, we reveal distinct temperature-dependent Gibbs energies for vacancies and antisites in the B2-ordered MoTa. Vibrational pair distribution analysis, performed using an accurate machine-learning potential, demonstrates that the difference in thermal contributions arises from the vibrational phase spaces of the investigated point defects.

MM 11.6 Tue 11:30 SCH/A215

Modelling Bulk and Confined High-entropy Materials — •Chen-Chen Er[1,2], Tom Barnowsky[1,2], and Rico Friedrich[1,2] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden Rossendorf, Dresden

High-entropy materials (HEMs) are single-phase multi-component disordered systems with unique electronic, mechanical, and thermal properties that are promising for applications in the energy and electronics sectors. HEMs include disordered ceramics such as carbides, nitrides, or oxides with ordered anion sublattices and disorder on the metal cation sites. Generally, five or more cation species are required to maximize configurational entropy.

In our work, efficient modelling of the disordered systems is conducted based on an ensemble of ordered structures as implemented in the partial occupation algorithm (POCC) [1] within the AFLOW framework [2,3]. Predictive descriptors including the entropy forming ability (EFA) [4] and disordered enthalpy-entropy descriptor (DEED) [5] are crucial to assess synthesizability. Here, we present new results for several bulk and confined high-entropy ceramics.

[1] K. Yang *et al.*, Chem. Mater. **28**, 6484 (2016).
[2] M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023).
[3] S. Divilov *et al.*, High Entropy Alloys Mater. **3**, 178 (2025).
[4] P. Sarker *et al.*, Nat. Commun. **9**, 4980 (2018).
[5] S. Divilov *et al.*, Nature **625**, 66 (2024).

MM 12: Materials for the Storage and Conversion of Energy III / Functional Materials I

Time: Tuesday 10:15–12:45 Location: SCH/A216

MM 12.1 Tue 10:15 SCH/A216

Harmonising Symmetry and Spin: Unveiling Giant Rashba Splitting and Diverse Topological Phases in Composite Quantum Materials — •Arijeet Sarangi, Rajib Sarkar, and Sudip Chakraborty — Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Prayagraj - 211019, India

We present a systematic theoretical study of ABX-type composite quantum materials crystallizing in non-centrosymmetric hexagonal structures, carried out through high-throughput DFT calculations. Approximately 50 candidate systems were screened to explore the interplay between structural symmetry breaking, strong SOC and emergent electronic properties. Our investigation reveals a striking coexistence of Rashba spin splitting and topologically nontrivial band topology across this materials family, with Rashba coefficients and band inversions strongly dependent on atomic ordering and chemical composition. To complement the band-structure analysis, we perform Berry phase calculations, which confirm the topological character of selected states and identify Berry curvature hotspots near avoided crossings. Building upon this, we evaluate the spin Hall conductivity and orbital Hall conductivity for representative compounds, demonstrating substantial intrinsic values comparable to those in established topological semimetals. These findings point to a strong potential for dissipationless spin and orbital current generation, key ingredients for next-generation spintronic and orbitronic devices. These results establish a promising design space for multifunctional applications, bridging spintronics and topological electronics.

MM 12.2 Tue 10:30 SCH/A216

TiO_2 meets water: Band alignment and spectral properties for solar-driven catalysis using Koopmans spectral functionals — •Marija Stojkovic[1], Edward Linscott[2,3], and Nicola Marzari[1,2,3] — [1]Theory and Simulations of Materials (THEOS), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Center for Scientific Computing, Theory and Data, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland — [3]National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

Photocatalytic water splitting has drawn considerable attention for renewable energy production. Thanks to its favorable band gap and band-edge positions, titanium dioxide has remained one of the most promising materials since its first reported photocatalytic water splitting. However, conventional computational approaches often struggle to accurately predict band gaps and band alignments. Here, we showcase the capabilities of Koopmans spectral functionals for evaluating photocatalysts* properties, showing how these can accurately predict band structures and level alignments for rutile, anatase, and brookite TiO_2. Furthermore, we investigate the impact of explicit water on band alignment at TiO_2-water interface by combining advanced molecular dynamics methods with electronic-structure Koopmans calculations.

MM 12.3 Tue 10:45 SCH/A216

Theoretical Calculation of Finite-Temperature X-Ray Absorption Fine Structure: Application to Sodium K-Edge in NaCl — Philipp Hönicke[1,2], Yves Kayser[3], and •Pouya Partovi-Azar[4] — [1]Helmholtz-Zentrum Berlin (HZB), Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — [3]Max Planck Institute for Chemical Energy Conversion, Stiftstr. 34-36, 45470 Mülheim an der Ruhr, Germany — [4]Institute of Chemistry, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale), Germany

A comprehensive computational framework for calculating the full X-ray absorption fine structure (XAFS) through quantum-chemical simulations is presented. The near-edge region is accurately captured using time-dependent density-functional perturbation theory applied to core excitations, while *ab initio* molecular dynamics provides sampling of core-excitation energies and interatomic distance distributions for interpreting extended X-ray absorption fine structure (EXAFS) features. Owing to the efficiency of the approach, the total spectrum can be decomposed into contributions from bulk, defective, and surface environments, which commonly coexist in experimental systems. The methodology is demonstrated for sodium at the Na K-edge in NaCl, where the predicted spectra show good agreement with experimental measurements on thin film samples. This strategy offers a practical route to generating chemically specific XAFS cross-section data for elements that remain challenging to characterize experimentally.

MM 12.4 Tue 11:00 SCH/A216

Spin-Charge Coupling at Mixed Fe/Cr Nodes Governs Optical Gaps in MIL-100 Photocatalysts — •Sabuhi Badalov[1], Patrick Länger[2], Jürgen Senker[2], and Harald Oberhofer[1] — [1]Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth — [2]Chair for Inorganic Chemistry III and Northern Bavarian NMR Centre, University of Bayreuth

With a view on photocatalytic CO_2 reduction, we investigate how mixed metal Fe/Cr nodes in MIL-100 metal organic frameworks (MOFs) influence the MOFs electronic and optical response. Using hybrid level density functional theory (DFT) on models of Fe_3O, Fe_2CrO, $FeCr_2O$ and Cr_3O, we map the evolution of spin-resolved edge levels and Kohn-Sham holes during the stepwise substitution of Fe with Cr. Time-dependent DFT calculations reveal dense $O(2p)\rightarrow M(3d)$ ligand-metal charge transfer (LMCT) bands, appearing between approximately 3.5 and 4.5 eV. From these we derive composition-dependent optical band gaps and $\lambda_{\max}$ values. The calculated trends, modest red/blue shifts of the first bright excitation and systematic hardening of the LMCT manifold with increasing Cr content, quantitatively agree with the experimentally obtained gaps. Our combined theoretical/experimental approach provides a deep microscopic insight into the influence of the Fe/Cr mixed metal centers on spin topology, band edges, and optical absorption. Ultimately, our work points the way towards a rational design of MIL-100 for maximal CO_2 conversion.

15 min. break

MM 12.5 Tue 11:30 SCH/A216

Beyond Ion Dynamics: Efficient Charge Transport Simulations including Electrons at Battery Scales — Matteo Rinaldi, Karsten Reuter, and •Christian Carbogno — Fritz-Haber-Institut der MPG, Berlin

Small polarons, i.e., atomically localized excess charges, are fundamental for charge transport in energy materials. A quantitative modeling of their dynamics is challenging, though, since it typically requires not only long time and length scales, but also an account of electronic degrees of freedom at an *ab initio* level. In this work, we overcome this hurdle via a machine-learning interatomic potential that explicitly accounts for small polarons, which are incorporated as semi-classical degrees of freedom that adiabatically follow the nuclei. Using HSE06 calculations [1] as training data, we validate the approach for $BiVO_4$ and further demonstrate its power for lithium titanium oxide (LTO), a prototypical anode material featuring polarons [2]. By running accelerated sampling and large-scale molecular dynamics simulations, we clarify the mechanisms that drive ionic and polaronic transport as well as their coupling in LTO. This reveals that polarons do not merely serve as spectators, but thermodynamically adapt to the much slower ionic motion. This results in an increase of ionic conductivity, in line with experimental measurements. For the first time, this theoretically corroborates the occurrence of a correlated polaron-ion dynamics with profound implications for the design of energy materials.

[1] S. Kokott *et al.*, J. Chem. Phys. **161**, 024112 (2024).
[2] M. Kick *et al.*, ACS Appl. Energy Mater. **4**, 8583 (2021).

MM 12.6 Tue 11:45 SCH/A216

Ion Transport in Mixed-Halide Lithium Argyrodites from Machine Learning Potentials — ●Yufeng Xu, Takeru Miyagawa, Waldemar Kaiser, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Lithium argyrodites Li_6PS_5X (X=Cl, Br, I) are structurally and chemically complex solid electrolytes. Their ionic conductivity is strongly affected by static forms of disorder, including sulfur-halide anti-site defects [1] and compositional disorder introduced through halide mixing [2]. In this study, we use the MACE message-passing architecture [3] together with machine-learning molecular dynamics to examine ion transport mechanisms in both pure and mixed-halide Li_6PS_5X. We analyze how static and dynamic disorder in mixed-halide systems shapes Li ion diffusion, and how these changes in ion conduction are reflected in the vibrational spectra of the argyrodites. References: [1] B.J. Morgan, Chem. Mater., 2021, 33, 6, 2004-2018. [2] S.V. Patel et al. Chem. Mater., 2021, 33, 4, 1435-1443. [3] I. Batatia et al. J. Chem. Phys., 2025, 163, 184110.

MM 12.7 Tue 12:00 SCH/A216

Positron Annihilation Studies of Nuclear and Highly Oriented Pyrolytic Graphite — ●Jagoda Urban-Klaehn, Arvin Cunningham, and William Windes — Idaho National Laboratory, 1955 Fremont Ave, Idaho Falls, ID 83415 USA

Graphite is a life-limiting component in nuclear reactor design thus its microstructure characterization and the effects of extreme conditions are of great importance.

We examined nuclear graphite materials of different origin, porosity and grain sizes by use of Positron Annihilation Lifetime Spectroscopy (PALS).

We determined that each type of graphite has its specific signature with trapping lifetimes in the range: 360-410 ps, and the most important factor was the grain size. Graphite with the coarse grain showed less positron trapping compared to fine grain which agrees with literature.

Graphite that was heat-treated (2300 C) showed a significant increase in positron trapping thus changes in the microstructure. PALS studies on Highly Oriented Pyrolytic Graphite (HOPG) polycrystalline specimens showed less trapping due to its polycrystalline nature. We are planning to use ELBE slow positron beam at different temperatures to study isotropic graphite defects formation enthalpy as well as crystalline graphite*s depth profiling.

MM 12.8 Tue 12:15 SCH/A216

Positron annihilation spectroscopy for atomic defects in functional materials — ●Maciej Oskar Liedke, Eric Hirschmann, Jyoti Verma, Sebastian Klug, and Andreas Wagner — Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328, Germany

Positron annihilation spectroscopy (PAS) is a highly effective method for the characterization of point defects and their agglomerates in functional bulk materials and thin films. The method provides access to defect concentration in the range of 0.01-100 ppm, which is common for most material classes, including metals, semi-, and superconductors. The utilization of the radiation source ELBE at HZDR in Dresden, which delivers a pulsed positron beam, enables depth profiling by varying the kinetic energy of positrons. The integration of PAS techniques with density functional theory calculations facilitates understanding of defect types and local chemistry at the defected crystal sites. In this contribution, we will present few highlights from positron studies and discuss the role of defects in wide-bandgap semiconductors, such as Ga2O3, in addition to superconducting Nb-based coatings, and high-entropy alloys intended for fusion applications. The presentation will emphasize the control over transitions between different polymorphs of Ga2O3 driven by ion irradiation and resulting defect microstructure. Furthermore, we will demonstrate the correlations between deposition parameters and defect landscapes in Nb alloys. We will conclude discussing healing processes in CrFeMnNi subjected to Fe-ion irradiation, which is analogous to neutron radiation in nuclear systems.

MM 12.9 Tue 12:30 SCH/A216

Operando X-ray Absorption Spectroscopy studies of the X-ray exposed active and passive fiber preforms and their recovery properties upon UV-laser light — ●Ali KARATUTLU[1,2], Esra KENDIR TEKGÜL[1], Iremnur DURU[1,2], Timuçin Emre TABARU[2], Latif Ullah KHAN[3], Messaoud HARFOUCHE[3], and Bülend ORTAÇ[1] — [1]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [2]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey — [3]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME), Allan, 19252, Jordan

In the development of active fiber preforms and active fibers containing rare-earth (RE) ions such as Yb+3 ions for 1-micron laser applications, the determination of the local environment around the Yb+3 ions is of paramount importance for their high optical-optical efficiency. In the long-term operation or when exposed to the gamma or X-ray exposures, the unwanted structural units are usually associated with the defects called color centers. This study demonstrates the formation of photodarkening upon gamma and X-ray exposures and operando X-ray absorption spectroscopy to determine the structural change around Yb+3 ions or Ge+4 ions with different doping levels before and after the irradiation of X-rays.

MM 13: Data-driven Materials Science: Big Data and Workflows I

Time: Tuesday 10:15–12:45 Location: SCH/A251

MM 13.1 Tue 10:15 SCH/A251

Surface reconstruction via automated LEED analysis based on Bayesian optimization — ●Xiankang Tang and Hongbin Zhang — Institute of Materials Science, Technische Universitat Darmstadt, 64287 Darmstadt, Germany

Recent advances in machine learning have enabled the automation of many material characterization processes, which are essential for realizing autonomous experimentation for solid-state materials in the near future. Low-energy electron diffraction (LEED) is a fundamental technique in surface science, providing structural reconstruction information encoded in the energy-dependent intensity modulation of diffracted beams. However, the complexity of data analysis and the computational demands have limited the broader adoption of quantitative LEED in routine surface structure determination. In this work, we implement a Bayesian optimization-based approach to automatize the LEED I(V) analysis, where the best matching structures can be obtained for the experimental I(V) curves by minimize the R-factor between the experimental and simulated I(V) data. This approach can bee combined with density functional calculations or atomisitic simulations to further accelerate the recommendation of plausible structures by minimizing total energies.

MM 13.2 Tue 10:30 SCH/A251

Structural relaxations for nonstoichiometric alloys without forces — ●Luca Numrich and Hongbin Zhang — Insitute of Materials Science, Technische Univerität Darmstadt, Darmstadt, Germany

Advances in machine learning and first-principles electronic-structure methods are accelerating materials design, focusing on stoichiometric compounds. Coherent potential approximation (CPA) is a standard approach for alloys with chemical disorder but there is no compatible implementation for forces, hindering the investigation of structural relaxations for nonstoichiometric alloys. For example, in many Ni-based Heusler alloys, a high-temperature disordered B2 phase transforms into the fully ordered $L2_1$ structure upon cooling via a second-order B2-$L2_1$ order-disorder transition.

In this work, we integrate Bayesian optimization (BO) with CPA as implemented in the exact muffin-tin orbitals (EMTO) code to identify low-energy crystal structures for nonstoichiometric alloys, as demonstrated for Ni-Mn-Ga-X Heusler alloys. Symmetry analysis is used to reduce the number of independent Wyckoff coordinates, which serve as parameters for BO, while the energy per atom computed via EMTO-

CPA defines the objective function to be minimized. Using a Gaussian process surrogate model with a parallel upper confidence bound acquisition function, the framework autonomously proposes candidate structures with progressively lower energies. Thus, instead of a relaxation via interatomic forces, an acquisition function is guiding the relaxation.

MM 13.3 Tue 10:45 SCH/A251

A Python-based workflow for phase identification and mapping via Raman spectroscopy — •Felix Drechsler[1], Mahnaz Mehdizadehlima[2], Cameliu Himcinschi[1], David Rafaja[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09599 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Materials Science, D-09599 Freiberg, Germany

Raman spectroscopy is a powerful tool for identifying phases and compounds. It is highly sensitive to both chemical and structural variations and is particularly attractive due to its minimal sample preparation requirements. This makes it well suited for fast phase identification and the determination of spatial phase distributions, complementing established techniques such as X-ray diffraction, element mapping via X-ray spectroscopy, and phase mapping using electron backscatter diffraction. However, phase-resolved analysis of Raman mappings remains challenging, as it involves processing high-dimensional data matrices and robust identification relies on comparing the complete spectrum with references.

In this talk, we present a Python-based workflow developed to address this challenge. The approach employs multivariate analysis methods and integrates mathematical similarity metrics with reference datasets to enable robust and reproducible phase identification. The proposed workflow provides an efficient way to construct Raman phase maps and offers a valuable tool for material characterization.

MM 13.4 Tue 11:00 SCH/A251

Automated Prediction of Phase Stability with ab-initio Accuracy — •Prabhath Chilakalapudi, Marvin Poul, Jan Janssen, and Jörg Neugebauer — Computational Materials Design, Max-Planck-Institute for Sustainable Materials, Düsseldorf

Developing sustainable metallic alloys-free of toxic elements and compatible with circular synthesis-requires novel and efficient ways to explore large composition spaces. A key bottleneck is the automated, abinitio-accurate prediction of temperature-composition phase diagrams, where experimental phase data is limited or difficult to obtain.

We present a reproducible, automated workflow that uses Machine-Learned Interatomic Potentials (MLIPs) such as Atomic Cluster Expansion (ACE)[1] and non-equilibrium thermodynamic integration (Calphy[2]) to compute free energies and phase stabilities. By analysing key approximations including point-defect models, different entropic contributions, and free-energy interpolation schemes, we quantify the reliability of the calculated phase boundaries and provide meaningful “error bars” on the diagram. The workflow is demonstrated for representative binary alloys and is structured for gradual scaling to multicomponent systems. We leverage the pyiron[3] workflow framework for reproducible and efficient automation, to accelerate the discovery of sustainable materials.

[1] R. Drautz, Phys. Rev. B 100, 249901 (2019).
[2] S. Menon et al., npj Comput. Mater. 10, 261 (2024).
[3] J. Janssen et al., Comput. Mater. Sci. 163, 24-36 (2019).

15 min. break

MM 13.5 Tue 11:30 SCH/A251

Towards Disorder-Aware Materials Discovery - Recognizing and Modeling Crystallographic Disorder — •Konstantin S. Jakob[1], Aron Walsh[2], Karsten Reuter[1], and Johannes T. Margraf[1,3] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Imperial College London — [3]Universität Bayreuth

Recent computational materials discovery efforts have led to an enormous number of predictions of previously unknown, potentially stable inorganic, crystalline materials. However, these efforts are currently limited to predicting perfectly crystalline materials. As a consequence, many of these predictions cannot be verified in experiments, where kinetic effects, defects, and crystallographic disorder can be crucial. Here, we discuss disorder as a current frontier in materials discovery. To this end, we show that machine learning classification models can reliably recognize disordered materials and demonstrate that a significant fraction of computationally predicted materials are likely disordered [1]. On the example of compositionally complex transition metal ferrite spinels, we then demonstrate how machine learning interatomic potentials and Monte Carlo sampling can be used to tackle such disordered systems efficiently.

[1] K.S. Jakob, A. Walsh, K. Reuter, and J.T. Margraf, Adv. Mater. e14226 (2025).

MM 13.6 Tue 11:45 SCH/A251

Efficient Exploration of the Unknown: Distance-Based Active Learning with SISSO Descriptors and Mendeleev Similarities for Materials Discovery — •Sreejani Karmakar[1], Akhil S. Nair[1,2], Lucas Foppa[1], and Matthias Scheffler[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Freie Universität Berlin, Berlin, Germany

The performance of AI models depends strongly on the distribution of their training data, which ideally should be independent and identically distributed. Materials-science datasets often violate this condition, containing redundancy and bias that hinder the discovery of statistically rare high-performance materials. Active learning (AL) helps by building concise, diverse training sets, introducing underrepresented materials classes. Commonly, AL relies on uncertainty estimates derived from the variance of model ensembles[1], but these are frequently overconfident and limit AL efficiency. We introduce an alternative strategy that selects candidate materials based on their distance from the existing training set in a low-dimensional descriptor space[2]. These descriptors, derived via SISSO (sure independence screening and sparsifying operator) symbolic regression approach. This distance-guided approach outperforms ensemble-based uncertainty AL, successfully identifying perovskites with exceptional properties. Adding the Mendeleev similarity metric further improves dataset diversity and supports efficient navigation of unexplored material space.

[1] A. Nair et al., npj Comput. Mater., 11, 150, 2025. [2] D. Wu et al., Inf. Sci., 474, 90, 105, 2019.

MM 13.7 Tue 12:00 SCH/A251

Where Are Large Language Models Actually Useful for Materials Design? — •Hedda Oschinski, Maximilian L. Ach, David Greten, Konstantin S. Jakob, Christian Carbogno, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

The rapid development of large language models (LLMs) and LLM-based agents has opened new possibilities for accelerating materials discovery and design. In this work, we explore their potential in the context of solar cell materials, a class of systems requiring complex, multi-property optimization across chemistry and materials science. By systematically evaluating a range of tasks for a well-known test set of Elpasolites - from context preparation and descriptor prioritization to design hypothesis generation and autonomous validation within an agent framework - we identify where current LLMs provide genuine utility and where critical limitations remain. Our findings offer a grounded perspective on how these tools can be integrated into materials discovery workflows, and what developments are needed to expand their impact in the future.

MM 13.8 Tue 12:15 SCH/A251

Predictive and interpretable machine learning models for thermodynamics tuning of metal hydrides for hydrogen storage — •Sinan S. Faouri[1], Kai Sellschopp[2,3], Claudio Pistidda[3], and Paul Jerabek[3] — [1]Mechanical and Industrial Engineering Department, Applied Science Private University, Amman, Jordan — [2]Department of Chemical and Process Engineering, University of Canterbury, Christchurch, New Zealand — [3]Institute of Hydrogen Technology, Helmholtz-Centre Hereon, Geesthacht, Germany

Metal hydrides remain among the most promising materials for solid-state hydrogen storage due to their tunable thermodynamic behavior. However, predicting key properties such as equilibrium pressure and hydrogenation enthalpy remains challenging, especially across diverse alloy systems. In this work, we explore feature-based machine learning strategies to model these thermodynamic quantities from elemental descriptors and derived structural features. The study combines experimental and computational data to identify the most relevant predictors governing hydrogen absorption thermodynamics. Particular attention is given to the relationship between atomic-scale size parameters, electronic features, and their collective influence on pressure-enthalpy correlations. The results demonstrate that data-driven approaches can reveal non-obvious structure-property relationships and guide the search for alloys with optimized storage performance. The presented framework offers a step toward integrating machine learning with physical insights for accelerated discovery of functional hydrides.

MM 13.9 Tue 12:30 SCH/A251

Score-based diffusion models for accurate crystal structure inpainting and reconstruction of hydrogen positions — •Timo Reents[1], Arianna Cantarella[2], Marnik Bercx[1], Pietro Bonfà[2,3], and Giovanni Pizzi[1] — [1]PSI Center for Scientific Computing, Theory and Data, CH-5232 Villigen PSI, Switzerland — [2]Department of Physics and Earth Sciences, University of Parma, IT-43124 Parma, Italy — [3]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, University of Modena and Reggio Emilia, IT-41125 Modena, Italy

Generative AI methods are rapidly evolving to speed up and improve materials discovery. Diffusion based models can not only be adopted to generate new materials with desired properties but also to reconstruct crystal structures for which structural information is only partially available. In this work, we use Microsoft's mattergen [1], a diffusion based model originally designed to generate new stable crystal structures, and extend it to reconstruct missing hydrogen sites in crystal structures reported in experimental databases. This is particularly useful as the experimental measurement of hydrogen sites with standard XRD is typically challenging due to weak scattering of hydrogen. We show how to leverage image inpainting approaches known from computer vision, combined with universal machine learning interatomic potentials, to improve the success rate of correctly identifying the missing sites or finding lower energy configurations while significantly lowering the computational cost with respect to a direct DFT approach.

[1] Zeni, C. et al., Nature 639, 624-632 (2025)

MM 14: Liquid and Amorphous Materials I

Time: Tuesday 11:30–12:45 Location: SCH/A315

MM 14.1 Tue 11:30 SCH/A315

Shining Light on Gold-in-Gallium: DFT Insights into Photocatalytic Benzyl Alcohol Oxidation — •Oliver Conquest[1], Chung Nguyen[2], Sarina Sarina[2], and Catherine Stampfl[1] — [1]School of Physics, The University of Sydney, Sydney, Australia — [2]School of Chemical and Biomolecular Engineering, The University of Sydney, Sydney, Australia

Recent experimental results have shown that pure liquid Ga with an oxide later does not perform well as a photocatalyst for Benzyl alcohol conversion to Benzaldehyde. When Au nanoparticles (Au NP) are introduced into the system, it emerges as an excellent Benzyl alcohol conversion photocatalyst. The Au NP develop an ultra-thin amorphous-GaO_x (a-GaO_x) skin when placed in liquid Ga, the a-GaO_x in the presence of Au is expected to play an important role in the photoreaction. Therefore, understanding the reaction mechanism requires atomic level investigation into the a-GaO_x/Au(111), and Au(111)/a-GaO_x/Ga interfaces. We perform molecular dynamics and density functional theory (DFT) calculations to provide insight into the charge and photoexcited properties of the Au(111)/a-GaO_x/Ga heterostructures with a careful emphasis on the a-GaO_x layer. The DFT calculations of the a-GaO_x/Au(111) interface demonstrate the charge transfer characteristics between the Au(111), a-GaO_x Ga-liq layers and provide a new detailed understanding of the photocatalytic mechanisms at play.

MM 14.2 Tue 11:45 SCH/A315

Reactive Edges and Inevitable Adsorption in Carbon Nanomembranes — •Levin Mihlan[1], Filip Vuković[2], Andrei Postnikov[3], Verena Müller[4], and Jürgen Schnack[1] — [1]Universität Bielefeld, Germany — [2]TU Wien, Austria — [3]Université de Lorraine, France — [4]Friedrich-Schiller-Universität, Germany

Carbon nanomembranes (CNMs) are nanometer-thin materials synthesized via electron-induced crosslinking of aromatic self-assembled monolayers. These membranes can be functionalized for various applications, initially serving as molecular filters. In addition to their internal structure, the precise elemental composition is not yet fully understood [1]. Therefore a first-order prediction for ultraviolet photoelectron spectroscopy (UPS) was developed based on DFT-calculated densities of state. Combined with theoretical carbon-only CNM model structures and an analysis of the near-zero binding-energy region, this approach enables statements regarding the saturation of different regions as well as the presence of reactive edges and dangling bonds. Since these regions are highly unstable under ambient conditions, physisorption and chemisorption of elements such as hydrogen and oxygen are to be expected. In this work, various CNM model structures are systematically investigated using this methodology, ultimately supporting the presence of such depositions, provided that other observations are valid.

[1] Dementyev, Petr, et al. "Carbon Nanomembranes from Aromatic Carboxylate Precursors" ChemPhysChem 21.10 (2020): 1006

MM 14.3 Tue 12:00 SCH/A315

Volume increase of silica glass due to water intercalation and silanol group formation — Manuel Enns[1], Wolfgang Körner[1], Christian Elsässer[1,2], and •Daniel F. Urban[1,2] — [1]Fraunhofer Institut für Werkstoffmechanik IWM, Freiburg, Germany — [2]Freiburger Materialforschungszentrum FMF, Albert-Ludwigs-Universität Freiburg, Germany

We present a theoretical study on the change of volume of silica glass due to the intercalation of molecular water and the formation of silanol groups. By a statistical representative set of density functional theory calculations, we obtained a volume increase per mole of molecular water in amorphous SiO_2 of 2.5 cm^3/mol. In comparison, for the reaction of water to silanol groups we found on average a 3.5 times larger volume increase of 8.7 cm^3/mol. Our results show that the exothermic dissolution of H_2O into silanol pairs is not restricted to small rings of size three and four. We find an equal distribution of reaction energies over all ring sizes which we explain by the structural relaxation and the related energy gain of the entire amorphous neighbourhood. Statistically, most exothermic dissolution of H_2O may happen at five-membered rings since they outnumber the three- and four-membered rings in amorphous SiO_2. Our findings shed new light on the underlying mechanisms and the size of the volume change of the water intercalation in silica glass and we discuss our findings with respect to previous experimental and theoretical work.

MM 14.4 Tue 12:15 SCH/A315

Insights into the interplay of relaxation and crystallization of Vit106a glass — •Lukas Musiol[1], Merlin Kempf[2], Lukas Musiol[1], Remi Daudin[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Université de Grenoble Alpes, CNRS, Grenoble INP, Laboratoire SIMaP, Grenoble, France

Metallic glasses are metastable systems that show relaxation behavior towards a local energy minimum and crystallize when heated sufficiently above their glass transition temperature (Tg). Different modes of relaxation can be accessed by varying the combination of relaxation time and temperature. At temperatures significantly lower than Tg only β-relaxation is expected, corresponding to local rearrangements of few atoms. For temperatures close to Tg and for long times only α-relaxation is observed which corresponds to collective rearrangements in the glass. While these two relaxations are often considered independent, a growing body of evidence shows that they are linked [J. Phys. Chem. Lett., 3 (2012), 735; Intermetallics, 93 (2018), 101]. Additionally few attempts have been made to understand how structural changes during relaxation influence crystallization behavior.

Vit106a as a model system of bulk metallic glasses has been investigated concerning the relaxation dynamics and changes in crystallization behavior using conventional scanning calorimetry correlated to strutural analyses using transmission electron microscopy-based methods.

MM 14.5 Tue 12:30 SCH/A315

Unraveling the Correlation Between Populated Site Energies, Activation Barriers and Saddle Point Energies in Solid Ion Conductors — •Martin Schäfer[1], Mohammad A. Badragheh[2], Michael Vogel[2], and Karl-Michael Weitzel[1] — [1]Universität Marburg, Marburg, Germany — [2]T.U. Darmstadt, Darmstadt, Germany

Transport phenomena in disordered materials are governed by a complex potential energy landscape that includes a distribution of local energy minima (sites), saddle point energies and local energy barriers. An understanding of the connection of these properties is essential to unravel the transition between local hops and long-range transport.

In this work, the populated site energy distribution (PSED) is experimentally determined by the Charge Attachment Induced Transport (CAIT) technique that yields concentration dependent diffusion coefficients and activation energies by comparison of measured concentration depth profiles to calculated profiles gained by Nernst-Planck-Poisson modeling [1]. The distribution of local barriers is probed through Nuclear Magnetic Resonance (NMR) measurements [2]. For Li3B7O12, the FWHM of the PSED is determined to be 250 meV while the activation energies show a FWHM of about 440 meV suggesting that the apparent energy distribution of saddle points must be significantly broader than the distribution of site energies.

[1] V.H. Gunawan, M. Schäfer, and K.-M. Weitzel, Phys.Chem.Chem.Phys., 26, 14430 (2024)

[2] M.A. Badgragheh, E. Winter, M. Vogel, unpublished results

MM 15: Phase Transformations I

Time: Tuesday 14:00–15:45 Location: SCH/A215

MM 15.1 Tue 14:00 SCH/A215

Quantum Geometric Injection and Shift Optical Forces Drive Coherent Phonons — •Luke Pimlott and Habib Rostami — University of Bath, Bath, United Kingdom

We identify injection and shift rectified Raman forces, which are phononic counterparts of the photogalvanic effect, that drive lattice vibrations and trigger transient emergent properties. These forces are governed by the quantum geometric tensor, a phononic shift vector, and interband asymmetries in the electron-phonon coupling. As a response to pulsed light, the injection force induces displacive atomic motion, while, unlike conventional impulsive mechanisms, the shift force produces impulsive atomic displacement in the resonant interband absorbing regime when time-reversal symmetry is broken. Using the bilayer Haldane model, we quantify the injection and shift forces acting on interlayer shear phonons through both analytical and numerical methods. Strikingly, we reveal strong tunability, both in magnitude and direction, of the rectified forces by varying the driving frequency and magnetic flux, uncovering a distinct quantum geometric mechanism for ultrafast and coherent manipulation of quantum materials.

MM 15.2 Tue 14:15 SCH/A215

Charge Density Wave Transition in ZrTe$_3$ from First Principles — •Josu Diego López and Matteo Calandra Buonaura — University of Trento, Trento, Italy

ZrTe$_3$ is a quasi-one-dimensional compound that undergoes a charge density wave (CDW) transition at 63 K with a propagation vector of $\mathbf{q}_{\mathrm{CDW}} = (0.07, 0, 0.33)$ in reciprocal-lattice units and characterized by a very sharp Kohn anomaly in reciprocal space. Although Fermi surface nesting between the quasi-1D bands has been widely invoked to explain this instability, a complete first-principles characterization of the lattice dynamics is still lacking. In particular, the phonon modes at the CDW wavevector have never been computed, even within the harmonic approximation, leaving open fundamental questions regarding the role of the electron-phonon interaction in this material.

In this work, we analyze from first principles the electronic and vibrational properties of the high-temperature phase of ZrTe$_3$. We show that only the correct characterization of the Fermi surface yields an imaginary harmonic phonon mode consistent with the observed CDW. Having access to the harmonic phonons at the critical wavevector also enables the calculation of the electron-phonon interaction at $\mathbf{q}_{\mathrm{CDW}}$, providing a framework to directly compare the electron-phonon mechanism with the nesting scenario in driving the CDW formation.

Funded/Co-funded by the European Union (ERC, DELIGHT, 101052708).

MM 15.3 Tue 14:30 SCH/A215

Coupled phase transition and valence fluctuations in Fe-doped $BaTiO_3$: a combined DFT and DMFT study — •Zhiyuan Li, Ruiwen Xie, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt Germany

Rational control of structural phase transitions in perovskites is a key challenge in materials design. In Fe-doped $BaTiO_3$(BTO), experiments observe a tetragonal-to-hexagonal transition, yet the governing microscopic mechanisms remain unclear. A critical control parameter is the Goldschmidt tolerance factor, which relies intimately on the dopant ionic radius and, consequently, the valence state. However, the valence of Fe in BTO remains a long-standing open question, with conflicting reports necessitating a treatment beyond standard DFT. Here, we employ Density Functional Theory (DFT) combined with Dynamical Mean-Field Theory (DMFT) to investigate this interplay. DMFT reveals that the Fe dopant exhibits strong valence and spin fluctuations, which are significantly suppressed by oxygen vacancies to stabilize a high-spin state. Integrating these electronic insights, our total-energy calculations identify three cooperative mechanisms driving the phase transition: tolerance factor variations, Jahn-Teller distortions, and oxygen vacancy formation. Then a systematic quantitative analysis was performed on these three factors. These findings provide a unified microscopic understanding of defect-mediated phase control.

MM 15.4 Tue 14:45 SCH/A215

Interface structure and migration in phase transformations between Fe_3O_4 and Fe_2O_3 — •Martina Ruffino[1], Baptiste Bienvenu[1], Xuyang Zhou[2], Guangyi Guo[1], Barak Ratzker[1], Dierk Raabe[1], and Yan Ma[3] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]Xi'an Jiaotong University, Xi'an, China — [3]TU Delft, The Netherlands

Although redox phase transformations between hematite (Fe_2O_3) and magnetite (Fe_3O_4) entail long-range diffusion, they are known to occur on well-defined $(111)_{\mathrm{mag}}||(0001)_{\mathrm{hem}}$ habit planes, and to maintain the oxygen sublattice fixed up to a change in stacking sequence (fcc and hcp arrangement for Fe_3O_4 and Fe_2O_3, respectively). Moreover, hematite formations during magnetite oxidation, as well as magnetite formations in hematite during reduction, are often observed to be of lenticular shape. In this study, we propose interfacial disconnections (i. e. steps with dislocation character) suitable for the accomplishment of these phase transformations. Using atomistic simulations with an atomic cluster expansion (ACE) potential developed for iron and its oxides, we calculate the equilibrium structures of the disconnections and we study their motion as a means to transform magnetite into hematite and vice-versa. We then validate theoretical calculations experimentally by investigating i) partially oxidised magnetite and ii) partially reduced polycrystalline hematite. Using transmission electron microscopy, we analyse the hematite/magnetite interfaces, characterising them as faceted interfaces containing steps; we observe good agreement with the simulated disconnection structures.

MM 15.5 Tue 15:00 SCH/A215

Grain boundary thermodynamics away from idealized boundaries: How line defects affect stability — •Tobias Brink[1], Swetha Pemma[1,2], Lena Langenohl[1], Saba Saood[1], Yoonji Choi[1], Rebecca Janisch[2], Christian H. Liebscher[2], and Gerhard Dehm[1] — [1]MPI for Sustainable Materials, Düsseldorf, Germany — [2]Ruhr-Universität Bochum, Germany

The concept of grain boundary (GB) phases (or "complexions") was developed to describe how the atomic structure and/or chemistry of GBs depend on external conditions, such as temperature or chemical potential. Analogous to bulk phases, GB phases also affect material properties. Even in the case of pure metals, structural GB transformations impact diffusivity and GB mobility. Simulation studies often concentrate on special, symmetric boundaries, which are easy to describe. It is unlikely, however, that their behavior can be generalized to the variety of imperfect GBs in a real polycrystal.

Here, we use atomistic simulations with empirical potentials to investigate thermodynamics of asymmetric GBs in Cu. Symmetric $\langle 111 \rangle$ tilt boundaries exhibit two GB phases. These also exist in asymmetric GBs, but contain multiple line defects (disconnections) that enable the deviation from the symmetric GB plane. We found the same defects in thin film samples using scanning electron transmission microscopy. Most importantly, their presence alters the thermodynamic stability of the two GB phases, even for very small deviations from the symmetric GB. We conclude that defects of defects have to be considered in interface thermodynamics.

MM 15.6 Tue 15:15 SCH/A215

Size effects on phase change: solid-state wetting vs. coherency stress — •Yong Li[1] and Jörg Weissmüller[2,1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Coherent phase transformations in interstitial solid solutions or intercalation compounds with miscibility gaps are crucial to the behavior of energy storage materials, particularly metal hydride and lithium-ion compounds nanoparticles. Prior studies often attribute size-dependent phase transformation behavior either to solid-state critical-point wetting at particle surfaces or to coherent stresses from solute-saturated surface layers. We introduce a hybrid numerical approach that couples atomistic grand canonical Monte Carlo simulations with continuum mechanics analysis of coherency-stress, allowing wetting and mechanical constraints to be simulated simultaneously or independently, thereby decoupling their respective contributions. For material parameters representative of realistic interstitial solutions, we find that solid-state wetting has only a minor influence, whereas coherency stress dominates the size dependence. Mechanical interactions reduce phase-transformation hysteresis at small sizes and increase solute binding in the solid, thereby lowering the chemical potential 'plateau' at the phase coexistence.

MM 15.7 Tue 15:30 SCH/A215

Critical-point wetting at crystal surfaces: Cahn-Hilliard residuum and occurence of first-order wetting transition — •Marine Bossert[1], Yong Li[2], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Hydrogen Technology, Helmholtz Center Hereon, Geesthacht, Germany

Since its publication in 1958, the work by J.W. Cahn and J.E. Hilliard on the free energy of non-uniform systems [1] has been the basis for numerous studies, such as phase-field simulation of microstructure evolution or solute segregation to lattice defects. Cahn and Hilliard found that the second derivative (Laplacian) of the composition field governs the excess energy of systems with conserved networks of sites - such as crystals. A partial integration of the excess energy gives the gradient-square representation, which has been used in all follow-up works in an approximate form that neglects the partial integration residuum. Inspecting critical-point wetting at the surface of an Ising-type FCC crystal with a miscibility gap, this study shows that the solutions obtained with the (exact) second derivative or with the (approximate) gradient-square expressions for the free energy are in fact qualitatively different: the first-order wetting transition predicted by the gradient-square approach is not confirmed by the second-derivative one. Moreover, atomistic Monte-Carlo simulations confirm the absence of a first-order transition. [1] Cahn, J. W., & Hilliard, J. E. (1958).The Journal of Chemical Physics, 28(2), 258-267.

MM 16: Functional Materials II

Time: Tuesday 14:00–15:45 Location: SCH/A216

MM 16.1 Tue 14:00 SCH/A216

Low and High Dose Gamma Radiation Effect on Germanium-Doped Optical Fibers: Investigation of Color Centers — •Esra Kendir Tekgül — Bilkent University UNAM, Institute of Materials Science and Nanotechnology, Ankara, 06800, TURKEY

Ge-doped optical fibers are widely used in sensing, data transmission, and space technologies, making their radiation resistance crucial. Gamma irradiation creates radiation-induced defects that form color centers, degrading optical transmission. In this study, five Ge-doped fibers and one quartz fiber were exposed to gamma rays of 0.5-50 kGy. RIA values at 550, 600, 680, and 755 nm were measured before and after irradiation, and color centers were identified from the RIA spectra. GeX, Ge-NBOHC, and GeY defects were attributed to Ge contributions, whereas ODC(II), STH1, and STH2 were attributed to the SiO2 matrix. NA and FTIR results showed radiation-induced changes in refractive index and a decrease in NA. Overall, the findings highlight the potential of Ge-doped fibers for radiation-hard applications and dosimetric sensing.

MM 16.2 Tue 14:15 SCH/A216

Switching applications in optical circuits using the electrochromic properties of LiMn2O4 — •Vinit Kumar Agarwalla[1], Yug Joshi[2], Guido Schmitz[1], and Mayank Kedia[3] — [1]Institut für Materialwissenschaft, Universität Stuttgart, Stuttgart Germany — [2]Max Planck Institute for Sustainable Materials, Dusseldorf, Stuttgart — [3]Institut für Photovoltaik, Universität Stuttgart, Stuttgart Germany

Optical communication depends on the accuracy with which the path of light is controlled to minimize signal loss in waveguides. The current method of optimizing the path of light is to maintain the waveguide's refractive index using the thermooptic effect. The waveguide consists of a core in which light travels, surrounded by cladding material to ensure total internal reflection, and a third protective outer layer. Here, I propose using electrochromic lithium manganese oxide(LiMn*O*, LMO) as a waveguide cladding. The primary wave from the core extends into the cladding known as evanescent waves, so changing the cladding*s refractive index changes the evanescent waves' path and thus the entire path of the light. Previous work has shown a change in refractive index in the visible region. Building on that, we measured IR reflectance spectra showing continuous visible-to-IR transitions, 100% reflectance, and resonance shifts with lithiation. Calculations show that a 38 μm waveguide can induce a π phase shift at 1550 nm. We also propose various delithiation methods to alter optical properties without degrading the optical structure.

MM 16.3 Tue 14:30 SCH/A216

In-Situ Activation of a Monolithic SrTiO3 Single Crystal for Room Temperature Hydrogen Sensing — •Karl-Michael Weitzel, Timo Kassubek, and Kevin Rein — Department of Chemistry, Philipps-Universität Marburg, Marburg, Germany

The development of reliable, fast, and cost-effective hydrogen sensors is of increasing importance for the safe implementation of a hydrogen-based economy. This work presents a novel and simple single-step method to convert an insulating strontium titanate (SrTiO3) single crystal into a highly sensitive, monolithic hydrogen sensor that operates at room temperature. The activation is achieved by applying a moderate DC electric field (100 V/cm) across a symmetric Pt/SrTiO3/Pt capacitor structure at 180 °C in a pure hydrogen atmosphere (200 mbar). This process causes a drastic and stable reduction in the material's resistance by several orders of magnitude. We propose a model of "field-induced chemical doping" to explain this transformation. The resulting activated crystal exhibits excellent hydrogen sensing properties at room temperature, detecting molecular hydrogen (H2) over an exceptionally wide partial pressure range from 0.0001 mbar to 1000 mbar with an accuracy of a few percent. The sensing mechanism is based on the reaction of hydrogen with the activated SrTiO3 sample, involving the release of electrons back into the conduction band and lowering the device's resistance. This monolithic approach opens a new pathway for designing robust and easy-to-fabricate chemical sensors from wide-bandgap oxides.

MM 16.4 Tue 14:45 SCH/A216

The laser-induced synthesis of Co-MOFs, the investigation of optic, gase sorption, DFT and sensor properties — Saliha MUTLU[1,2], Bülend ORTAÇ[2], Ali KARATUTLU[2,3], Taylan GÖRKAN[2], Engin DURGUN[2], Dilek SÖYLER[4], Saniye SÖYLEMEZ[4], Jelena LILLEPÄG[5], Volkan FILIZ[5], Nergis ARSU[6], and •Sevil SAVAŞKAN YILMAZ[1] — [1]Karadeniz Technical University Chemistry Department, Trabzon, Türkiye — [2]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [3]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey — [4]Department of Biomedical Engineering, Necmettin Erbakan University, Konya, 42090 Turkey — [5]Helmholtz-Zentrum Geesthacht, Institute of Polymer Research, Max-Planck-Str. 1, 21502 Geesthacht, Germany — [6]Yildiz Technical University, Department of Chemistry, Davutpasa Campus, Istanbul, 34220

Turkey

High-power rapid laser-induced synthesis of MOFs has drawn significant attention due to the rapid and effective preparation conditions for Zn- and Ni-MOFs. In this study, the Co-MOF microcrystals yield visible light photoluminescence with relaxation times on the order of ns, showing controllable properties, including low-temperature paramagnetic state transition, supported by magnetic measurements and DFT calculations. Outstanding performance in gas sorption and electrochemical sensing has been demonstrated with low separation costs and ultra-low LODs for dopamine, respectively.

MM 16.5 Tue 15:00 SCH/A216

First-Principles Study of Electronic and Optical Properties of Mo-Doped $CsPbBr_3$ Perovskites — Said Al Azar[1], Anas Al-Reyahi[2], •Saleh Bashaish[3], and Marwan Mousa[4] — [1]Zarqa University, Zarqa, Jordan — [2]Hashemite University, Zarqa, Jordan — [3]Al-Ahliyya Amman University, Amman, Jordan — [4]Jadara University, Irbid, Jordan

$CsPbBr_3$ perovskites, particularly when doped, show great promise for tandem solar cells and advanced optoelectronics. This study employs density functional theory (DFT) and semi-classical Boltzmann transport theory to comprehensively investigate the structural, electronic, magnetic, thermoelectric, and optical properties of Mo-doped $CsPb_{(1-x)}Mo_xBr_3$ (x = 0, 0.25, 0.5, 0.75). Our calculations confirm the structural stability of all compositions and reveal a transformative electronic behavior: Mo-doping induces a ferromagnetic half-metallic state. Notably, the $x = 0.5$ composition exhibits an ideal band gap for solar applications (1.872 eV via mBJ) and a high spin-up figure of merit (zT) approaching unity at room temperature. Additionally, enhanced absorption in the infrared region suggests potential for IR photodetectors. These findings establish Mo-doped $CsPbBr_3$ as a compelling multifunctional material for spintronic and high-efficiency optoelectronic devices.

MM 16.6 Tue 15:15 SCH/A216

Optimizing NiTi Interatomic Potentials Through Atomic Cluster Expansion — •Petr Šesták[1,2], Petr Jaroš[1], Miroslav Černý[2], and Petr Sedlák[1] — [1]Institute of Thermomechanics Czech Academy of Sciences, Prague, Czechia — [2]CEITEC, Brno University of Technology, Brno, Czechia

In this work, we present an interatomic potential for NiTi based on the Atomic Cluster Expansion, developed using the Pacemaker software package. We validate this potential by comparing it against the results of simulations using other interatomic potentials, quantum-mechanical calculations, as well as our own experimental data. Our quantum-mechanical calculations utilize density functional theory (DFT) within the generalized gradient approximation (GGA) to determine the ground-state structural, electronic, thermodynamic, and elastic properties of NiTi in low-temperature (martensitic) phase. The target properties include elastic constants, phonon spectra calculations, and vacancy formation energy. Specifically, the stress-strain method was employed to compute the full tensor of the second-order elastic constants and assess the mechanical stability of the studied phases, ensuring that the results are consistent with those obtained using other established potentials.

MM 16.7 Tue 15:30 SCH/A216

Response of NiTi martensite to mechanical loading — •Miroslav Černý and Petr Šesták — Central European Institute of Technology, CEITEC, Brno University of Technology, Purkyňova 123, Brno, Czechia

Shape-memory alloys are unique materials capable of undergoing large reversible strains and exhibiting the shape-memory effect, which is driven by external changes of temperature. These remarkable properties are based on a martensitic transformation between austenite (high-temperature phase) and martensite (low-temperature phase). The NiTi shape memory alloy has become the most widely used shape memory material in industrial, high-tech, and medical ap-plications due to its unique thermal and mechanical properties.

In this work we aim at fundamental understanding of the behavior of twins in the martensite structure under mechanical loading. For this purpose, we constructed computational supercells representing both the perfect and twinned martensite and studied their responses to shear and tensile loading. Such calculations are computationally very demanding when using ab initio approaches. Therefore, we employed machine learning to develop a new interatomic potential, tailored specifically for the martensite struc-ture. Computationally accessible predictions based on the potential were benchmarked from first principles.

MM 17: Data-driven Materials Science: Big Data and Workflows II

Time: Tuesday 14:00–15:45 Location: SCH/A251

MM 17.1 Tue 14:00 SCH/A251

Modelling Diffusion Kinetics in Refractory High Entropy Alloys Using Graph Neural Network Database Models — •Klemens Lechner[1], Jiyao Zhang[1], Peter Wagatha[2], Wolfram Knabl[2], Helmut Clemens[1], and David Holec[1] — [1]Department of Materials Science, Montanuniversitaet Leoben — [2]Plansee SE

Refractory high-entropy alloys (RHEAs) offer exceptional mechanical and thermal properties, such as high-temperature strength, and may exhibit high-temperature oxidation and corrosion resistance. However, their stability at high temperatures has yet to be confirmed. Nonetheless, even thermodynamically unstable solid solutions can have useful applications if the decomposition is slow. This is inherently connected with the (self-)diffusion kinetics. In this study, we present a workflow for the systematic investigation of diffusion kinetics in RHEAs. The necessary diffusion barriers are predicted using a graph neural network (GNN). We train the GNN using an active learning cycle involving molecular statics simulations with a universal machine-learning interatomic potential (uMLIP). The training data of migration barriers are calculated using the Nudged Elastic Band method. By varying the amount of training data, the GNN can be trained to an accuracy that, in theory, can fully mimic that of the uMLIP but with a more efficient computation. This is crucial for larger-scale modeling applications, e.g., the kinetics of decomposition, ordering or clustering of specific elements. We demonstrate the usage and performance of the GNN to quantify self-diffusion in Mo-Nb-Ta-W alloys using the Kinetic Monte Carlo method.

MM 17.2 Tue 14:15 SCH/A251

Broken neural scaling laws in machine learning for optical properties of metals — •Max Grossmann, Marc Thieme, Malte Grunert, and Erich Runge — Institute of Physics and Institute of Micro- and Nanotechnologies, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Neural scaling laws guide the development of machine-learning models and their training datasets. Here, we investigate them in the context of materials science, where data are inherently costly and scarce, using dielectric functions of metals as an example. We compute dielectric functions for 205,224 intermetallic compounds using high-throughput *ab initio* calculations and train two multi-objective graph neural networks, OptiMetal2B and OptiMetal3B—the latter incorporating three-body interactions—to predict the complex interband dielectric function and the Drude frequency. Systematic variations in the number of training data and model parameters reveal so called "broken" neural scaling laws. Data scaling follows a smoothly broken power law, with steeper slopes occurring above 20,000 materials. In contrast, parameter scaling follows a conventional power law but saturates at around ten million parameters. Including three-body interactions improves accuracy by about 12% but leaves scaling slopes essentially unchanged. These findings suggest that, in the context of spectroscopy, expanding high-quality datasets is a more effective way to improve machine-learning models than optimizing network architectures, increasing body order, or merely increasing network size.

MM 17.3 Tue 14:30 SCH/A251

Simultaneous Learning of Static and Dynamic Charges — Philipp Stärk[1], •Philip Loche[2], Marcel Langer[1], Henrik Stooss[1,3], Michele Ceriotti[2], and Alexander Schlaich[1,3] — [1]Stuttgart Center for Simulation Science, University of Stuttgart, Germany — [2]Laboratory of Computational Science and Modeling, École

Polytechnique Fédérale de Lausanne, Switzerland — [3]Institute for Physics of Functional Materials, Hamburg University of Technology, Germany

Long-range interactions and electric response are essential for accurate modeling of condensed-phase systems, yet remain challenging for atomistic machine learning. Static charges modulate Coulomb interactions, while dynamic charges such as atomic polar tensors describe the response to external electric fields. We compare strategies for learning both types of charges: independent models; coupled learning with or without an isotropic dielectric correction; and coupled learning with an environment-dependent screening. While screening corrections are crucial in the coupled case, assuming homogeneous, isotropic screening fails in heterogeneous systems such as water clusters. Learning a local screening restores accuracy for dynamic charges but offers negligible improvement over independent models while increasing computational cost.

MM 17.4 Tue 14:45 SCH/A251

A high-throughput study of heterostructures with polar discontinuities — •Maria Andolfatto[1,2,3], Junfeng Qiao[2,1], Davide Campi[3], and Nicola Marzari[1,2] — [1]PSI - Switzerland — [2]EPFL - Switzerland — [3]Unimib - Italy

Heterostructures composed of two bulk insulating materials with different polarizations can exhibit localized conductive states at the interfaces and could lead to a wide range of technological applications. Currently, most studies focus on perovskite-based materials to engineer such heterostructures, whose number and performance is limited. This project aims to identify new candidate heterostructures exhibiting interface-localized conductive states by leveraging high-throughput computational screening. Starting from thousands of bulk materials, we compute the polarization and we systematically identify thousands of possible interface combinations. Finally, we analyze the resulting localized density of states of thirty-one heterostructures to assess the formation of two-dimensional electron gases (2DEGs).

MM 17.5 Tue 15:00 SCH/A251

Leveraging Koopmans band structure for exciton characterization in materials — •Miki Bonacci[1], Nicola Colonna[1], Edward Linscott[1], and Nicola Marzari[1,2] — [1]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [2]Theory and Simulation of Materials (THEOS), Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland

Exciton characterization is crucial for several materials applications, ranging from energy transport and storage technologies to photocatalysis, plasmonic, sensing. The ab initio state-of-the-art approach is many-body perturbation theory (MBPT), in particular the Bethe-Salpeter equation (BSE) [1]. This is usually built on top of computationally demanding G0W0 quasiparticle (QP) band structures (BSE@G0W0 approach). In this work, we demonstrate how it is possible to construct the BSE Hamiltonian starting from Koopmans functionals [2] eigenvalues as the main ingredient for the BSE Hamiltonian (BSE@KI), obtaining optical spectra with comparable accuracy with respect to the BSE@G0W0, at reduced computational cost. Automated workflows to compute BSE@KI are provided within the AiiDA workflow engine [3].

[1] Onida et al., Rev. Mod. Phys., 74(2), 601-659 (2002)
[2] Dabo et al., Phys. Rev. B, 82, 115121 (2010)
[3] Huber et al., Sci. Data, 7(1):300 (2020)

MM 17.6 Tue 15:15 SCH/A251

Many-body perturbation theory vs. density functional theory: A systematic benchmark for band gaps of solids — •Marc Thieme[1,2], Max Grossmann[1], Malte Grunert[1], and Erich Runge[1] — [1]Institute of Physics and Institute of Micro- and Nanotechnologies, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Institute of Applied Physics, Friedrich Schiller Universität, 07743 Jena, Germany

The band gap is one of the most important material properties for optoelectronic applications. However, predicting band gaps remains a challenging task in materials science. Here, we benchmark many-body perturbation theory against density functional theory, the workhorse of computational materials science, for predicting the band gaps of solids. We systematically compared four GW variants—G_0W_0 using the plasmon-pole approximation (G_0W_0-PPA), full-frequency quasiparticle G_0W_0 (QPG_0W_0), full-frequency quasiparticle self-consistent GW (QSGW), and QSGW augmented with vertex corrections in W (QS$G\hat{W}$)—against the currently best-performing and popular density functionals. Our results show that the QS$G\hat{W}$ produces band gaps so accurate that they can even flag questionable experimental measurements, albeit at an extremely high computational cost. To balance accuracy and efficiency, we identify lower-cost alternatives, such as the QPG_0W_0 and a rescaled version of the QSGW, which achieve nearly the same accuracy as the QS$G\hat{W}$ while being significantly more efficient, making them promising candidates for generating high-fidelity datasets in machine-learning-driven materials discovery.

MM 17.7 Tue 15:30 SCH/A251

Learning G_0W_0 Self-Energies in Real Space with Equivariant Neural Networks — •Elisabeth Keller, Karsten W. Jacobsen, and Kristian S. Thygesen — CAMD, DTU Physics, Kongens Lyngby, Denmark

Many-body G_0W_0 calculations provide highly accurate quasiparticle energies for semiconductors and insulators beyond standard density-functional theory, but at a much higher computational cost.

To overcome this limitation, we use equivariant neural networks to replace the explicit G_0W_0 self-energy evaluation. The networks are trained on G_0W_0 self-energies from GPAW projected onto an atom-centered LCAO basis. Using this representation, we investigate how the real-space localization of the self-energy enables learning from atomic configurations.

MM 18: Liquid and Amorphous Materials II

Time: Tuesday 14:00–15:30 Location: SCH/A315

MM 18.1 Tue 14:00 SCH/A315

Influence of Phosphorus Content on the Symmetry and Correlation Length of the Medium-Range Order in Pd-Ni-P Bulk Metallic Glasses — •Hongshuai Li, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Pd-Ni-P metallic glass is known as an excellent glass former, which enables systematic investigation of how variations in phosphorus (P) content affect its structural characteristics. In this study, we investigate the influence of P concentration on the dominant correlation length and the local symmetries of motifs within Pd-Ni-P metallic glass using fluctuation electron microscopy (FEM) and angular correlation microscopy. In FEM, the relationship between normalized variance and probe size can be used to examine the medium-range order (MRO) in amorphous materials. Our experimental results reveal that, as the composition deviates from the eutectoid composition Pd40Ni40P20, the correlation lengths associated with the dominating motifs undergo significant changes. Moreover, the volume fraction of the medium-range order increases as the P content diverges from the eutectoid composition. Regarding the symmetry analysis, the P content exerts a strong impact on the four-, five-, and six-fold symmetries. Specifically, as the P content moves away from the eutectoid composition, five-fold symmetry becomes prominent relative to the four- and six-fold symmetries.

MM 18.2 Tue 14:15 SCH/A315

Decoupling Structural and Mechanical Behavior in CuZr Metallic Glasses — •Askar Kvaratskheliya[1], Jürgen Eckert[1,2], and Daniel Şopu[1,3] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Technical University of Leoben, Leoben, Austria — [3]Technical University of Darmstadt, Darmstadt, Germany

Although lacking of long range order symmetry, metallic glasses (MG) possess a high degree of short- and medium-range order that governs their macroscopic properties. Particularly, in case of CuZr MG, network of five fold symmetry clusters defines the degree of local order. These motifs resist shear, stabilize energy minima, and inhibit strain localization. In this study, we systematically decouple the contributions of distinct motif perturbations by simulating irradiation-induced structural states through targeted atomic dilution. Specifically, we construct post-irradiation analogs of $Cu_{64}Zr_{36}$ MG by systematically removing atoms according to their local motifs. This approach enables decoupling of the influence of local topology from the overall degree of rejuvenation. We investigated how perturbation of specific motifs alters relaxation, stress distribution, and mechanical strength. Recent advances in high-performance computing have enabled a clear shift toward large-scale, high-throughput molecular dynamics workflows. Leveraging this paradigm, we performed an extensive parameter sweep consisting of hundreds of independent molecular dynamics simulations, systematically varying temperature and structural perturbation protocols.

MM 18.3 Tue 14:30 SCH/A315

Influence of Xe swift heavy ions irradiation on the mechanical properties of PdNiP bulk metallic glasses — •Maren Jeromin[1], Marilena Tomut[1,2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str.10, 48149 Münster — [2]GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt

Pd40Ni40P20 bulk metallic glass samples that had been subjected to different relaxation states were investigated by nanoindentation and laser scanning microscopy (LSM) for irradiation effects induced by swift heavy ions. The samples were irradiated with 630 MeV Xe-ions at the UNILAC accelerator at GSI in Darmstadt. During irradiation, the samples were partially covered with honeycomb- patterned masks to enable direct comparison between irradiated and non-irradiated areas. LSM revealed a distinct swelling step at the mask boundary, whose height increased with ion fluence and varied systematically with the relaxation state of the material. The observed swelling is attributed to ion track formation, where localized melting and rapid re-solidification generates excess volume due to cooling rates exceeding the initial quenching rate. Nanoindentation measurements demonstrated a fluence-dependent decrease in hardness; however, the hardness of irradiated regions consistently remained higher than that of pristine samples. These findings offer new insight into the structure modification of bulk metallic glasses under medium-mass swift ion irradiation, where elastic collision effects increasingly compete with ion track formation governed by electronic energy-loss processes.

MM 18.4 Tue 14:45 SCH/A315

A ReaxFF study of the covalency-driven cracking-to-shearing transition in metal-metalloid glasses — •Shansi Liao[1], Jürgen Eckert[1,2], and Daniel Sopu[1,3] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Technical University of Leoben,Leoben, Austria — [3]Technical University of Darmstadt, Darmstadt, Germany

Revealing the atomistic origins of failure in amorphous solids remains challenging. In metal-metalloid glasses, mechanical response is strongly governed by the breaking and reformation of covalent bonds which cannot be adequately captured by non-reactive interatomic potentials. Here, large-scale reactive molecular dynamics simulations using a ReaxFF potential that includes angular constraints for covalent bonding reveal a composition-dependent transition from cleavage cracking to shear banding in model CuSi glasses. During loading, a highly connected, rigid Si-rich network suppresses strain delocalization, generating mechanically unstable regions characterized by shear-induced reductions in coordination number and severe distortions of Si-Si-Si bond angles. These unstable regions serve as energetically favorable pathways along which the crack advances. As Cu content increases, reduced angular rigidity promotes widespread shear transformation and shear-band-mediated plasticity. In contrast, the modified embedded-atom method potential, which intrinsically overestimates the angular flexibility of the Si-rich networks, fails to reproduce this transition. Our results show that angular rigidity of the interatomic potential is a key descriptor of plasticity in metal-metalloid glasses.

MM 18.5 Tue 15:00 SCH/A315

Macroscopic response of $Pd_{40}Ni_{40}P_{20}$ **Bulk Metallic Glasses to GeV** ^{238}U **Ion irradiation** — •Richard von Destinon, Maren Jeromin, Marilena Tomut, and Gerhard Wilde — Institut für Materialphysik, Universität Münster, Münster, Germany

Ion tracks formed by localized heating due to intense electronic excitations of the target atoms offer new pathways to tailor the mechanical properties of bulk metallic glasses. In this work, we investigate the effects of swift heavy ion irradiation on macroscopic behavior such as the hardness, swelling and strain-rate sensitivity on the well-characterized bulk metallic glass $Pd_{40}Ni_{40}P_{20}$. The samples were thermally relaxed at $0.94T_g$ and subsequently irradiated with 1.14 GeV U ions at the UNILAC accelerator at GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt. By using aluminum degraders of different thicknesses, the energy loss of the ions at the sample surface and their corresponding penetration depths were systematically varied. Characterization was carried out using Laser Scanning Microscopy (LSM) as well as nanoindentation with displacement depths up to 0.3 μm. The results show a pronounced increase of swelling as well as a decrease in hardness with increasing irradiation fluences. The strain-rate-sensitivity increases at higher fluences, suggesting that the increased structural heterogeneity within the irradiated metallic glass alters the local stress distribution, affecting the shear band propagation.

MM 18.6 Tue 15:15 SCH/A315

Compositional and Surface Variations in Sasanian Early Islamic Glasses from Gorgan, Ray, and Istakhr — •Farahnaz Bayat Nejad[1], Mohammadamin Emami[2], Rémy Chapoulie[3], and Farzaneh Bayat Nejad[4] — [1]Islamic Azad University, Central Tehran Branch, Tehran, Iran — [2]Art University of Isfahan, Isfahan, Iran — [3]Archéosciences Bordeaux, UMR 6034 CNRS, Université Bordeaux Montaigne, Pessac, France — [4]Islamic Azad University, Central Tehran Branch, Tehran, Iran

This study investigates the compositional and microstructural characteristics of Sasanian*Early Islamic glasses from Gorgan, Ray, and Istakhr. Laser-Induced Breakdown Spectroscopy (LIBS), Scanning Electron Microscopy with Energy-Dispersive X-ray Spectroscopy (SEM-EDX), and Hyperspectral Imaging (HSI) were used to assess elemental composition, surface morphology, and colorant phases. Distinct variations in Ca/K/Na ratios reflect differences in raw materials and production recipes across the three sites. SEM-EDX reveals heterogeneous corrosion layers and localized devitrification, especially in Istakhr samples with silica-rich alteration crusts. HSI spectra identified absorption features of Fe**, Mn, and Cu** chromophores associated with glass coloration. These results provide insight into technological choices and raw material exchange networks in Late Antique Iran, demonstrating the power of non-destructive, multi-analytical methods in archaeometric glass research.

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 Technology, 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 structural 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 investigate 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].

[1] D.Hamelberg et. al, J. Chem. Phys. 2004, 120, 11919
[2] P. Kumar & S. Yashonath, J. Am. Chem. Soc. 2002, 124, 3828

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.

[1] S. Kümmel, J. Roth, J. Phys. D: Appl. Phys. 58, 415302 (2025)

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.

[1] L. H. Goodman, E. S. Bililign, B. W. Keller, S. G. Kenny, and J. Krim, J. Appl. Phys. 124 (2018) 024502
[2] Ph. Ortner, M. Umlandt, N. Lomadze, S. Santer, and M. Bekir, Analyt. Chem. 95 (2023) 15645
[3] H. F. Tiersten, J. Acoust. Soc. Am. 59 (1976) 879
[4] J. P. Valentin, J. Appl. Phys. 57 (1985) 492

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 $\mathrm{Ni}_{1+x}\mathrm{Ti}_{1-x}$ 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 $\mathbf{Mg_3(Sb,Bi)_2}$ 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 $\mathrm{Mg_3(Sb,Bi)_2}$-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 $\mathrm{Sb_{0.6}Bi_{1.4}}$ 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).

MM 20: Topical Talk: Shigenobu Ogata

Time: Wednesday 9:30–10:00 Location: SCH/A251

Topical Talk MM 20.1 Wed 9:30 SCH/A251

Neural Network Atomistic Modeling of Dislocation Plasticity in Ceramics — •Shigenobu Ogata and Shihao Zhang — The University of Osaka, Osaka, Japan

Dislocations in ceramics are increasingly recognized as levers for toughening intrinsically brittle materials and for tailoring functional responses. Yet atomistic simulation of their plasticity remains difficult because ceramic bonding combines ionic and covalent character, dislocation cores are often nonstoichiometric and charged, and core structures can be highly extended in complex lattices - features that exceed the fidelity of empirical interatomic potentials. Here, we develop neural network potentials (NNPs) for dislocation plasticity in three representative functional ceramics - ZnO, GaN, and SrTiO3. The NNPs accurately reproduce charged and nonstoichiometric core structures, slip barriers, and the long-range electrostatic interactions between charged dislocations. Leveraging these models, we examine plasticity via nanopillar compression and nano-indentation, finding excellent agreement with experimental observations. The results establish a practical workflow for constructing NNPs that enable detailed, large-scale atomistic modeling of dislocation behavior in ceramics and open new avenues for predictive exploration of plastic deformation and property tuning in functional ceramic systems.

MM 21: Phase Transformations II

Time: Wednesday 10:15–13:00 Location: SCH/A215

MM 21.1 Wed 10:15 SCH/A215

On the nature of solutal melting in Cu-Pd — •Nagarjuna Remalli[1], Huai Zhang[1,2], Nisha Singh[1], Nuria Navarrete[1], Julien Zollinger[3], and Florian Kargl[1,4] — [1]Institute for Frontier Materials on Earth and in Space, German Aerospace Center (DLR), 51147 Cologne, Germany — [2]Department of Mechanical Engineering, University of Alberta, AB T6G 2G8 Alberta, Canada — [3]Université de Lorraine, Institut Jean Lamour, 54000 Nancy, France — [4]Foundry Institute, Fundamentals of Solidification, RWTH Aachen University, 52072 Aachen, Germany

We report on the kinetics of the solid-liquid (s-l) interface during solutal melting of isomorphous Cu-Pd melting couples. Using X-ray radiography (XRR) with sub-second time resolution the solutal melting dynamics along with the evolution of solute concentration fields was investigated. To this end circular melting couples of different thicknesses (220 μm and 460 μm) were in-situ monitored in an isothermal field at 1090°C slightly above the melting point of copper (1085°C) and well below the one of palladium (1555°C).

Sample thickness dependent differences in dissolution speed were observed which are suggested to be related with buoyancy-driven convective flow. By comparing SEM analysis results of the re-solidified Cu-Pd alloys with the in-situ results good agreement was found. Persistent non-equilibrium conditions were found at the s-l interface at the end of melting, independent of sample thickness or melting mechanism.

MM 21.2 Wed 10:30 SCH/A215

Chemoelastic effects, phase equilibria, and uphill diffusion in Cu-Pd nanoparticles — •Idan Klein, Feitao Li, and Eugen Rabkin — Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Haifa 3200003, Israel

We fabricated nanoparticles (NPs) of Cu-40 at.% Pd alloy via solid state dewetting and subsequent slow-cooling of Cu-Pd bilayers deposited on a sapphire substrate. We observed that some nanoparticles which experienced partial transformation from a disordered A1 FCC phase to the ordered B2 β-CuPd exhibited compositional discontinuity, with the ordered phase being richer in Pd. This compositional discontinuity was associated with fully or partially coherent interphase boundary. At the same time the FCC particles that did not experience any transformation, the fully transformed β-CuPd particles, and partially transformed particles with incoherent interphase boundary exhibited homogeneous distribution of the components. We developed a thermodynamic model which demonstrated that misfit-strain from the coherent interface influences the thermodynamics of the system, depressing the transformation temperature. Re-distribution of the components causes changes to the lattice parameter of each of the phases, mitigating the misfit between them, reducing free energy and encouraging the phase transformation.

MM 21.3 Wed 10:45 SCH/A215

Mechanism of structure formation during electrochemical dealloying — •Gideon Henkelmann[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

During electrochemical dealloying of a solid solution, atoms of the more noble species rearrange by surface diffusion to form a connected nanoporous structure with a characteristic length scale. Details of the underlying nanoscale self-organization process, specifically the criteria that select this characteristic length scale, remain to be understood. Here, we study this issue by kinetic Monte Carlo simulations. While previous studies started out with corroding a planar single-crystal surface, our approach starts by forming an internal cavity and follows the evolution of the surface of the growing void. This allows us to focus on passivation or bifurcation of the corrosion front in a realistic scenario with curved and rough surfaces. We find that passivation is governed by simple geometric criteria related to the enrichment of the more noble species on the pore surface. Furthermore, the variation of the resulting structure size with the overpotential may be rationalized by a Gibbs-Thomson-type scaling law.

MM 21.4 Wed 11:00 SCH/A215

ab-initio investigation of short-range order in Fe-Si-Al alloys — •Daniil Khodachenko[1], Franco Moitzi[1,2], Andrei Ruban[2], Oleg Peil[2], and Vsevolod Razumovskiy[1,2] — [1]Christian Doppler Laboratory for digital materials design guidelines for mitigation of alloy embrittlement, Leoben Austria — [2]Materials Center Leoben Forschung GmbH, Leoben Austria

Unique electromagnetic properties of steels with silicon and aluminum make them an excellent choice for the production of transformers and electric motors. These so-called electrical steels have enhanced energy efficiency due to reduced core losses and enhanced magnetic permeability. However, increasing the concentration of silicon and aluminum beyond a critical amount leads to significantly reduced ductility, which makes production very challenging.

The theoretical origin of these embrittlement effects is still not fully understood, as ab initio modeling based on Density Functional Theory (DFT) is rather challenging, due to requiring large supercells and complex magnetic interactions. Such first-principles simulations frequently use approximations that assume a fully random distribution of the alloying elements. However, real systems are not perfectly random, due to atomic interactions, which result in short-range ordering (SRO) of the atomic sites. We investigate atomic SRO phenomena using accurate DFT- and Green's function-based methods to study effective cluster interactions and their magnetic state dependence. Finally, we perform Monte-Carlo simulations to investigate phase transitions and the effect of SRO in these materials.

MM 21.5 Wed 11:15 SCH/A215

Ordering in Mo-Cr-Ti-Al refractory high-entropy alloys via machine learned interatomic potential — •Jiyao Zhang[1], Klemens Lechner[1], Markus Masswohl[2], Petra Spörk-Erdely[2], and David Holec[1] — [1]Department of Materials Science, Montanuniversität Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria — [2]Institute of Materials Science, Joining and Forming, Graz University of Technology, Kopernikusgasse 24/I, 8010 Graz, Austria

Refractory high-entropy alloys (RHEAs) offer exceptional mechanical and thermal properties, such as excellent high-temperature strength, making them favorable competitors to nickel-based superalloys. Origin of the superior high-temperature performance of the Mo-Cr-Ti-Al RHEA can be tracked to its two-phase microstructure of disordered BCC and ordered B2 phases. Modeling RHEAs poses significant challenges, as accurate density functional theory (DFT) calculations are extremely time-consuming, a difficulty worsened by the alloys' complex compositions. Universal machine learning interatomic potentials (UMLIPs) have recently emerged as a promising solution. Trained on vast DFT datasets, UMLIPs enable near-DFT accuracy for large-scale simulations of thousands of atoms. In this work, we utilize UMLIPs in mixed Monte Carlo/Molecular Dynamics simulations to evaluate the thermal stability of ordered versus disordered states in Mo-Cr-Ti-Al system as a function of the Al contents. Furthermore, we analyze the impact of composition on order/disorder transition temperature and elastic properties. We validate our findings against experimental data.

15 min. break

MM 21.6 Wed 11:45 SCH/A215

Shear-stress dependent formation of Si-polymorphs during saw dicing analyzed by raman spectroscopy — •Zainab Zainab[1,2], Jörg Debus[2], and Hannes Kurtze[1] — [1]Bernburger street 55, 06366 Köthen (Anhalt) — [2]August-Schmidt-Str. 4, 44227 Dortmund

Raman spectroscopic analysis of diced silicon wafers reveals that the saw cutting process generates considerable amounts of metastable silicon polymorphs (BC8/R8) along with the original diamond-cubic structure (DC-Si). We demonstrate that the formation of these phases exhibits a distinct spatial distribution that correlates with the shear stress profile imposed by the rotating blade. The DC-Si signal is strongest near the bottom of the cut (wafer tape side), while BC8 and R8 phases are most concentrated near the top surface at the blade entry point. This gradient arises from differences in the mechanical stress state: at the top, the steeper blade angle generates substantial shear stress in addition to normal compressive stress, facilitating shear-induced phase transformation at locally applied pressures. At the bottom, the nearly parallel blade trajectory produces predominantly normal stress with minimal shear, suppressing the formation of metastable phases. Additionally, we find that specific feed rates enhance phase transformations and intensify the spatial gradient. These findings confirm that shear stress is the critical enabling factor for polymorph formation during mechanical processing of silicon, consistent with recent studies showing dramatic reduction in transformation pressures under non-hydrostatic conditions.

MM 21.7 Wed 12:00 SCH/A215

Investigating the temperature-driven structural phase transition in α-In2Se3: A Raman study — •Saswata Talukdar, Mitanshi Gupta, Devesh Negi, Suvodeep Paul, Shalini Badola, Shivani Tripathi, Ravi Shankar Singh, and Surajit Saha — Indian Institute of Science Education and Research Bhopal, Bhopal, 462066, India

In recent years, the complex characteristics and polymorphic nature of indium selenide (In2Se3) have distinguished it as a prominent candidate among 2D semiconductors for memory and nano-electronic applications. Despite comprehensive research on its thermal, electrical, and optical properties, the structural dynamics, especially the phase transitions over temperature, remain elusive. In this work, temperature-dependent Raman spectroscopy of bulk α-In2Se3 reveals well-defined spectral signatures corresponding to its multiple polymorphic phases, providing direct evidence of its structural transitions. Our results also show that the phase transition is governed not solely by temperature, but it is further influenced by the local strain, which forms wrinkles on the surface of the material, playing a crucial role in directing the transition pathway. Moreover, comparative Raman measurements on exfoliated flakes highlight a pronounced thickness-dependent modulation of the transition behavior, underscoring the critical role of dimensionality in governing phase stability and evolution. Altogether, this work presents a comprehensive picture of the phase transitions in In2Se3, offering valuable insights for its integration into future high-performance phase-change memory applications.

MM 21.8 Wed 12:15 SCH/A215

Transforming martensite in Ni-Mn-Ga within picoseconds — •Klara Lünser[1,2], Yuru Ge[3,4], Fabian Ganss[3], Daniel Schmidt[5,6], Daniel Hensel[5], Mike J. Bruckhoff[7], Bruno Neumann[3,4], Mariana Brede[5], Sakshath Sadashivaiah[8,9], Markus E. Gruner[7], Peter Gaal[5,6], and Sebastian Fähler[3] — [1]University Duisburg-Essen — [2]RCFEMS, Bochum — [3]HZDR, Dresden — [4]TU Dresden — [5]Leibniz IKZ, Berlin — [6]TXproducts, Hamburg — [7]CENIDE, University of Duisburg-Essen — [8]Helmholtz-Institut Jena — [9]GSI Darmstadt

Martensitic transformations are driving a wide range of emerging applications, including high-stroke actuation, mechanocaloric refrigeration, and thermoelastic energy harvesting. However, systematic investigations of the fast dynamics and fundamental speed limits of martensitic transformations are scarce. In this study, we employed a synchrotron-based time-resolved diffraction technique to investigate the martensitic transformation induced by 200 fs laser pulses. Our results show that the transformation from martensite to austenite occurs within 100 ps, limited by the synchrotron probe pulse duration. We also demonstrated that an appropriate laser fluence and undercooling can complete a full transformation cycle within 5 ns, the fastest value reported for martensitic transformation. Our study highlights the importance of analyzing the lattice temperature during martensitic transformations and discusses the need for and limits of this approach. Furthermore, we found that stress must be considered as a competing influence on the martensitic transformation, in addition to temperature.

MM 21.9 Wed 12:30 SCH/A215

In-situ view on contact and solutal melting of Al-Cu — •Florian Kargl[1,2], Matthias Kolbe[1], and Nagarjuna Remalli[1] — [1]Institute for Frontier Materials on Earth and in Space, German Aerospace Center, Cologne, Germany — [2]Foundry Institute, Fundamentals of Solidification, RWTH Aachen University, Aachen, Germany

Melting plays an important role in many technical processes such as casting, additive manufacturing, etc. but is far less understood than solidification. We report on the kinetics of the solid-liquid interface during contact and solutal melting of Al-Cu melting couples. Al-Cu melting couples consisting of an Al-annulus and a Cu-disc in close contact were processed in an isothermal temperature field. The melting process was in-situ monitored with X-radiography with a sub-second time resolution determining interface kinetics and liquid composition changes. For contact melting a temperature below the melting points of Al and Cu but above the eutectic temperature was chosen. For solutal melting the sample was processed above the melting point of Al. We observed contact melting to be initiated along Cu-grain boundaries with intermetallic layers representing the entire phase diagram forming between the liquid and the still solid Cu. The layer structure has been verified post-mortem by optical imaging and quantified by SEM-EDX. Solutal melting was found to be dependent on sample thickness with buoyancy convection increasing the reaction speed in thicker samples. Further, asymmetric reaction patterns were observed to arise due to Al2O3-layer build-up and/or initial Al2O3-presence at the Al-Cu interface and/or partial Al-detachment during melting.

MM 21.10 Wed 12:45 SCH/A215

Forming bicontinuous microstructures by distributed internal melting at the Ni3Sn4 peritectic — •Zhongyang Li[1], Lukas Lührs[1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg — [2]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

A recent study on peritectic melting of TiAg suggests that a bicontinuous structure can be obtained through liquid film migration (LFM) during annealing. Without the requirement of mass exchange with the environment, peritectic melting is free of the restrictions on sample size. To date, application of this method is limited to TiAg. In this work, the intermetallic compound Ni3Sn4 is selected as the new parent system for peritectic melting. After annealing and quenching, spherical clusters are obtained, consisting of crystallographically aligned Ni3Sn2 ligaments and interpenetrating Sn phase. The phase decomposition proceeds via the LFM mechanism, i.e. complete melting of Ni3Sn4 and growth of Ni3Sn2 across the melt layer. Constitutional supercooling, induced by a composition gradient within the melt, promotes cellular growth of Ni3Sn2 nuclei, resulting in a ligament structure. Based on previous studies on peritectic and partial melting, we propose the concept of distributed internal melting, which utilizes the internal premelting sites (vacancies, dislocations and grain boundaries) to initiate LFM and generates bicontinuous structures through heat treatment.

MM 22: Data-driven Materials Science: Big Data and Workflows III

Time: Wednesday 10:15–12:45 Location: SCH/A216

MM 22.1 Wed 10:15 SCH/A216

Hashing It Out: Overcoming the Duplicate Structure Filtering Bottleneck for Large Data Sets — •Julian Holland, Juan Manuel Lombardi, Chiara Panosetti, and Karsten Reuter — Fritz Haber Institute, Berlin, Germany

With the increasingly data-rich landscape of computational chemistry research, new bottlenecks to material property elucidation have emerged stemming from data processing. Duplicate detection is often an essential data processing step for active learning, global optimization, and general PES exploration algorithms to ensure efficiency and functionality. Such duplication checks typically scale unfavorably with the number of structures, potentially taking longer to perform than the data generation. Hashing-based methods, which have decoupled scaling with dataset size, circumvent this but are conventionally too rigid to reliably find duplicates. In this talk, we present a democratic hashing duplicate detection algorithm that is flexible enough to detect duplicate structures with arbitrarily similar, but distinct, global descriptors nearly instantly. The uniqueness of the structure can be determined by an ensemble of hash functions associated with a set of randomly perturbed global descriptors. We compare the performance of our duplicate detection algorithm against conventional distance-matrix-based methods and introduce a standardized suite of duplicate detection benchmarks. Our algorithm is not only faster but often significantly more robust at detecting known duplicates.

MM 22.2 Wed 10:30 SCH/A216

MC3D: The Materials Cloud FAIR and full-provenance materials database — •Michail Minotakis — PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland

Carefully curated databases of materials and their properties have become invaluable resources for a range of applications, from property prediction using machine learning techniques to materials discovery. Here, we introduce MC3D, the Materials Cloud three-dimensional database, in which more than 95% of the available materials are, to date, classified as experimentally known. This database is derived from structures sourced from three major databases: the Pauling File, the Inorganic Crystal Structure Database, and the Crystallography Open Database. After careful curation, the final collection of 72,609 unique stoichiometric compounds is refined using density-functional theory calculations at the PBEsol level, executed in Quantum ESPRESSO and leveraging the SIRIUS library for optimized GPU performance. The AiiDA materials informatics infrastructure (http://aiida.net) manages each workflow stage, ensuring full traceability and preserving simulation provenance. The results are freely accessible in the MC3D section of Materials Cloud (https://mc3d.materialscloud.org) and are already being used as a starting point for materials discovery projects, such as novel thermoelectrics, electrides, superconductors, or materials displaying a large nonlinear Hall effect.

MM 22.3 Wed 10:45 SCH/A216

Building a FAIR Community around Parsing — •Nathan Daelman[1], Alvin N. Ladines[1], Esma Boydas[1], Martin Kuban[1], Bernadette Mohr[1], Sascha Klawohn[1], Rubel Mozumber[1], Christina Ertural[2], Silvana Botti[3], Joseph F. Rudzinski[1], Lauri Himanen[1], and FAIRmat Team[1] — [1]Inst. für Physik, Humboldt-Universität zu Berlin — [2]Department of Materials Chemistry, Federal Institute for Materials Research and Testing, Berlin — [3]RC-FEMS and Faculty of Physics, Ruhr University Bochum

NOMAD [nomad-lab.eu][1, 2] is an open-source data infrastructure for materials science data. One of its most praised features is how NOMAD allows for direct ingestion of various software output formats. This gives data producers access with minimal effort to the whole toolkit infrastructure system regardless of their choice of simulation code. As the NOMAD community extends into related scientific disciplines, parsing procedures should grow alongside and empower casual users to contribute too. To this end, I will be presenting two new parsing frameworks: (i) Mapping Annotation which connects code-specific formats to the NOMAD interoperable schema, while gracefully handling syntatic concerns; (ii) an agentic LLM interface for hooking up third-party parsers via the Model Context Protocol (MCP). Finally, I will highlight how both approaches fit into NOMAD Plugins and NOMAD Actions.

[1] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).
[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).

MM 22.4 Wed 11:00 SCH/A216

Uncertainty Propagation in Machine-learned Interatomic Potentials — •Haitham Gaafer, Jan Janssen, and Jörg Neugebauer — Computational Materials Design, Max-Planck-Institute for Sustainable Materials, Düsseldorf

Accurate multiscale materials modeling requires that uncertainties be quantified and propagated consistently from the electronic-structure level to macroscopic property predictions. Machine-learned interatomic potentials (MLIPs), trained on density-functional theory (DFT) reference data, now routinely reach near-DFT accuracy at dramatically reduced computational cost. Yet the connection between fitting errors in an MLIP and uncertainties in derived physical properties, such as bulk moduli or phase stabilities, remains insufficiently understood. We present a data-driven pyiron workflow designed to analyze how uncertainties originating in MLIP training propagate into thermomechanical property predictions. As a case study, we construct diverse DFT training sets for Cu, Ag, and Au using the Automated Small SYmmetric Structure Training (ASSYST) workflow, and fit computationally efficient atomic cluster expansion (ACE) potentials employing a minimal basis optimized to reach a target root-mean-square error. These potentials are subsequently used to determine equations of state and to quantify uncertainties in key properties, including the equilibrium lattice constant, bulk modulus, and its pressure derivative. Our results provide a transparent link between MLIP fitting quality and property reliability, offering a systematic route for uncertainty-aware atomistic modeling.

MM 22.5 Wed 11:15 SCH/A216

Accurately predicting thermal conductivity using non-equilibrium molecular dynamics simulations and machine-learned force fields — •Florian Unterkofler[1], Lukas Legenstein[1], Sandro Wieser[2], and Egbert Zojer[1] — [1]Graz University of Technology, Austria — [2]TU Wien, Austria

With the rise of machine-learned interatomic potentials, simulations have become an even more crucial tool for predicting material properties. We previously achieved accurate predictions of experimentally observed thermal conductivity of acenes, using system-specific, machine-learned Moment Tensor Potentials (MTPs) within a lattice dynamics approach.[1] To obtain a complementary real-space perspective, we now investigate whether comparable accuracy can be achieved using non-equilibrium molecular dynamics (NEMD).

Here, we present the workflow required to obtain accurate and reliable predictions when applying MTPs in NEMD simulations. We show that, due to the inherently stochastic nature of both MD and MTP training, a thorough statistical analysis of multiple simulations with different initial conditions and different realizations of the MTP is necessary. Furthermore, we highlight the importance of selecting appropriate training data to generate robust MTPs. When these considerations are taken into account, we achieve an excellent agreement between experiments, lattice-dynamics, and NEMD results, with NEMD simulations providing tools to investigate heat-transport bottlenecks in real space.

[1] L. Legenstein et al., *npj Comput Mater* 11, 29 (2025)

15 min. break

MM 22.6 Wed 11:45 SCH/A216

Data-efficient training of interatomic potentials using finite-temperature DFT structures — •Martin Schlipf[1], Sudarshan Vijay[1,2], and Georg Kresse[1,3] — [1]VASP Software GmbH, Berggasse 21/14, 1090 Vienna, Austria — [2]Department of Chemical Engineering, Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra 400076 India — [3]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Kolingasse 14-16, A-1090 Vienna, Austria

We successfully generated a database of 150,000 unique finite-temperature structures using VASP and a "one-shot" DFT method to systematically sample atomic environments across the periodic ta-ble. Despite the small size of our training set compared to the millions typically used for foundation models, our resulting interatomic potentials achieve a force prediction error of 72 meV/Å. This performance is of the same magnitude as current state-of-the-art foundation models when tested against the same high-quality dataset. This result demonstrates that focusing on data quality and chemical diversity at finite temperatures is as impactful as massive data quantity. Furthermore, we showcase the computational infrastructure that made it possible to integrate interatomic potentials into an ab-initio software and discuss necessary enhancements to electronic optimization methods to compute magnetic materials more reliably.

MM 22.7 Wed 12:00 SCH/A216

MACE-based Machine Learning Interatomic Potentials for Iron-Nickel Alloys: Validation Across Composition and Pressure Ranges — •Kushal Ramakrishna[1], Mani Lokamani[1], and Attila Cangi[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), D-01328 Dresden, Germany — [2]Center for Advanced Systems Understanding (CASUS), D-02826 Görlitz, Germany

Machine-learned interatomic potentials have emerged as powerful tools bridging quantum-level accuracy with mesoscale simulations in computational materials science. We present a comprehensive evaluation of MACE models for iron-nickel alloys across a wide range of compositions and pressures, with direct relevance to Earth's core modeling and industrial applications. We construct special quasirandom structures (SQS) to simulate random iron-nickel alloy configurations and train MACE models on density functional theory datasets combined with experimental validation data. Extensive short-range order analysis confirms improved chemical randomness for larger supercells, critical for faithful property sampling. Multiple MACE flavors are systematically compared against experimental measurements for structural and elastic properties in both body-centered cubic and face-centered cubic phases. Our results demonstrate that fine-tuned MACE models achieve remarkable predictive accuracy for equation-of-state behavior and elastic properties across all compositions. This approach successfully bridges computational predictions with experimental observations, enabling accelerated materials discovery for technologically relevant transition metal alloys.

MM 22.8 Wed 12:15 SCH/A216

Benchmarking the MACE Foundation Model for Solid-State Ion Conductors — •Takeru Miyagawa, Yufeng Xu, Levon Satzger, Waldemar Kaiser, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Recent progress in foundation model machine learning potentials (MLPs) has demonstrated promising transferability and accuracy across diverse material classes [1, 2]. Instead of being trained from scratch for each new system, these large pretrained models aim to provide broadly accurate force and energy predictions that can be refined for new chemistries with comparatively small datasets. This offers a complementary route to traditional system-specific MLPs and may reduce the cost of studying complex ionic materials.

Here, we benchmark the MACE foundation model [2] on representative solid-state ion conductors (SSICs) through direct comparison with first-principles calculations. We assess its accuracy for phonons and vibrational properties, characterize temperature-driven structural and phase transitions, and analyze ion transport across different phases. We then explore data-efficient DFT-based fine-tuning strategies to improve the foundation model's accuracy for SSICs and clarify the limits and strengths of pretrained representations in the context of ionic transport. References [1] Batatia, I. et al., Adv. Neural Inf. Process. Syst. 35, 11423-11436, 2022, [2] Batatia, I. et al., J. Chem. Phys. 163, 184110, 2025

MM 22.9 Wed 12:30 SCH/A216

MACE-μ-α: A Foundation Model for Molecular Dipole Moments and Polarizabilities — •Nils Gönnheimer[1,2], Venkat Kapil[3], Karsten Reuter[2], and Johannes T. Margraf[1,2] — [1]Universität Bayreuth — [2]Fritz-Haber-Institut der MPG — [3]University College London

Machine-learning interatomic potentials (MLIPs) have had a strong impact on computational chemistry, physics, and materials science in recent years by filling the accuracy gap between first-principles methods and classical force fields, at a fraction of the computational cost of the former. MLIPs are so far typically limited to predicting energies and forces, however, while other properties traditionally obtained from first-principles calculations have remained less accessible. Here, equivariant neural network architectures have led to enormous progress, as they allow the prediction of vectorial and tensorial properties on the same footing as energies and forces.

Here, we present the MACE-μ-α architecture for predicting dielectric properties based on the MACE MLIP framework. Trained on over 1.6 million organic systems, the corresponding foundation model allows the accurate prediction of molecular dipole moments and polarizabilities, as well as Raman and IR spectra (when combined with an MLIP). Notably, despite being trained on gas-phase molecules and clusters, the model also shows transferability to condensed systems such as molecular crystals.

MM 23: Topical Session: Dislocations in Functional Materials I (joint session MM/FM)

Time: Wednesday 10:15–11:30 Location: SCH/A251

MM 23.1 Wed 10:15 SCH/A251

Mechanical seeding of dislocations for room-temperature plasticity in ceramics — •Wenjun Lu[1], Jiawen Zhang[1], and Xufei Fang[2] — [1]Department of Mechanical and Energy Engineering, Southern University of Science and Technology, Shenzhen, 518055, China — [2]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe,76131, Germany

The pursuit of room-temperature ductile ceramics has long been hindered by their inherent brittleness. Here, we demonstrate a simple strategy to seed mobile dislocations at room temperature with densities up to 1014 m-2, enabling ceramics to sustain plastic compressive strains exceeding 30%. These dislocations multiply through cross-slip and motion, effectively suppressing brittle fracture without high-temperature processing. Using in situ nano-/micromechanical deformation and ex situ bulk tests, we bridge the length scales of plasticity and reveal a strong dependence of yield strength and flow behavior on dislocation density. Specifically, SrTiO3 micropillars transition from brittle fracture (dislocation-free) to plastic yield when mechanically seeded dislocations are present. Yield strength first decreases then rises with increasing dislocation density, reflecting complex structural evolution observed via transmission electron microscopy. These findings highlight dislocation engineering as a viable pathway toward ductile ceramics and open avenues for tuning their mechanical and functional properties through room-temperature dislocation plasticity.

Contribution: Wenjun Lu is the Speaker.

MM 23.2 Wed 10:30 SCH/A251

Impact of mechanically seeded dislocations on the mechanical properties of perovskite ceramics — •Jiawen Zhang[1], Xufei Fang[2], and Wenjun Lu[1] — [1]Southern University of Science and Technology, Shenzhen, China — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany

The inherent brittleness of functional ceramics severely hinders their engineering application. The strong ionic and covalent bonds in ceramics make dislocation nucleation, motion, and multiplication difficult at room temperature. Recent research challenges the conventional perception of ceramics as inherently brittle materials, with dislocations emerging as a promising avenue for enhancing their mechanical properties. By using a Brinell ball indenter to perform surface scratching, crack-free plastic deformation zones with tunable dislocation density can be generated on the ceramic surface. The dislocation generation mechanism and dislocation-dominated plastic deformation mechanism were investigated by introducing dislocations into perovskite SrTiO3 and KTaO3. Room temperature micropillar compression tests then revealed that as the mechanical seeded dislocation density increased,SrTiO3 exhibited a *brittle* to *ductile* transition as the dislocation density increased from ~1010 m-2 to ~1014 m-2. However, the (001) KTaO3 single crystal exhibits a *brittle* to *ductile* then to *brittle* transition as the dislocation density increased from ~1010 m-2 to ~1015 m-2. Additionally, the yield strength displayed a complex trend, initially decreasing and then increasing in these two perovskite oxide ceramics.

MM 23.3 Wed 10:45 SCH/A251

Dislocation interaction with a tilt low angle grain boundary in bi-crystal SrTiO3 — •Kuan Ding[1,2], Atsutomo Nakamura[3], Patrick Cordier[4,5], and Xufei Fang[3,6] — [1]Department of Materials and Earth Sciences, Technical University of Darmstadt, 64287 Darmstadt, Germany — [2]Max Planck Institute for Sustainable Materials, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [3]Department of Mechanical Science and Bioengineering, Osaka University, 1-3 Machikaneyama-chou, Toyonaka, Osaka, 560-8531, Japan — [4]Unité Matériaux et Transformations, Université de Lille, 59655 Villeneuve d'Ascq Cedex, France — [5]Institut universitaire de France (IUF), 75005 Paris, France — [6]Institute for Applied Materials, Karlsruhe Institute of Technology, Kaiserstr. 12, 76131 Karlsruhe, Germany

For applications of ceramics with dislocation-tuned mechanical and functional properties, it is pertinent to achieve dislocation engineering in polycrystalline ceramics. However, grain boundaries (GBs) are effective barriers for dislocation glide at room temperature. It is critical to understand the fundamental processes for dislocation-GB interaction. We investigated a bi-crystal SrTiO3 with a 4° tilt GB. Brinell indentation was used to generate a plastic zone at the mesoscale without cracking, allowing for direct assessment of GB-dislocation interaction. Together with dislocation etch pits imaging and transmission electron microscopy analysis, we observe dislocation pileup, storage, and transmission across the LAGB. Our observations reveal new insights into dislocation-GB interaction at room temperature at mesoscale.

MM 23.4 Wed 11:00 SCH/A251

Dislocation-Mediated Extraordinary Room-Temperature Plasticity in Inorganic Semiconductors — •Xiaocui Li[1] and Yang Lu[2] — [1]Department of Materials Science and Engineering, City University of Hong Kong, Kowloon, Hong Kong SAR, China — [2]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam, Hong Kong SAR, China

Inorganic semiconductors, with their ionic or covalent bonds, are typically brittle at room temperature, restricting their use in flexible electronics. Our recent study reveals that all-inorganic perovskite (CsPbX3, X=Cl, Br, I) single-crystal micropillars can achieve extraordinary room-temperature plasticity with average plastic strain of ~64% (Nat. Mater. 2023, 22, 1175). They can be morphed into distinct geometries without cracks or cleavage. The deformation is mediated by partial dislocations on {011}<0-11> slip system, featuring four equivalent variants that address the lack of deformation pathways in ionic crystals. Sequential activation of variants prevents strain hardening and crack formation caused by dislocation reactions. First-principles calculations attribute this plasticity to low slip barriers enabling sustained deformability and strong Pb-X bonds preserving crystal integrity. Leveraging this deformability, we developed shape-customizable optoelectronic devices that maintain stable functional properties and bandgap energies post-deformation. This discovery overturns the notion of brittleness in inorganic semiconductors, and provides a foundation for advanced applications in flexible electronics and deformable sensors.

MM 23.5 Wed 11:15 SCH/A251

Dislocations as Key Enablers on the Road to Functional and Resilient Oxide Ceramics — •Oliver Preuss[1], Enrico Bruder[2], Zhangtao Li[3], Yinan Cui[3], Jinxue Ding[1], Philippe Carrez[4], and Xufei Fang[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Division Physical Metallurgy, Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany — [3]Department of Engineering Mechanics, Tsinghua University, PR China — [4]Materials and Transformations Unit, Université Lille, Lille, France

Designing oxide ceramics that unite high mechanical resilience with strong functional performance is challenging. We show that introducing ultra-high dislocation densities ($\approx 10^{15}$ m^{-2}) into materials such as MgO and $SrTiO_3$ provides a direct route to enhance both damage tolerance and functional properties. Cyclic Brinell ball scratching at room temperature generates near-surface, dislocation-rich zones of arbitrary size and shape. These regions markedly alter fracture behaviour, arresting propagating cracks and suppressing crack initiation, as demonstrated by Vickers indentation and quasi-in situ DCDC tests. Crystal-plasticity phase-field simulations reproduce the observed toughening mechanism. The dislocation networks also improve transport properties, increasing electrical conductivity while reducing thermal conductivity by nearly half: an advantageous combination for thermoelectric performance. This work establishes a practical strategy for dislocation engineering to achieve oxide ceramics with combined mechanical robustness and enhanced functionality.

MM 24: Invited Talk: Andrea Bachmaier

Time: Wednesday 15:00–15:30 Location: SCH/A251

Invited Talk MM 24.1 Wed 15:00 SCH/A251

Recent advances in processing of rare-earth free MnBi magnets by severe plastic deformation — •Andrea Bachmaier[1], Lukas Weissitsch-Reiner[1], Martin Kraus[1], Michael Meindlhumer[2], and Stefan Wurster[1] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences — [2]Department of Materials Science, Montanuniversität Leoben

Magnetic materials are key materials needed for Green energy technologies. The research on rare-earth free magnetic materials has increased significantly in recent years, driven by supply chain issues, environmental and social concerns.

Severe plastic deformation processing of magnetic materials and its influence on the magnetic properties have attracted increasing research interest in the last years.

In this contribution, the use of high-pressure torsion deformation to synthesize the rare-earth free α-MnBi phase is in focus. Our recent experimental results of the process-structure-property relationships that link chemistry, synthesis and processing parameters with microstructure evolution and magnetic properties are discussed. An emphasis is put on detailed characterization of the microstructure by backscattered electron imaging, electron backscattered diffraction as well as x-ray diffraction utilizing high energy synchrotron radiation since it strongly influences the magnetic properties.

MM 25: Interface Controlled Properties, Nanomaterials, and Microstructure Design I

Time: Wednesday 15:45–17:00 Location: SCH/A215

MM 25.1 Wed 15:45 SCH/A215

Confined but Active: Atomic-Scale Dynamics of Gallium and Silver Intercalation in Graphene/SiC — •Nadire Nayir[1], Qian Mao[2], Malgorzota Kowalik[2], and Adri van Duin[2] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]The Department of Mechanical Engineering, The Pennsylvania State University, PA, US

Metal intercalation at the interface of epitaxial graphene and SiC offers a powerful approach for stabilizing covalently bonded materials in two dimensional form [1-2]. This talk focuses on the atomic-level modeling of 2D metals (i.e. Ga and Ag) grown via confinement heteroepitaxy [2]. The intercalation mechanisms differ notably between metals. Combined photoemission electron microscopy and multiphysics simulatiosn reveal that while metal de-intercalation emerge in all cases, their re-intercalation dynamics vary markedly. For Ag, reversible de- and re-intercalation occurs through defects. In contrast, Ga exhibits irreversible de-intercalation characterized by faster kinetics. Multiphysics simulations integrating ReaxFF and Density functional theory simulations uncover the origin of these distinct behaviors, showing that Ga atoms bind more strongly to graphene than Ag atoms consistent with the faster, irreversible diffusion kinetics observed experimentally. Overall, the findings highlight that both the thermophysical properties of the intercalated metal and its interactions with defective graphene critically determine the intercalation behavior. [1] Nature materials 19 (6), 637-643(2020) [2] Small 20 (11), 2306554(2024)

MM 25.2 Wed 16:00 SCH/A215

Accelerating grain boundary segregation studies in ferritic steels with machine learned interatomic potentials — •Han Lin Mai[1], Tilmann Hickel[2], and Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials GmbH, Dusseldorf, Germany — [2]BAM Federal Institute for Materials Research and Testing, Berlin, Germany

The segregation of solute and impurities to grain boundaries (GBs) can critically alter the mechanical properties of steels. To predict segregation phenomena, ab-initio methods such as density functional theory (DFT) are frequently used, but their computational expense limits the size of the model GBs viable for computation. This limitation has rendered access to segregation statistics out of reach and therefore has hindered our understanding of segregation phenomena. Here, we present a machine learned interatomic potential (MLIP) for multiple Fe-X binary alloys that predict segregation energies approaching ab-initio accuracy with automated dataset generation techniques. We use these potentials to conduct high-throughput segregation studies to generate segregation energy spectra and compare these to those commonly found in GBs accessible to DFT studies. Commonly purported relationships between GB quantities such as excess volume, site volume and GB energies and the strength of segregation binding of solutes and impurities are re-examined and revised.

MM 25.3 Wed 16:15 SCH/A215

Defect Phase Diagrams for Exploring Chemo-Structural Coupling in Ni Grain Boundaries — •Prince Mathews[1], Ali Tehranchi[1], Jörg Neugebauer[2], and Tilmann Hickel[1,2] — [1]Federal Institute for Materials Research and Testing (BAM), Berlin, Germany — [2]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

The knowledge-driven framework of defect phase diagrams (DPDs) offers an effective and systematic approach to design materials with tailored properties. Unifying bulk and defect thermodynamics along with the consideration of structural and chemical complexities around defects, DPDs advance the fundamental understanding of defects and can also provide a pathway for guided microstructure design. In this work, we apply the framework of DPDs using ab-initio calculations to evaluate the stability of defect phases and investigate defect phase transformations in Ni grain boundaries. In competition with the nearest intermetallic phase, Nb containing defect phases are stable in $\Sigma5$ [001]/(310) whereas Nb containing defect phases are not stable in $\Sigma3$ [110]/(111) grain boundaries. Moreover, our findings indicate the preference of solutes to segregate at sites around defects with partial column occupations. Furthermore, with the application of a sub-lattice based model, we present the insights on grain boundary site column coverages as a function of temperature. In addition, we discuss a new approach for determining a characteristic defect width using the solute distribution probability across the defect which facilitates the integration of defects into the CALPHAD methodology.

MM 25.4 Wed 16:30 SCH/A215

Non-Hermitian physics and exceptional points at Z2 Weyl semimetal*ferromagnet junctions — •Tong Wang[1], Robert Amelung[2], and Flore Kunst[1,2] — [1]Max Planck Institute for the Science of Light, Staudtstraße 2, 91058 Erlangen, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Non-Hermitian systems extend beyond the framework of Hermitian quantum mechanics and allow for the description of open systems with loss and gain. The study of non-Hermitian physics leads to an enrichment of topological phases of matter and practical applications in photonics and sensing. Here we study the junction between a metallic ferromagnet and a Z2 Weyl semimetal [1], where a combined time-reversal symmetry and reflection symmetry leads to degenerate helical Fermi arcs on certain surfaces. The couplings at the material interface give arise to a complex self-energy in the Green's function [2], rendering the effective Hamiltonian of the Fermi arc surface states non-Hermitian. We show that non-Hermiticity can break a degenerate Fermi arc into pairs of exceptional point, and the resulting exceptional phase persists for a wide parameter range regarding the magnetization of the ferromagnet and topological mass term of the semimetal. We also discuss the how the exceptional points may influence physical properties of the Z2 Weyl semimetal. [1] T. Morimoto and A. Furusaki, Phys. Rev. B 89 235127 (2014). [2] E. J. Bergholtz and J. C. Budich, Phys. Rev. Res 1 012003(R) (2019).

MM 25.5 Wed 16:45 SCH/A215

Theory Unravels Electro-Ionic Metal-Support Interactions at Supported Electrocatalyst Nanoparticles — •Yufan Zhang, Tobias Binninger, Jun Huang, and Michael Eikerling — Theory and Computation of Energy Materials, Institute of Energy Technologies, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Electrochemical energy conversion requires electrocatalysts to accelerate reactions. Most theoretical studies used idealized planar electrodes, whereas real catalysts typically consist of supported nanoparticles (NPs) with heterogeneous compositions and structures that lead to unique electronic and ionic properties.

In this talk, I will present results from our recently published paper [1]. Using density-potential functional theory, we calculate the contact electrification of a Ag NP and a Au support. While traditional view believes that electron redistribution is confined to the NP-support contact interface, we reveal that it also occurs at the NP's external surface, directly influencing the catalytically active sites. The electron redistribution generates an electric field in electrolyte surrounding the supported NP, which further leads to ion separation. The support-induced charge perturbations at the NP's external surface can be no longer described by the classical concept of the potential of zero charge for planar electrode. To address this, we define a global and two local characteristic potentials. It is demonstrated that the electronic and ionic effects are strongly coupled at supported NPs, and are therefore best described as electro-ionic metal-support interactions (EIMSI).

[1] Y. Zhang, et al., Phys. Rev. Lett. 134, 066201 (2025).

MM 26: Transport in Materials: Diffusion, Charge, or Heat Conduction I

Time: Wednesday 15:45–17:00 Location: SCH/A216

MM 26.1 Wed 15:45 SCH/A216

Theoretical investigation of the conductivity of the LiMnPO$_4$ Battery Material — •Franz Winkler and Harald Oberhofer — Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth

Developing better batteries and thus battery materials is a crucial step in humanity's urgent energy transition. Thereby, theory can play an important role in characterizing and understanding the properties of the involved materials. In this contribution we present our work on olivine LiMnPO$_4$ which exhibits some desirable properties such as a high energy density and a high potential and thus operating voltage. However, its adoption is hampered by a bad conductivity. In order to understand the barriers to conductivity and suggest potential remedies we compute electronic and ionic transport properties and how they could be influenced by defects.

The electron and hole band transport mobilities are calculated using Hubbard-corrected electronic density functional theory (DFT+U), both for antiferromagnetic and paramagnetic LiMnPO$_4$ as well as materials derived by substitution. For ionic conductivity we determine the minimal energy path of the Li ions via the nudged elastic band (NEB) method. To reduce calculational cost and enable larger systems, we use machine learned force fields and refine these models via DFT to transition states. Li ions are transported in LiMnPO$_4$'s 1D channels. However these diffusion paths can be blocked by antisite defects. As those very strongly limit ionic transport we investigate their stability with first-principle DFT, phonon and thermodynamics calculations.

MM 26.2 Wed 16:00 SCH/A216

Multiscale modeling of cooperative defect dynamics in MoS$_2$ — •Aaron Flötotto[1,2], Erich Runge[1,2], and Christian Dressler[1,2] — [1]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [2]Technische Universität Ilmenau, Institut für Mikro- und Nanotechnologien, Ilmenau, Germany

Chalcogen vacancies strongly influence the electrical and memristive properties of transition metal dichalcogenides including MoS$_2$. However, capturing their dynamics at device-relevant time and length scales is challenging due to the high energy barriers associated with individual atomic jumps [1]. We have developed a multiscale framework for MoS$_2$ that uses *ab-initio* molecular dynamics to generate training data for machine-learning force fields. This step reveals the motifs of cooperative sulfur-vacancy migration and cluster formation [2]: (i) Vacancy migration almost exclusively occurs by vacancy-assisted hopping, implying non-linearities and suggesting memristive behavior; (ii) An energy barrier comparable to lab temperatures protects long vacancy lines against splitting into smaller vacancy clusters.

These insights are incorporated into a Monte-Carlo model that reproduces several key experimental observations and enables the prediction of device level quantities, such as the vacancy-density-dependence of the diffusion coefficient of sulfur vacancies in MoS$_2$.

[1] Q. Chen, et al. , ACS Nano 12, 7721-7730 (2018), doi: 10.1021/acsnano.8b01610.

[2] A. Flötotto, et al., arXiv:2508.13790 (2025).

MM 26.3 Wed 16:15 SCH/A216

Coupled Spin–Orbital–Lattice Interactions in FeO: A DFT+U and Heisenberg Analysis — •Hao Chen, Christoph Freysoldt, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf, Germany

Wüstite (FeO) is a prototypical correlated oxide where spin, orbital, and lattice degrees of freedom are intricately coupled. In addition, significant deviations from stoichiometry can occur via oxygen vacancies and Fe^{2+}/Fe^{3+} mixed valency. Local lattice distortions and orbital reorientations around such defects can modify magnetic exchange pathways and thus the defect formation energies. Using DFT+U, we investigate how the orbital orientation in Fe^{2+} correlates with structural strain and magnetic interactions. Our results reveal a well-defined correlation between the minority-spin t_{2g} occupation and the rhombohedral distortion parameter, giving rise to four distinct symmetry-broken orbital states. By mapping total-energy differences between these orbital configurations onto an effective Heisenberg model, we show that the exchange constants are sensitive to orbital orientation, evidencing strong superexchange–orbital coupling. This framework provides quantitative insight into the competition between Jahn–Teller-like lattice distortions and anisotropic magnetic exchange arising from orbital orientation. Building on this, the study provides a unified DFT+U-based picture of spin–orbital–lattice coupling in FeO and establishes a consistent energetic framework for incorporating spin and orbital effects into defect calculations.

MM 26.4 Wed 16:30 SCH/A216

Quantum interference in higher pseudospin fermions — •Gargee Sharma and Arpan Gupta — Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016 India

We construct a unified theory of quantum-interference corrections in disordered pseudospin-s fermions described by $k{\cdot}\mathbf{S}$ Hamiltonians. Employing the rotation-group structure of SU(2), we derive closed-form wavefunctions, scattering and vertex corrections, and Cooperon kernels valid for arbitrary pseudospin s in two and three dimensions. A universal "parity rule" emerges: integer s (orthogonal symmetry, $T^2 = +1$) yields weak localization, half-integer s (symplectic, $T^2 = -1$) yields weak antilocalization, while interband and intervalley scattering renormalize the prefactor via a finite Cooperon-mass matrix. Explicit results for $s = \frac{1}{2}$ and $s = 1$ reproduce graphene and spin-1 Weyl limits and verify the general scaling laws. Our approach resolves the long-standing ambiguity in interband scattering, providing an analytic route for arbitrary s and concrete predictions for multifold-fermion materials.

MM 26.5 Wed 16:45 SCH/A216

Effects of strong electron-electron interactions on the conductivity of free-standing graphene — •Maksim Ulybyshev[1], Adrien Reingruber[1], and Kitinan Pongsangangan[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Würzburg, Germany — [2]Department of Physics, Faculty of Science, Mahidol University, Bangkok, Thailand

Transport in strongly correlated systems is often described using the Boltzmann equation, where correlation effects enter through the collision integral. In practice, the collision integral is usually evaluated with a number of approximations, such as computing scattering amplitudes only up to tree-level diagrams. These approximations become unreliable when interactions are sufficiently strong.

Free-standing graphene provides a representative example, as the effective coupling constant of its low-energy effective field theory exceeds unity. Using unbiased Quantum Monte Carlo (QMC) simulations on lattices with up to 102x102 unit cells and long-range Coulomb interactions, we investigate both the DC and optical conductivity of free-standing graphene. We find that the optical conductivity remains essentially unaffected by interactions, whereas the DC conductivity exhibits a strong dependence on both temperature and interaction strength. We then compare these results with kinetic-theory calculations based on the Boltzmann equation, highlighting how the QMC data can guide improvements in the accuracy of the collision integral.

MM 27: Topical Session: Dislocations in Functional Materials II (joint session MM/FM)

Time: Wednesday 15:45–17:15 Location: SCH/A251

Topical Talk MM 27.1 Wed 15:45 SCH/A251

Dislocations in perovskite oxides: similarities and differences — •Pierre Hirel — Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France

The experimental discovery of room-temperature ductility in strontium titanate $SrTiO_3$ in 2001, has revealed the surprising mobility of dislocations in $\langle 110\rangle\{110\}$ slip systems. Atomic-scale simulations have contributed to resolving the core structure of these dislocations, and their role in the ductile-brittle transition. Since then, similar ductile behaviour was found in related perovskite oxides $KNbO_3$ and $KTaO_3$. However, other perovskites like $BaTiO_3$ or $CaSiO_3$ remain essentially brittle at room temperature, despite having the same crystal lattice and similar chemical compositions as ductile perovskites.

MM 27.2 Wed 16:15 SCH/A251

Probing the Known Unknown of the Dislocation Dynamics in Oxides and Semiconductors — •Liming Xiong — NC State University, Raleigh, NC, USA

Dislocation dynamics in oxides and semiconductors are widely aware, but its exact nature and impact on the properties and functionality of these materials are not fully understood yet. One reason is that the well-established knowledge for dislocation dynamics in metals often can't fully explain or even fail when used for oxides and semiconductors. To fill this knowledge gap, here we will present a concurrent atomistic-continuum computational tool for probing the dislocation dynamics in oxides and semiconductors. This tool has a unique feature to accommodate the motion/multiplication of μm-long dislocations together with the atomic-scale core structure evolution along the dislocation within all within one single model. Taking dislocation-seeded SrTiO3 and ZnS as sample materials, we will: (i) map the core structure/stress along a dislocation line to its local charge states and motion mechanism; (ii) measure the dislocation mobility and its dependence on stress, temperature, dopant concentration, charge states, electrical field, light illumination, and dislocation line lengths ranging from nanometers to micrometers; (iii) predict how local internal stress builds up when a mesoscale dislocation slip interacts with an atomically structured grain boundaries, and how such a high local stress may initiate a crack in turn. A consolidation of such simulation data into constitutive rules needed by higher-scale models for interpreting experimental observations will be also discussed.

MM 27.3 Wed 16:30 SCH/A251

Electric Field Effects on Dislocation Motion in SrTiO3 via Mesoscale Indentation — •Alexander Frisch[1], Daniel Isaia[2], Oliver Preuss[2], and Xufei Fang[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany

Dislocations in perovskite oxides have the potential of tuning functional properties of electroceramics, however their behavior and stability under externally applied electric fields remain elusive. Therefore, we investigated the effect of high densities of dislocations onto the dielectric breakdown behavior of SrTiO3, a model perovskite material. Lower dielectric breakdown strengths were found in the high-dislocation-density samples, engineered through the Brinell scratching method. Further, the effect of a 2 kV/mm electric field on the introduction and mobility of dislocations in SrTiO3 was investigated. While no changes to the dislocation plastic zone size, depth, or dislocation distribution were observed, the results suggest the stability of pre-engineered dislocation structures in perovskite oxides under applied electric fields. These results will be interpreted in the context of the dislocation charge state, associated electric field forces, and defect-modified electrical/thermal conductivity.

MM 27.4 Wed 16:45 SCH/A251

Generating a "ferroelectric metal" by preferential reduction of dislocations in $BaTiO_3$ — •Christian Rodenbücher[1], Gustav Bihlmayer[2], Carsten Korte[1], and Kristof Szot[3] — [1]Forschungszentrum Jülich GmbH, Institute of Energy Technologies (IET-4), 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-1), 52425 Jülich, Germany — [3]University of Silesia, Institute of Physics, 41-500 Chorzów, Poland

Redox processes in transition metal oxides are of high relevance for sensors, information technology, superconductivity, and energy conversion. Perovskites with mixed ionic-electronic conductivity, such as $BaTiO_3$, are of particular interest because oxygen nonstoichiometry controls electronic charge carriers and thus conductivity. Surprisingly, thermal reduction in vacuum can induce metallic behaviour with conductivities far exceeding predictions from point-defect chemistry. To clarify the origin of this metallic state, we investigate the electronic transport, electronic structure, and chemical composition of $BaTiO_3$ single crystals during annealing and cooling under ultrahigh vacuum. Surface-sensitive techniques such as XPS and LC-AFM allow us to correlate electronic structure changes with the insulator-to-metal transition. We find that surface-layer dislocations act as preferential reduction sites, forming conducting filaments that yield macroscopic metallic behaviour despite minimal overall oxygen loss. Metallic behaviour persists into the ferroelectric phase. Nanoscale mapping shows that metallic filaments and piezoelectrically active regions coexist thus explaining how a "ferroelectric metal" can exist.

MM 27.5 Wed 17:00 SCH/A251

Dislocation dynamics in Ni-based superalloys: atomistic simulations and uncertainty quantification — •Geraldine Anis, Thomas Hudson, and Peter Brommer — University of Warwick, Coventry CV4 7AL, UK

Ni-based superalloys exhibit extraordinary strength at high temperatures. This strengthening effect is largely attributed to precipitation strengthening, where dislocations are hindered by precipitates present in their microstructure. In our work, we model dislocation trajectories obtained from Molecular Dynamics (MD) simulations of Ni-Ni_3Al. A reduced model was developed to describe dislocation-interface interactions within this system, which captures important features of the MD dislocation trajectories. The developed model was tested on a representative system and was shown to capture a range of qualitatively different dislocation behaviour. The model parameter distributions were then determined using Differential Evolution Monte Carlo (DE-MC) sampling and a Gaussian process surrogate model. The present approach offers a means of identifying atomistic-scale parameters, which can be used to inform larger length scale simulations of dislocations. Determining parameter distributions using DE-MC means that parameter uncertainties can be propagated through a hierarchy of multiscale models. We illustrate how such uncertainty propagation can be achieved by considering a dislocation mobility law with quantified uncertainties in pure Ni. This work is part of a wider study aiming to model the deformation behaviour of Ni-based superalloys with a focus on quantifying and propagating uncertainties.

MM 28: Members' Assembly

Welcome to this general meeting of the DPG-SKM division MM! All of you, presenters of MM talks or posters and other interested participants of this conference, are cordially invited to this meeting. We will come together in a relaxed atmosphere, supported by drinks and pretzels (at least) for personal exchange. We will award the poster prizes, discuss the current conference, and ask for your suggestions for future Topical Sessions in MM, Symposia, and invited speakers. Take this opportunity to share your ideas regarding our MM program for our next DPG spring meeting.

Time: Wednesday 17:15–18:45 Location: SCH/A251

All members of the Metal and Material Physics Division are invited to participate.

MM 29: Invited Talk: Philipp Pelz

Time: Thursday 9:30–10:00 Location: SCH/A251

Invited Talk MM 29.1 Thu 9:30 SCH/A251
Three dimensional sub-Ångström resolution imaging from 4D-STEM experiments — •Philipp Pelz — Friedrich Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Electron ptychography is rapidly emerging as a way to turn scattered high-energy electron waves into precise three-dimensional atomic maps, effectively solving a challenging inverse problem that links measurement, modeling, and reconstruction. By combining multi-slice physics, joint optimization, and automated data collection, we can now recover sub-Ångström 3D structures even when the experiment violates classical limits in electron microscopy such as depth of focus and tomographic completeness. These methods dramatically expand the range of materials and volumes that can be imaged at true atomic resolution, opening the door to data that is richer, more robust, and more compatible with theory and simulation. I will present several results that bridge experiment and computational modeling through a unified, physics-based reconstruction framework, show applications to nanomaterials and outline our ambitions to scale the method to larger volumes.

MM 30: Interface Controlled Properties, Nanomaterials, and Microstructure Design II

Time: Thursday 10:15–11:45 Location: SCH/A215

MM 30.1 Thu 10:15 SCH/A215
Statistics of Shear-Coupled Grain Growth in Polycrystals — •Marco Salvalaglio[1], Caihao Qiu[2], Jian Han[2], and David J. Srolovitz[3] — [1]Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — [2]Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong SAR — [3]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam, Hong Kong SAR

Grain growth in polycrystals, the coarsening of crystalline domains with different orientations, is traditionally viewed as a capillarity-driven process governed by interfacial energy minimization. However, grain-boundary migration can also induce, and in turn couple to, shear deformation, making microstructure evolution sensitive to externally applied stress. At the microscopic level, this behavior arises from the motion of disconnections, steps with dislocation character constrained at grain boundaries. Using a multi-phase-field (PF) framework that incorporates disconnection flow through coarse-graining, we demonstrate that accounting for shear coupling enables realistic grain-growth behavior in single-component polycrystals. Simulations reproduce recent experimental observations of weak correlations between grain boundary velocity and curvature. We then use PF simulations to analyze key aspects of microstructure evolution, including grain-size distributions, grain-shape evolution, and statistical characterization of the evolving network.

MM 30.2 Thu 10:30 SCH/A215
Revealing nanovoids in growth-resistant regions of nanocrystalline Pd–Au using atom probe tomography — •Johannes Wild[1], Fabian Andorfer[4], Svetlana Korneychuk[2,3], Jules M. Dake[4], Dorothée Vinga Szabó[1,2,3], Stefan Wagner[1], Carl E. Krill III[4], and Astrid Pundt[1,2] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology — [3]Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe Institute of Technology — [4]Institute of Functional Nanosystems, University of Ulm

Nanocrystalline Pd–Au produced by inert gas condensation (IGC) shows extreme abnormal grain growth (AGG) upon heat treatment. In some cases, narrow regions of residual nanocrystalline material resist coarsening entirely, persisting between abnormally grown grains exceeding 100 μm. We investigate these growth-stagnant regions using site-specific SEM/FIB lift-outs, atom probe tomography (APT) and TEM. FIB cross-sections reveal that these nanocrystalline regions are significantly more porous than the surrounding matrix, and APT reconstructions from them exhibit a strongly elevated density of OH-containing clusters, which are largely absent elsewhere. By analysing local ion-density variations during field evaporation into voids, we show that these OH clusters correspond to nanovoids in the material. Correlating porosity with grain morphology, we find that the most porous regions exhibit the strongest resistance to grain growth, indicating that nanoscale porosity is a key factor in stabilizing the nanocrystalline grain structure in IGC Pd–Au (manuscript submitted).

MM 30.3 Thu 10:45 SCH/A215
Vacancy-mediated extreme abnormal grain growth in inert gas-condensed nanocrystalline Pd–Au: when what's missing runs the show! — Fabian Andorfer[1], Johannes Wild[2], Jürgen Markmann[3,4], Markus Ziehmer[1], Jules M. Dake[1], Torben Boll[2], Dorothée Vinga Szabó[2,5,6], Stefan Wagner[2], Astrid Pundt[2,5], and •Carl E. Krill III[1] — [1]Inst. of Functional Nanosystems, Ulm University — [2]Inst. for Applied Materials, KIT — [3]Inst. of Hydrogen Technology, Helmholtz-Zentrum Hereon — [4]Inst. of Materials Physics and Technology, TUHH — [5]Inst. of Nanotechnology, KIT — [6]Karlsruhe Nano Micro Facility (KNMFi), KIT.

Inert gas-condensed Pd–Au exhibits extreme abnormal grain growth (AGG), marked by a small number of grains growing dendritically through a matrix of nanocrystallites, eventually reaching sizes of $100\,\mu$m or more. The triggers for rapid growth of abnormal grains (emergence) and for maintaining this growth advantage (persistence) remain unclear. Annealing under hydrogen accelerates emergence without altering grain morphology, suggesting that the ~ 5 vol% porosity inherent to inert gas condensation not only pins matrix/matrix grain boundaries (GBs) but also governs where and when abnormal grains emerge. In nano-Pd–Au, pores can coarsen by vacancy diffusion along GBs, with larger pores growing at the expense of smaller ones. Small-angle x-ray scattering measurements support such an evolution in pore-size distribution. Vacancy transport, rather than variations in boundary mobility, appears to establish the spatiotemporal conditions for AGG in this system.

MM 30.4 Thu 11:00 SCH/A215
Small-angle x-ray scattering of nanoporous gold - a discussion of the structure factor and its implications for local order — •Celina Passig[1,2], Jürgen Markmann[2,1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Department Hybrid Materials Systems, Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Nanoporous gold (NPG) made by dealloying is a popular model system for studies of size and interface effects as well as microstructure evolution in nanomaterials. Here, we investigate to what extent information on the microstructural geometry may be obtained by Small-Angle X-Ray Scattering (SAXS). It is well established that NPG exhibits a sharp interference peak, indicative of a characteristic wavelength underlying its leveled-wave-like microstructure and, hence, of an exceptional degree of order. Remarkably, our measurements even reveal a secondary peak at larger wave number. We compare the experimental data to simulations for small-angle scattering of NPG generated (1) by kinetic Monte Carlo (KMC) studies of dealloying or (2) as leveled-wave structures. On that basis, we discuss in how far the secondary interference peak is intrinsic to the microstructure of idealized, uniform NPG and what information it provides on the geometry of that microstructure. Since the feature vanishes during coarsening, we inspect how this process affects the order of the ligament network.

MM 30.5 Thu 11:15 SCH/A215

Enhanced Field Emission Current Density in Chemically Engineered Multiwall Carbon Nanotube - Neodymium Oxide Heterostructures — •Anima Mahajan[1], Menaka Jha[2], and Santanu Ghosh[1] — [1]Department of Physics, Indian Institute of Technology, Hauz Khas, New Delhi -110016, India. — [2]Institute of Nano Science & Technology, Knowledge City, Sector-81, Mohali, Punjab-160062, India.

The MWCNT, neodymium oxide (Nd*O*), and MWCNT-Nd*O* heterostructure were successfully fabricated through a facile three-step synthesis process: the synthesis of MWCNT rods by the chemical vapor deposition technique, the synthesis of the Nd*O* nanoparticles by using the micellar-assisted solid-state route, and the fabrication of the MWCNT-Nd*O* heterostructure. Moreover, the MWCNT-Nd*O* heterostructure exhibits enhanced field emission properties, with a lower turn-on field of 2.4 V/*m compared to pure MWCNT and Nd*O*, which have turn-on fields of 3.6 and 3.8 V/*m, respectively. The emission current stability at a preset value of 6 V/*m over an 8-hour duration is found to be fairly good, characterized by current fluctuations within * 3% of the average value. The enhanced field emission (FE) performance of the MWCNT-Nd*O* heterostructure is attributed to its high enhancement factor (β) of ~3.3*10*.

MM 30.6 Thu 11:30 SCH/A215

Exploring Superconductivity in Misfit Nanodevices — •Sushmita Chandra and Claudia Felser — Nöthnitzer Str. 40, 01187 Dresden

Recently, MISFIT layered compounds (MLCs) have attracted considerable attention in the field of 2D materials due to their unique structure, crystallographic diversity, and chemical tunability. Typically, MLCs can be represented by the general formula $[(MX)(1+\delta)]m[(TX2)n]$ with m, n = 1, 2, 3, where M = Sn, Sb, Pb, Bi, rare-earth elements; T = Ta, Nb, Mo, etc., and X = S, Se, Te. The lattice mismatch between the distorted rock salt MX layers and hexagonal TX2 counterparts creates a strained interface in the MLCs which allows a charge transfer from one layer to another, leading to a wealth of fascinating physical phenomena and modulations in the electronic structure. Although MLCs have been extensively studied for their potential applications in thermoelectrics, the fabrication of nanodevices with single- or multilayer MISFIT crystals is a challenging task and has not been explored at all. In this talk, I will present the fabrication of nanodevices based on high-quality MISFIT single crystals. I will also correlate how the misfit strain is associated with the superconducting transition and affects the electronic transport in these natural van der Waals heterostructures.

MM 31: Transport in Materials: Diffusion, Charge, or Heat Conduction II

Time: Thursday 10:15–13:00 Location: SCH/A216

MM 31.1 Thu 10:15 SCH/A216

Thermal Transport through Benzene-1,3,5-Trisamide Fibers — •Eberhard Lukas Flöter and Fabian Pauly — Universität Augsburg, Augsburg, Germany

Benzene-1,3,5-trisamides (BTAs) are a group of chiral and polar molecules which consist of a benzene ring, three amide groups and various side groups. Hydrogen bonding between the amide groups lets the BTAs assemble to columns. These columns pack into hexagonal structures, forming fibers. Since BTAs are chiral and polar, there are multiple configurations that these structures can take. We use nonequilibrium molecular dynamics (NEMD) methods and force fields to model thermal transport through BTA fibers in various configurations. In the presentation we discuss how thermal transport depends on side groups, molecular stacking and defects.

MM 31.2 Thu 10:30 SCH/A216

Phonon Interference in Single-Molecule Junctions — Sai C. Yelishala[1], Yunxuan Zhu[1], •Pablo M. Martinez[2,3], Hongxuan Chen[4], Mohammad Habibi[1], Giacomo Prampolini[5], Juan Carlos Cuevas[3,6], Wei Zhang[4], Guilherme Vilhena[2], and Longji Cui[1,7] — [1]Paul M. Rady Department of Mechanical Engineering, University of Colorado Boulder, USA — [2]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain. — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain. — [4]Department of Chemistry, University of Colorado Boulder, USA — [5]Istituto di Chimica dei Composti Organo Metallici (ICCOM-CNR), Italy. — [6]Condensed Matter Physics Center (IFIMAC), Spain — [7]Materials Science and Engineering Program and Center for Experiments on Quantum Materials, University of Colorado Boulder, USA.

Wave interference opens a new route to control transport properties and has been widely studied in electronic and photonic materials. However, interference of phonons, which govern thermal transport in insulators, has been poorly characterized due to experimental challenges. We report the observation of phonon interference at room temperature in molecular-scale junctions. This is enabled by custom-developed scanning thermal probes which can track heat flowing through a single molecular junction at a time. Using isomers of oligo(phenylene ethynylene)3 with either para- or meta-connected centre rings, we reveal a 40% reduction in thermal conductance for the latter. Quantum-mechanically accurate simulations show this difference arises from the destructive interference of phonons through the molecular backbone.

MM 31.3 Thu 10:45 SCH/A216

Phunky.jl - A Multithreaded Phonon Spectral Function Calculator In Julia — •William L. Wenig and Nakib H. Protik — Humboldt-Universität zu Berlin, Berlin, Germany

The ability to compute the phonon properties of materials is crucial for the understanding of physical phenomena such as transport and spectroscopy. At present, several code packages exist that allow ab initio access to phonon computations. These codes are mostly written in traditional languages such as Python, Fortran, or C++. In this talk we present Phunky.jl, a new tool for computing the harmonic and anharmonic phonon properties of materials. The tool is written in Julia, a language that has been designed specifically for scientific computation. It allows researchers to write software at a high level of abstraction, while generating code that runs at speeds faster or comparable to that of more traditional languages in this domain. Phunky.jl is written in an extensible manner so that one can easily expand and interface it with phonon transport solvers. We will highlight the capabilities of Phunky.jl by calculating the phonon spectral quantities for a selection of materials.

MM 31.4 Thu 11:00 SCH/A216

Understanding How Pressure Enhances Heat Transport in Organic Semiconductors — •Lukas Legenstein[1,2], Sandro Wieser[1,3], Michele Simoncelli[4], and Egbert Zojer[1] — [1]Graz University of Technology, Austria — [2]Montanuniversität Leoben, Austria — [3]TU Vienna, Austria — [4]Columbia University, USA

Understanding how lattice thermal conductivity changes under pressure is increasingly important in materials science, yet difficult to predict because materials exhibit a variety of behaviors, ranging from monotonic increases or decreases to anomalous trends. Molecular crystals, including organic semiconductors, stand out for exhibiting unusually large pressure-induced increases relative to their (ultra-)low thermal conductivities.

Our test system, naphthalene, crystallizes in a herringbone stack, a packing motif common in most π-conjugated organic semiconductors. Measurements up to 2 GPa from previous literature show an isotropic thermal conductivity that is up to four times higher than at ambient conditions. By combining highly accurate machine-learned potentials with the Wigner transport equation, we not only reproduce these findings but also elucidate how compression affects naphthalene's anisotropic thermal conductivity and how phonon tunneling becomes less relevant with increasing pressure. Finally, we trace the pressure-induced enhancement to frequency upshifts and the associated modifications in phonon scattering.

MM 31.5 Thu 11:15 SCH/A216

Building Trust in Ab Initio Machine-Learning Potentials for Extreme Materials – Applications to Strongly Anharmonic Ceramics and Thermal Insulators — •Shuo Zhao[1], Kisung Kang[1,2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at FHI, Max Planck Society — [2]School of Materials Science and Engineering, Chonnam National University

Thermal insulating ceramics and semiconductors often exhibit significant anharmonicity, particularly associated with rare events such as Frenkel defect creation and rattling phonon modes. These phenomena not only disrupt the phonon picture and the conventional perturbative methods for heat transport, but also pose challenges for the effective and trustful training of machine-learned interatomic potentials (MLIPs). Our contribution describes the implementation of a framework that combines the non-perturbative Green-Kubo formalism with a sequential, uncertainty guided active learning scheme using `AlmoMD`[1] with equivariant neural networks `NequIP`[2] and `So3krates`[3]. The approach is demonstrated by application to possibly ultra-low thermal conductivity materials[4]. Our results not only substantiate reliable predictions of thermal conductivity for strongly anharmonic systems but also pave the way for the accelerated exploration and design of novel thermal insulators.

[1] K. Kang, *et al.*, *Phys. Rev. Mater.* **9**, 063801 (2025). [2] S. Batzner, *et al.*, *Nat. Commun.* **13**, 2453 (2022). [3] J.T. Frank, *et al.*, *Nat. Commun.* **15**, 6539 (2024). [4] T.A.R. Purcell, *et al.*, *Npj Comput. Mater.* **9**, 112 (2023).

15 min. break

MM 31.6 Thu 11:45 SCH/A216

Probing Lattice Anharmonicity and Thermal Transport in Ultralow-κ Materials Using Machine Learning Interatomic Potentials — •Soham Mandal[1], Ashutosh Srivastava[2], Tanmoy Das[1], Abhishek Singh[2], and Prabal Maiti[1] — [1]Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India — [2]Materials Research Centre, Indian Institute of Science, Bangalore 560012, India

Crystalline solids with ultralow lattice thermal conductivity (κ) are promising candidates for thermoelectric and thermal-barrier applications, yet understanding heat transport in such strongly anharmonic systems remains challenging. Perturbative frameworks such as the Boltzmann transport equation (BTE) are unreliable when anharmonicity is large and higher-order phonon scattering cannot feasibly be computed. Here, we develop machine-learning interatomic potentials (MLIPs) to study heat transport in TlAgSe and $Cs_2PbI_2Cl_2$ and compare three transport formalisms: Green-Kubo (GK), BTE, and the Wigner transport equation (WTE). BTE underestimates κ, while WTE improves agreement but slightly overpredicts due to neglected higher-order scattering. The non-perturbative GK framework captures full anharmonicity and closely matches the experimental κ value. Phonon scattering rates exceeding the Ioffe-Regel limit and the degree of anharmonicity $\sigma^A > 0.5$ confirm the strongly anharmonic nature of both materials. This MLIP-integrated framework advances predictive understanding of ultralow-κ heat transport and supports future materials design.

MM 31.7 Thu 12:00 SCH/A216

Current-voltage curves of transformer oils: Analytical and numerical results — •Markus Bier — Technische Hochschule Würzburg-Schweinfurt, Schweinfurt, Germany

High-voltage transformers contain oil, which should allow for convective heat transport while sustaining electrical insulation. These oils are complex fluids composed of various molecular and colloidal species which, over time, give rise to the formation of charged entities due to numerous, by now not entirely known and fully understood mechanisms. A widely used technique to diagnose transformer oils are current-voltage curves, which can exhibit remarkable and non-trivial transient features upon polarisation of a relaxed oil or repolarisation of an electrically stressed oil. Theoretical modelling provides a bottom-up approach to link current-voltage curves to the underlying charge transport processes. The present contribution reports on analytical and numerical results obtained within theoretical investigations of reaction-drift-diffusion models based on Poisson-Nernst-Planck (PNP) theory. After presenting an analytical solution of the PNP equations for a semi-infinite system in the non-equilibrium steady state as well as analytical cross-over boundaries between different repolarisation regimes, the main features of numerical transient current-voltage curves for polarisation and repolarisation are discussed.

Reference: M. Bier, ”Non-equilibrium steady states of electrolyte interfaces”, New J. Phys. 26, 013008 (2024).

MM 31.8 Thu 12:15 SCH/A216

Interband effects in the matrix Boltzmann transport equation — •Elena Trukhan and Nakib H. Protik — Department of Physics and CSMB, Humboldt University of Berlin

The current state-of-the-art ab initio method for computing electronic transport properties relies on the Boltzmann transport equation (BTE). However, the BTE fails to capture certain quantum effects, most notably interband coherence. To address this limitation for phonon transport, Simoncelli et al [1]. developed an approach based on the Wigner transport equation, which incorporates these effects by including the off-diagonal terms of the density matrix. This framework was later adapted to electrons by Cepellotti and Kozinsky [2]. Their method, however, involves several critical simplifications; for instance, it ignores kinetic corrections and treats the collision integral within a relaxation time approximation (RTA). Also, modern derivations rely on the assumption of a band-diagonal form of the interaction self-energies, which might not hold generally. In this work, we derive a more general electronic transport equation from a Green’s function formalism. Using a modified Kadanoff-Baym Ansatz, we carefully track the terms that survive various standard approximations in the Dyson equations in the band representation, explicitly include electron-impurity and electron-phonon interactions, keeping self-energy in non-diagonal form and present a framework that captures interband coherence while moving beyond the RTA.

[1] M. Simoncelli, et al., Phys. Rev. X 12, 041011 (2022) [2] A. Cepellotti and B. Kozinsky, Mater. Today Phys. 19, 100412 (2021)

MM 31.9 Thu 12:30 SCH/A216

Coulomb and phonon scattering limited transport in doped systems — •Nakib H. Protik and Dwaipayan Paul — Humboldt-Universität zu Berlin, Berlin, Germany

In this talk we present an extension of the elphbolt [1] transport code package that includes the Coulomb interactions among the charge carriers. We perform ab initio calculations to study the effect of these interactions on the transport properties of doped systems over a range of temperatures. Specifically, we probe the charge carrier hydrodynamics in these systems and identify the relative roles of the Coulomb and phonon scattering in the realization these transport regimes. We provide a comparison with recent measurements and comment on the violation of the Wiedemann-Franz law.

[1] N. H. Protik, C. Li, M. Pruneda, D. Broido, and P. Ordejón, The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations, npj Computational Materials 8, 28 (2022).

MM 31.10 Thu 12:45 SCH/A216

Stoichiometric Locking in the High State of Charge in Solid Ion Conductors: A Kinetic Monte Carlo Study — •Roya Ebrahimi Viand, Chiara Panosetti, Christoph Scheurer, Karsten Reuter, and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin

The advancement of solid-state batteries critically relies on a deep understanding of ion transport in crystalline electrolytes and electrode active materials. We present a kinetic Monte Carlo (kMC) approach with fast update rules for transition propensities that enables efficient simulation of systems with long-range Coulomb interactions. Our study systematically probes the effects of state of charge (SOC), temperature, and applied external electric field on ionic mobility. We observe a pronounced mobility minimum near 100% SOC, where ions freeze in a low-energy Coulomb superlattice configuration that persists even under applied electric fields. Deviations from stoichiometry dramatically enhance transport by introducing defect pathways, with nearly symmetric behavior for ion and vacancy diffusion. By decomposing the state of charge into a reference and an excess carrier concentration (ΔSOC), we find that the intrinsic mobility per excess carrier remains approximately constant across different SOC values, revealing that transport is fundamentally mediated by the ΔSOC disrupting the reference structure. Analysis of effective activation energies across different SOC values reveals behavior consistent with percolation-controlled transport, where the availability of defect-mediated pathways strongly influences the energy landscape for ion diffusion.

MM 32: Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom I

Time: Thursday 10:15–12:45 Location: SCH/A251

Topical Talk MM 32.1 Thu 10:15 SCH/A251

High-Throughput Nanomechanics and Data-Driven Workflows for Mapping Composition-Microstructure-Property Landscapes — •Ruth Schwaiger — Forschungszentrum Juelich, Institute of Energy Materials and Devices, IMD-1: Structure and Function of Materials, Juelich, Germany

Combinatorial and high-throughput (CHT) methods are enabling nanoscale mechanical studies that span broad compositional and microstructural spaces with unprecedented efficiency. This talk presents an integrated perspective on how automated nanoindentation, combinatorial thin-film libraries, and machine-learning analysis jointly accelerate the discovery of composition-microstructure-property relationships.

Combinatorial thin-film libraries provide dense, continuous coverage across multicomponent compositions, enabling systematic mapping of phase formation, defect structures, and mechanical response. For example, CHT workflows applied to Ni-Al coatings captured structural transitions and hardness trends across the phase diagram, enabling development of a mechanistic hardness model that integrates grain-size, solid-solution, and phase-fraction strengthening. To extract intrinsic material properties from such heterogeneous datasets, data-driven analysis methods, ranging from physics-informed regression to unsupervised clustering, allow the identification of mechanically distinct regions, quantification of data sufficiency, and robust separation of compositional, microstructural, and defect-driven effects.

MM 32.2 Thu 10:45 SCH/A251

Reliability of Interatomic Potentials for Surface- and Size-Dependent Mechanical Behavior — •Sriram Anand, Jan Janssen, Jörg Neugebauer, and Erik Bitzek — Computational Materials Design, Max-Planck-Institute for Sustainable Materials, Düsseldorf

Material properties at the nanoscale differ markedly from the bulk, largely due to the increased surface-to-volume ratio. Surface stresses in particular are thought to modify the elastic response and contribute to the anomalous mechanical behavior of nanoobjects. These effects are typically investigated using atomistic simulations; however, the interatomic potentials used in such studies are generally not fitted to surface stresses. As a consequence, both the quantitative values (e.g., Young's modulus) and, to a lesser extent, the deformation mechanism of nanoobjects obtained from simulations may deviate from physical reality.

Here, we present a systematic study of surface stresses, nonlinear elasticity, and stacking-fault energies in FCC metals as predicted by a broad set of classical and machine-learning interatomic potentials. Using first-principles data as reference, we compile a benchmark database of these key quantities and demonstrate - through tensile deformation of nanowires - how the choice of potential can markedly influence simulated mechanical properties and deformation behavior. Our benchmark of surface stresses, higher-order elastic constants, and fault energies provides a robust foundation for the accurate design of reliable next-generation nanoelectromechanical devices.

Topical Talk MM 32.3 Thu 11:00 SCH/A251

Expanding nanoindentation capabilities: Data-driven and novel experimental approaches — •Michael Wurmshuber[1], Matthias Glosemeyer[1], Pouya Hassanzadeh Sarhangi[1], Verena Maier-Kiener[2], Heinz Werner Höppel[1], and Matthias Göken[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Montanuniversität Leoben, Leoben, Austria

As material discovery and manufacturing accelerate through artificial intelligence and additive manufacturing, high-throughput materials characterization is essential to ensure fast-paced material development. Here, nanoindentation with its capability to measure small material volumes and individual microstructural constituents in a quick manner, has the edge over classical slow-paced mechanical testing. Since Oliver and Pharr's groundbreaking work, nanoindentation has developed to extract not only hardness and modulus but numerous other mechanical properties through specialized indentation protocols. This talk presents two approaches to further extend the information space we receive from nanoindentation. First, we introduce a novel spherical indentation technique enabling local mapping of inelastic backstrain via loading-unloading-reloading experiments, allowing for the mapping of underlying geometrically necessary dislocation networks. Second, we demonstrate how artificial neural networks and ensemble methods can accelerate flow curve characterization from standard Berkovich nanoindentation. Together, these advances demonstrate how data-driven and experimental innovations can significantly expand the information accessible from nanoindentation measurements.

15 min. break

Topical Talk MM 32.4 Thu 11:45 SCH/A251

Additive Manufacturing and Nanomechanics - where is the Link? — •Ralph Spolenak — Laboratory for Nanometallurgy, Department of Materials, ETH Zurich, Switzerland

While size effects in mechanical properties of metals created by whisker growth and thin films had been known since the 1950s, the introduction of micro- and nanoscale subtractive manufacturing (also known as focused ion beam milling) became a game changer as it allowed to study size effects practically independent of the material and its microstructure. The contribution will focus on additive micro- and nanoscale manufacturing with voxel sizes down to 30 nm and how both the manufacturing process (with regards to microstructure control and chemistry) as well as the dimension influences mechanical properties. Comparison will be made to sputter deposited materials including self-organized microstructure, such as nanoporosity by dealloying or local pore formation by Kirkendall voiding, as well as nanostructured reactive multilayers. Finally, the potential combination of subtractive and additive processes will be discussed.

MM 32.5 Thu 12:15 SCH/A251

Mechanical Behaviour of Nafion Membranes — •Mateja Jovanović[1,2,3], Matthias Baldofski[2], Nicolas Bernhard[2], Marcin Rybicki[2,4], Miljan Dašić[3], and Igor Stanković[3,5] — [1]Institute of Technical Sciences of the SASA, K. Mihailova 35/IV, 11000 Belgrade, Serbia — [2]Freudenberg Technology Innovation SE&Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany — [3]Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia — [4]Freudenberg e-Power Systems GmbH, Bayerwaldstrasse 3, 81737 München, Germany — [5]Departamento de Ingeneria Mecanica, Universidad Tecnica Federico Santa Maria, Av. Espana 1680, Valparaiso, Chile

Proton Exchange Membrane Fuel Cells (PEMFCs) utilise polymer membranes like Nafion, valued for their proton conductivity and mechanical integrity. In this work, we examine the stress-strain response of Nafion membranes, focusing on how hydration, crystallinity, and temperature modulate mechanical behavior, using molecular dynamics simulations. Here, we demonstrate that membrane hydration level and structural ordering fundamentally influence mechanical properties under applied stress. Water distribution and polymer chain dynamics are closely connected to the stress-strain response, suggesting that structural organization at the nanoscale is crucial in governing overall mechanical performance across different conditions. By integrating clustering algorithms, structural descriptors, and stress-strain analyses, this study provides a comprehensive view of how membrane architecture and environmental factors govern mechanical performance.

MM 32.6 Thu 12:30 SCH/A251

The Fracture toughness of thin films — •Mathias Göken[1], Benoit Merle[2], and Jun Lou[3] — [1]Department of Materials Science & Engineering I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Materials Science and Engineering, Universität Kassel, Germany — [3]Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, USA

The mechanical properties of thin films play a pivotal role for applications either as freestanding films or as coatings. So far, the understanding of the fracture toughness of very thin films and especially of their thickness dependence is limited. Bulge testing is a very reliable technique for characterizing the mechanical properties of thin films, where a freestanding film is subjected to a controlled pressure from underneath and the deflection of the film is recorded. Bulge tests have shown that the fracture toughness of ductile and soft Au drops down to extremely low values of only 2 MPam1/2 if the film thickness is reduced to 100 nm. On the other hand, single layer graphene has shown a fracture toughness of around 4 MPam1/2. In this paper the thickness dependence of the fracture toughness is discussed based on an old and simple basic fracture mechanics concept derived by Bluhm and Knott in the 1960th. It is shown, that based on this model it is easy to predict the fracture toughness of thin films and their thickness dependence. The results agree surprisingly well with the experimental data on graphene and Au thin films.

MM 33: Invited Talk: Stefan Nolte

Time: Thursday 15:00–15:30 Location: SCH/A251

Invited Talk MM 33.1 Thu 15:00 SCH/A251
LPBF with Ultrashort Laser Pulses - Additive Manufacturing Beyond Current Limits — •Stefan Nolte[1,2], Hagen P. Kohl[1], Lisa Matthäus[1], Tobias Ullsperger[1], Dongmei Liu[1], and Stephanie Lippmann[1] — [1]Friedrich Schiller University Jena, Institute of Applied Physics, Jena, Germany — [2]Fraunhofer Institute for Applied Optics and Precision Engineering IOF, Jena, Germany

Ultrashort-pulse lasers introduce additional degrees of freedom to powder bed fusion through the choice of pulse duration, repetition rate, and pulse energy. The short interaction times enable extremely high local temperatures and highly confined melt pools, with heat accumulation tunable through the pulse repetition rate. This allows precise control over melt dynamics, thermal gradients and cooling rates, which remain largely fixed in continuous-wave systems. A key outcome is accelerated solidification and pronounced grain refinement. The confined melt geometry and reduced heat accumulation suppress segregation, cracking, and vaporization-driven compositional shifts, enabling alloys and microstructures that are difficult to achieve with conventional laser melting. These processing characteristics contribute to improved mechanical uniformity, enhanced phase distribution, and greater design flexibility in alloy development. We will introduce the governing mechanisms of ultrashort-pulse interaction in metal additive manufacturing and highlight their impact through material case studies. Demonstrated benefits include grain refinement in Al-Si, dense and crack-free structures in refractory metals, and reduced vaporization with improved composition control in hypereutectic Al-Li.

MM 34: Hydrogen in Materials I

Time: Thursday 15:45–17:30 Location: SCH/A215

MM 34.1 Thu 15:45 SCH/A215
In-situ mechanical characterization of 316Ti hollow specimens in hydrogen environments - from ambient down to 20 K — •Elvina Gaisina, Simeon Eckerle, Camelia Schulz, Zahra Abbasi, Astrid Pundt, and Klaus-Peter Weiss — Karlsruhe Institute of Technology, Germany

The Application of Liquid Hydrogen (AppLHy) project explores the feasibility of a hybrid pipeline system transporting liquid hydrogen while simultaneously using the cold enables superconducting electrical energy transmission. Developing such a system requires a reliable understanding of material behavior under cryogenic conditions and exposure to hydrogen environments. However, conventional test setups that simulate these conditions are often large, complex, and require extensive safety measures to prevent hydrogen leakage. To provide a safer and more efficient testing method, this study presents an in-situ mechanical testing approach using hollow cylindrical specimens pressurized with gas. Austenitic stainless steel 316Ti, a widely applied cryogenic compatible material, was selected for testing. The hollow specimens were filled with hydrogen or helium at pressures up to 200 bar and subjected to tensile loading at temperatures ranging from ambient down to 20 K. The results show that some hydrogen-induced effects become noticeable primarily after substantial plastic deformation. Significant changes in mechanical properties and fracture behavior are observed only at 200 K.

MM 34.2 Thu 16:00 SCH/A215
In situ Micromechanical Investigation of Hydrogen Embrittlement Mechanisms in Fe3%Si — •Maral Sarebanzadeh[1], Svetlana Korneychuk[1,2], Rolf Rolli[1], Hans-Christian Schneider[1], Astrid Punt[1], Xufei Fang[1], and Christoph kirchlechner[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Insitute of Nanotechnology, Karlsruhe Institute Technology, Karlsruhe, Germany

Hydrogen embrittlement (HE) remains a critical limitation for the reliable use of hydrogen in structural applications. Among the proposed micromechanisms, hydrogen-enhanced localized plasticity (HELP) is widely discussed, suggesting that hydrogen facilitates dislocation motion and localizes deformation. However, its microstructural manifestation remains insufficiently understood and rarely observed directly. To address this, we investigate HE in Fe3%Si using in-situ micropillar compression combined with tritium charging, leveraging the advantage of probing a few dislocations in a well-defined geometry. Micropillar tests conducted before and after charging with a protium/tritium gas mixture show a strong increase in yield strength, indicating pronounced dislocation blocking rather than enhanced glide. We demonstrate that dislocations can lose mobility, with the activating stress increasing by a factor of 2-3. Transmission electron microscopy (TEM) and electron energy loss spectroscopy (EELS) investigations are being performed to identify hydrogen-containing features around dislocations and to clarify how hydrogen governs dislocation mobility in bcc materials such as Fe3%Si.

MM 34.3 Thu 16:15 SCH/A215
Theoretical study of temperature dependencies in HELP- and HEDE-based damage models on the fatigue behavior of ferritic steel by hydrogen — Alexandra Stark[1,2], Petra Sonnweber-Ribic[1], and •Christian Elsässer[2,3] — [1]Robert Bosch GmbH, CR, 71272 Renningen — [2]Fraunhofer IWM, 79108 Freiburg — [3]University of Freiburg, FMF, 79104 Freiburg

In this theoretical study, the influence of temperature dependencies in hydrogen embrittlement (HE) models on the fatigue damage of ferritic steel is investigated by using a coupled hydrogen-diffusion and crystal-plasticity finite-element simulation framework. We focus on the characteristic "bell-shaped" dependence of HE on temperature and examine its effects by means of HE models based on Hydrogen Enhanced Local Plasticity (HELP) and Hydrogen Enhanced Decohesion (HEDE) mechanisms. Hydrogen-induced fatigue damage is monitored by a fatigue indicator parameter (FIP): maximized damage occurs within a narrow temperature range consistent with experimental results reported in literature. Our results arise from an interplay of plastic strain localization and hydrogen trapping, combined with a sufficiently efficient supply of hydrogen. The findings of this study highlight how the interplay of hydrogen diffusivity, trap filling kinetics, and available diffusible hydrogen plays a critical role for the temperature dependence of HE. In addition, the influence of varying trap binding energies is explored, which has a substantial effect on both temperature behavior and induced fatigue damage.

MM 34.4 Thu 16:30 SCH/A215
Atomistically Informed Grain-Boundary Thermodynamics for Phase-Field Modelling of Hydrogen-Driven Microstructural Evolution in Aluminium — •Bharathi Ganesh Ganesan Sekar[1], Ali Tehranchi[1], Tilmann Hickel[1], and Nils Warnken[2] — [1]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — [2]University of Birmingham, Birmingham, United Kingdom

Hydrogen-driven microstructural evolution in polycrystalline aluminium (Al) is strongly influenced by grain-boundary (GB) structure and hydrogen (H) segregation. We aim to develop an atomistically informed phase-field framework to describe these effects, with relevance to hydride formation. Molecular-statics simulations were performed for representative FCC Al symmetric-tilt boundaries $\Sigma5(310)$, $\Sigma5(210)$, and $\Sigma3(111)$ to assess whether H segregation can initiate hydride formation. Instead, H induces defect-mediated structural transitions and shows distinct relaxation pathways during ingress and discharge. At high H content, the GB cleaves and free surfaces form. To generalise these insights, a library of 250 microstates was generated for each GB plane normal within the $\Sigma5$ family by sampling rigid-body translations and boundary-plane atomic fractions. This enables construction of GB energies as a function of plane normal, with temperature dependence introduced through Boltzmann weighting. H effects are included by evaluating segregation energies for the minimum-energy microstate of each plane normal, yielding H-chemical-potential-dependent GB energies. These results provide essential GB energetics for phase-field modelling of H-driven microstructural evolution in Al.

MM 34.5 Thu 16:45 SCH/A215

Understanding of hydrogenation induced planar defects in a proton-based battery material — •Yujun Zhao, Stefan Zaefferer, Yug Joshi, and Dierk Raabe — Max-Planck-Institut für Nachhaltige Materialien, Max-Planck-Straße 1, 40237 Düsseldorf, Deutschland

Research on nickel-metal hydride batteries provides valuable insights for advancing hydrogen storage systems. However, the battery cycle stability is limited by crystalline defects generated during hydrogenation. Therefore, an in-depth understanding of these defects is critical for improving the long-term cyclic performance of electrode materials. In this work, electrochemically charged hydrogen induces the formation of planar defects and dislocation bands in LaNi5 intermetallic compound. The correlations among crystallographic orientations, defect characteristics, and local hydrogen concentration were explored by multiscale characterization techniques, including electron backscattered diffraction (EBSD), electron channeling contrast imaging (ECCI), transmission electron microscopy (TEM), and atom probe tomography (APT). In particular, the atom probe evaporation behavior of LaNi5 along different orientations are revealed, clarifying the local magnification effect and the loss of spatial resolution. The influences of the planar defects on the evaporation behaviors of metallic elements and hydrogen atoms are also discussed.

MM 34.6 Thu 17:00 SCH/A215

Hydrogen Solution Energies at Microstructural Defects in Ferritic Steels — •Onur Can Şen[1,2,3], Santiago Benito[2], Sebastian Weber[2], and Rebecca Janisch[3] — [1]Max Planck Institute for Sustainable Materials, Germany — [2]Institute for Materials, Chair of Materials Technology, Ruhr-University Bochum, Germany — [3]ICAMS, Ruhr-University Bochum, Germany

Hydrogen is essential for sustainable industries but can also cause severe degradation through hydrogen embrittlement (HE). Trapping H at microstructural defects helps mitigate HE, though its efficiency depends on how each defect affects H solution energy.

This study combines experiments and DFT calculations to examine how microstructural defects in ferritic steels influence H trapping, focusing on different grain boundary (GB) types with and without segregants.

DFT was used to calculate solution energies at several special GBs in ferrite, both clean and with alloying elements (Cr, Cu, Ti) or vacancies, and these energies were linked to structural and electronic GB parameters.

Ferritic model alloys with varied compositions were produced and characterised. By optimizing processing, we increased the fraction of special GBs in the microstructure (Şen et al., JMRT (2025)).

The calculated solution energies serve as input for Oriani's model to predict thermal desorption spectra of these alloys.

Overall, this work shows how combining simulations and experiments clarifies the role of microstructural heterogeneities in HE.

MM 34.7 Thu 17:15 SCH/A215

Investigation of phase stability and defects in FeTi for H2 storage application — •Shankha Nag[1], Ali Tehranchi[1], Ruben Bueno Villoro[2], Christian Liebscher[2], Yuanyuan Shang[3], Claudio Pistidda[3], and Tilmann Hickel[1] — [1]Bundesanstalt für Materialforschung und -Prüfung, Berlin, Germany — [2]Fakultät für Physik und Astronomie, Ruhr Universität Bochum, Bochum, Germany — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany

Safe, durable, and efficient storage remains a central hurdle in hydrogen economy, where metal hydrides offer a promising route, particularly for stationary applications. Among these materials, FeTi stands out as a cost-effective system capable of reversible hydrogen uptake and release under near-ambient conditions. As part of BMBF-funded collaborative project GreenH2Metals, we performed atomistic simulations aimed at elucidating experimentally observed microstructural transformations such as formation of secondary phases and hydrides. We analyzed the thermodynamic stability of competing phases using ab initio calculations and examined chemical segregation as well as heterogeneous precipitation at dislocations and planar defects. Defect phase diagrams, along with the roles of vacancies and antisite defects in bulk diffusion, are explored in detail. The impact of various tramp elements on these processes is assessed through high-throughput calculations enabled by workflow frameworks such as pyiron. Together, these computational insights support a data-driven alloy design strategy for optimizing FeTi-based materials for sustainable hydrogen storage.

MM 35: Additive Manufacturing / Transport in Materials III

Time: Thursday 15:45–17:30 Location: SCH/A216

MM 35.1 Thu 15:45 SCH/A216

Tailoring Microstructure and Mechanical Properties of LPBF Ti-5553 Alloy by STA Heat Treatment — •Yang Lei[1,2], Parthiban Ramasamy[2], and Jürgen Eckert[1,2] — [1]Department of Materials Science, Chair of Materials Physics, Montanuniversität Leoben, Jahnstraße 12, A-8700 Leoben, Austria — [2]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, A-8700 Leoben, Austria

Ti-5553 is a metastable β titanium alloy widely used in aerospace gears due to its exceptional strength, toughness, and hardenability. However, Laser Powder Bed Fusion (LPBF) fabrication introduces significant limitations, particularly strong anisotropy and persistent columnar grains.

Solution Treatment and Aging (STA) offers a critical pathway to tailor these properties. This study investigates the microstructural evolution during STA, revealing a competition between nucleation driving force and diffusion kinetics that dictates the initial α-phase morphology. Notably, the columnar β grain size was restricted after heat treatment due to Zener pinning effect exerted by α precipitates, which impedes boundary migration and suppresses recrystallization.

Consequently, the specific microstructural features formed during solution treatment significantly influence subsequent aging behavior. Since β-grain refinement is inhibited, the enhancement in tensile strength is attributed primarily to Orowan strengthening via dispersed precipitates rather than Hall-Petch strengthening.

MM 35.2 Thu 16:00 SCH/A216

Electron Microscopy Investigation of AM316L before and after Heat Treatment: Implications for Hydrogen Diffusion — •Gabriele Palazzo[1,2,3], Kai Stefan Lagemann[1], Svetlana Korneychuk[1,2,3], Stefan Wagner[1], Christian Kübel[2,3], and Astrid Pundt[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Karlsruhe Nano Micro Facility, Karlsruhe, Germany

As hydrogen technologies evolve, understanding local hydrogen-metal interactions in structural alloys becomes critical. High-pressure hydrogen storage requires materials resistant to hydrogen embrittlement (HE). Austenitic stainless steels are promising, and selective laser melting (SLM) enables attractive properties but can reduce resistance to hydrogen environmental embrittlement (HEE). We investigate additively manufactured 316L (AM316L) steel and its interaction with dissolved hydrogen, focusing on microstructure evolution under directed heat treatments. SEM and (S)TEM with STEM-EELS/EDX map elemental distributions, while EBSD and STEM-ACOM resolve grain structure and sub-grain dislocation cells (SDC). Comparing as-

built and heat-treated states by ex-situ TEM and hydrogen diffusion measurements, we show that heat treatment alters the microstructure, reduces hydrogen diffusivity, and lowers HEE susceptibility [1].
[1] Kai Stefan Lagemann, Gabriele Palazzo, Tim Lucas Haag, Svetlana Korneychuk, Stefan Wagner, Christian Kübel, and Astrid Pundt. Manuscript submitted. 2026.

MM 35.3 Thu 16:15 SCH/A216

Diffusion processes in magnetron sputtered copper-gold thin films: layer design, argon pressure tuning and Kirkendall effect — •Oliver Wipf and Ralph Spolenak — Departement of Materials, ETH Zürich, Vladimir-Prelog-Weg 1-5/10, 8093 Zürich, Switzerland

Controlled Kirkendall voiding is a promising diffusion process to fabricate hollow nano- and micro-structures. This work extends the understanding and use of the Kirkendall effect as a route to fabricate voids in magnetron sputtered copper-gold thin films, a process with a high degree of control over the deposited thin films and a pathway to scalable, novel applications of diffusion self-organized thin film technology. To study the diffusion in the thin films, double and triple layered samples were fabricated using low and high argon gas pressures during the deposition. Annealing of the samples resulted in large voids located at the wafer to film interface and in the center of the film, depending on the layer structure. Using a comprehensive diffusion study, we demonstrate that diffusion in copper-gold thin film diffusion couples is dominated by vacancies moving, which leads to the growth of Kirkendall voids.

MM 35.4 Thu 16:30 SCH/A216

Visualizing lithium dynamics in battery electrodes by operando optical microscopy — •Monica Mead[1], Shihao Wei[1], Vidula Ambure[1], Nadine Kerner[1], Roham Talei[1], Yug Joshi[2], and Guido Schmitz[1] — [1]Max Planck-Institut für nachhaltige Materialien GmbH, Max-Planck-Straße 1, 40237 Düsseldorf — [2]Universität Stuttgart, Heisenbergstraße 3, 70569 Stuttgart

Typically, chemical diffusion coefficients of Li-ions in battery electrodes are measured by purely electrochemical methods such as potentiostatic or galvanostatic intermittent titration technique (GITT/PITT), cyclic voltammetry (CV) or electrochemical impedance spectroscopy (EIS). Surprisingly, the correspondingly determined diffusion coefficients vary within up to ten orders of magnitude. This cannot be explained solely by the influence of concentration dependence and microstructure. To clarify the origin and thereby understand which additional factors influence the ion transport, alternative methods have to be developed and applied. Therefore, we apply a method based on optical microscopy and the optical response upon Li intercalation in different Li-ion battery electrodes, such as lithium manganese oxide, lithium titanate, vanadium oxide and silicon. With this method, the transport along several hundreds of micrometres can be measured, which allows differentiation between different transport mechanisms (diffusion/transport across a kinetic barrier). We find that above-mentioned electrochemical methods tend to underestimate the diffusion coefficient. We discuss the origin with respect to the transport mechanism.

MM 35.5 Thu 16:45 SCH/A216

Kinetic analysis of lithium transport in silicon anode using operando optical microscopy — •Shihao Wei[1], Monica Mead[1], Yug Joshi[2], and Guido Schmitz[1] — [1]Heisenbergstraße 3, 70569, Stuttgart, Germany — [2]Max-Planck-Straße 1, 40237, Düsseldorf, Germany

Understanding lithium diffusion and phase transformation in silicon(Si) anodes is essential for the advancement of high-capacity lithium(Li)-ion batteries. In this work, Li transport behavior and phase evolution are investigated using an in-situ optical method, which enables direct visualization of phase movement and measure Li migration across phase boundaries, advantages not offered by conventional techniques, such as EIS, SIMS, and NMR. First, it is observed that the lithiation process on a semi-infinite plane is predominantly governed by diffusion-controlled parabolic growth, with minimal evidence of interface-controlled linear growth. The temperature dependence of transport is explored, quantified with an Arrhenius-like model, revealing the activation energy of diffusion and interfacial reaction. In contrast, delithiation exhibits markedly sluggish kinetics and behaves fundamentally differently. To investigate this behavior, smaller circular geometries with limited diffusion depth creating a 2D transport scenario are examined. In these confined structures, lithiation is demonstrated by a Deal-Grove-type model. Remarkably, during delithiation, instead of a distinct moving interface, the lithiated phase gradually fades as lithium ions leave. Such a difference implies that lithiation and delithiation follow distinct reaction pathways.

MM 35.6 Thu 17:00 SCH/A216

W diffusion in Mo-Ta alloys: temperature dependence and vacancy energetics — •Aditya Burla[1], Xiang Xu[2], Felix Kipke[1], Hartmut Bracht[1], Xi Zhang[2], Blazej Grabowski[2], Gerhard Wilde[1], and Sergiy V Divinski[1] — [1]Institut für Materialphysik, Universität Münster, 48149 Münster, Germany — [2]Institut für Materialwissenschaft, Universität Stuttgart, 70569 Stuttgart, Germany

Refractory metals and their alloys have gained renewed attention with the emergence of high-entropy alloy concepts, driven by their exceptional properties at elevated temperatures. However, despite their technological significance, diffusion data for refractory binary systems remain sparse, limiting predictive understanding of defect-mediated transport at high temperatures. This study addresses this gap by investigating tungsten diffusion in the binary Mo-Ta system. Diffusion profiles were measured using secondary ion mass spectrometry after annealing in the temperature range of 1373K to 2273K. A key focus is on correlating the diffusion behavior with the vacancy formation energies. Complementary computational analysis provides atomistic insights, revealing composition-dependent variations in vacancy energetics within the Mo-Ta system. Its influence on W diffusivity and activation energies is discussed. This combined approach provides a comprehensive framework for understanding W diffusion and vacancy-controlled transport in Mo-Ta alloys, offering valuable guidance for the design of advanced refractory materials.

MM 35.7 Thu 17:15 SCH/A216

Hydrogen Diffusion in ß-MoO$_3$ Thin Films Governed by Structural Changes — •Tim K. Hecker, Martin Becker, and Peter J. Klar — Institute of Experimental Physics I and Center for Materials Research, Justus Liebig University Giessen, Giessen, Germany

Hydrogen incorporation strongly alters the electronic, optical and structural properties of transition-metal oxides. In MoO$_3$, hydrogen intercalation forms H$_x$MoO$_3$ bronzes that exhibit reversible color changes, lattice distortions and notably higher hydrogen diffusion coefficients. Although these effects are central to electrochromic, catalytic, sensing and energy storage applications, the mechanisms of hydrogen transport remain poorly understood, especially in the metastable ß-phase. To address this, we performed electrochemical hydrogen insertion into ß-MoO$_3$ thin films covered by a PMMA layer, only allowing incorporation in a small, well-defined uncovered stripe. Hydrogen only enters through this gap and then diffuses laterally beneath the PMMA in a semi-infinite space. Using the electrochromic response of MoO$_3$ in combination with the Beer-Lambert law, we monitored the hydrogen concentration in-situ. These diffusion profiles were then analyzed with a deep-learning algorithm to extract concentration dependent diffusion coefficients. We identify two distinct increases in the diffusion coefficient as hydrogen concentration rises. Complementary Raman measurements during intercalation and deintercalation link these changes to partial structural transformations, each increasing the hydrogen diffusion coefficient by nearly one order of magnitude.

MM 36: Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom II

Time: Thursday 15:45–17:15 Location: SCH/A251

Topical Talk MM 36.1 Thu 15:45 SCH/A251

High-temperature micropillar compression for understanding dislocation-precipitates interactions in Ni-Based superalloys — •Subin Lee[1], Sangwon Lee[2], Pyuck-Pa Choi[2], and Christoph Kirchlechner[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea

The mechanical role of plate-like μ phases, topologically close-packed (TCP) precipitates, in Ni-based single-crystal superalloys was investigated using bulk and in situ SEM micropillar compression, supported by electron microscopy and APT. The μ phase showed strong temperature-dependent behavior: it remained rigid at room temperature, enforcing single-slip deformation, but became more compliant at 500 °C through bending and non-basal shearing.

Although acting as local obstacles to slip, μ phases consistently lowered the CRSS of micropillars. This softening resulted from deformation within the μ phase and from microstructural changes in the surrounding γ/γ' matrix. APT revealed Ta enrichment at the μ/γ' interface, enhancing γ' strengthening, while elastic mismatch shifted slip traces away from the interface by tens of nanometers.

Overall, these results highlight the dual role of μ phases. This integrated understanding of μ-phase deformation, interfacial chemistry, and matrix softening provides a fundamental mechanistic understanding for how TCP precipitation shapes the high-temperature mechanical behavior of Ni-based superalloys.

MM 36.2 Thu 16:15 SCH/A251

Nanomechanics of Silicon: Linking Phase Transitions to High-Temperature Plasticity — •Verena Maier-Kiener and Gerald Schaffar — Montanuniversität Leoben, Department materials Science, Leoben, Austria

This presentation focuses on phase transformations in silicon revealed through high-resolution nanoindentation techniques and their interplay with high-temperature deformation behavior. Using a novel unloading contact pressure approach with continuous stiffness measurement (CSM), pressure-induced phase transitions during indentation are investigated with improved precision. The method enables direct calculation of mean contact pressure during unloading and reveals the influence of load-holding segments on transformation onset, aligning well with high-pressure literature data, and was confirmed by Raman spectroscopy. To contextualize these findings, complementary high-temperature nanoindentation studies are discussed. In monocrystalline (100) silicon, a transition from phase transformation to dislocation-controlled plasticity occurs between 300°C and 400°C, with further changes above 800°C. Additionally, spherical nanoindentation on a 1.2μm silicon film at 500°C and 700°C extracts stress-strain behavior, confirming thermally activated dislocation glide. Together, these results provide a comprehensive view of silicon's mechanical response, bridging nanoscale phase transformation analysis with bulk high-temperature deformation mechanisms.

MM 36.3 Thu 16:30 SCH/A251

In situ TEM nanomechanics of neutron-irradiated nanocrystalline carbides and the role of amorphous shells in local mechanical response — •Elchin Huseynov — Institute of Radiation Problems of Ministry of Science and Education, 9 B.Vahabzade, Baku AZ 1143, Azerbaijan

Predicting the mechanical reliability of neutron-exposed ceramics remains challenging because classical micromechanical tests average over complex, irradiation-induced defect structures at the nanoscale. In particular, nanocrystalline carbides develop near-surface amorphous layers and defect-rich shells whose role in governing deformation and failure is still poorly quantified. This work introduces an in situ TEM-based nanomechanical workflow for neutron-irradiated nanocrystalline 3C-SiC. Reactor-irradiated nanoparticles at graded fluences serve as a model for plasma-facing and core structural ceramics. Ex situ HRTEM/SAED reveals pronounced agglomeration and a continuous amorphous shell up to 5 nm thick encasing a crystalline core. Building on this microstructural baseline, in situ TEM traction and gentle indentation experiments on nanoparticle films and micro-sized volumes are used to track shell stability and defect evolution under load via ring broadening, lattice-fringe de-coherence and defect coalescence at the shell/core interface. The results reveal a critical amorphous-shell thickness above which deformation concentrates in the disordered layer and promotes early crack initiation, whereas thinner or discontinuous shells favour more homogeneous load transfer across the crystalline core.

MM 36.4 Thu 16:45 SCH/A251

Mechanical Properties of Irradiated Zircaloy Cladding and Their Impact on Structural Integrity During Dry Interim Storage — •Tzu Yen Lin[1], Michel Herm[1], Volker Metz[1], Maria Vrellou[2], and Christoph Kirchlechner[2] — [1]Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal, P. O. Box 3640, 76021 Karlsruhe, Germany — [2]Karlsruhe Institute of Technology, Institute for Applied Materials, P. O. Box 3640, 76021 Karlsruhe, Germany

In Germany, spent nuclear fuel is planned for disposal in a deep geological repository after 2050. The SNF assemblies are stored in dual-purpose casks, while delays in repository commissioning may extend storage beyond licensed periods. Evaluating the safety of Zircaloy-4 cladding during extended dry storage requires assessing the effects of irradiation damage, hydride formation, and microstructural evolution. This work aims to establish a reliable micromechanical testing methodology for irradiated Zircaloy-4. As a precursor to irradiated samples, Electron Backscatter Diffraction (EBSD) and nanoindentation were performed on non-irradiated cladding in hydrogenated and non-hydrogenated states. EBSD revealed variations in grain size, texture, anisotropy, and dislocation density from manufacturing processes, with further increases from hydrides. Nanoindentation showed higher hardness and reduced modulus in hydride regions compared with the α-Zr matrix. Occasional pop-ins in load-displacement curves indicate dislocations or microstructural discontinuities, consistent with misorientation patterns observed in EBSD.

MM 36.5 Thu 17:00 SCH/A251

Experimental evidence and first-principles verification of deformation of basal twist grain boundaries in Ti — •Biaobiao Yang[1,2], Samuel Hémery[3], Wei Shao[1,2], Victoria Tucker[1,4], Michael S. Titus[1,4], Miguel A. Monclús[1], and Javier LLorca[1,2] — [1]IMDEA Materials Institute, C/Eric Kandel 2, Getafe, 28906 - Madrid, Spain — [2]Department of Materials Science, Polytechnic University of Madrid / Universidad Politécnica de Madrid, E.T.S. de Ingenieros de Caminos, 28040 - Madrid, Spain — [3]Institut Pprime, ISAE-ENSMA, Université de Poitiers, CNRS UPR 3346, Téléport 2, 1 avenue Clément Ader, BP 40109, Futuroscope-Chasseneuil Cedex, 86961, France — [4]School of Materials Engineering, Purdue University, 701 West Stadium Ave., West Lafayette, IN 47907, USA

Recent studies show that Basal Twist Grain Boundaries (BTGBs) are important fatigue-crack nucleation sites in Ti alloys. Micropillar compression combined with high-resolution microscopy revealed extremely easy interfacial shear: one basal grain slides over the other at very low critical resolved shear stresses (45-205 MPa), far below those required for common <a> basal slip. To explain this behavior, first-principles calculations were used to determine the grain boundary energies of BTGBs with different twist angles. The results show that variations in twist angle or in-plane translation produce only negligible changes in grain boundary energy, indicating intrinsically low shear resistance. Together, these experimental and computational findings clarify why BTGBs serve as potent crack-nucleation sites in Ti alloys.

MM 37: Development of Calculation Methods I

Time: Thursday 15:45–17:00 Location: SCH/A315

MM 37.1 Thu 15:45 SCH/A315

The two-particle Green's function in the particle-particle channel: A survey of approximations — •Caja Annweiler[1], Lucia Reining[2], and Claudia Draxl[1] — [1]Humboldt Universität Berlin, Berlin, Germany — [2]École Polytechnique, Palaiseau, France

While in general setting up and solving the Bethe-Salpeter equation (BSE) is out of reach for realistic systems, it provides an ideal starting point for constructing approximations. In the particle-hole channel, this has lead to established approaches such as the GW-level approximation to capture excitonic effects. This framework can be extended to the BSE in the particle-particle channel (pp-BSE), obtained by choosing a different time-ordering in the two-particle Green's function. The result is an equation describing the propagation of two particles (either electrons or holes). While formally similar to the ph-BSE, it is a promising alternative for the calculation of the exchange-correlation energy and yields important information for topics such as pair correlations in superconductors. Despite growing interest in the pp-BSE, systematic investigations of approximations remain scarce.

In the present work we consider a variety of approximations to the pp-BSE. For this purpose, exactly solvable model systems of interacting electrons provide valuable insights into the minimal ingredients needed to capture the key physics. We present approximations from many-body perturbation theory (HF, GW, etc.) at the level of the self-energy Σ and interaction vertex Ξ on small Hubbard models, with the aim of advancing our understanding of approximations in the pp-channel.

MM 37.2 Thu 16:00 SCH/A315

Reliable Super-Resolution for Real-Time Electronic Structure Theory — •Alexander Gorfer, Karsten Reuter, and Matthias Kick — Fritz-Haber-Institut der MPG, Berlin

Calculating excited state spectra of large systems is often prohibitively expensive with standard frequency-domain methods such as the Casida equations, the Bethe-Salpeter Equation (BSE), or Equation-of-Motion Coupled Cluster (EOM-CC). Real-time methods provide an alternative, as all modes are excited simultaneously. However, long simulation times are required to resolve narrow spectral features with traditional Fourier signal analysis, significantly limiting system size. Super-resolution methods such as Compressed Sensing promise high-resolution spectra from much shorter signals but assume the spectrum to be sparse, an assumption which breaks down in larger systems where sharp features are embedded in a quasi-continuum of smaller nearby peaks. To overcome this, we combine newly designed highly noise-tolerant super-resolution techniques with physically motivated filtering. Using approximate frequency information, we identify the brightest transitions and extract only these important modes from the time propagation. By doing so, we effectively precondition the problem for super-resolution, reducing the number of required time steps for signal reconstruction to a minimum. We demonstrate our approach on systems containing several hundred heavy atoms, achieving up to 20-fold speedups while maintaining spectral accuracy even for signals dominated by large continua.

MM 37.3 Thu 16:15 SCH/A315

Electron thermalization in TDDFT and Ehrenfest molecular dynamics — •Tobias Zier, Uday Panta, and David A. Strubbe — University of California, Merced, USA

A non-equilibrium electronic state will in general thermalize toward an equilibrium state due to electron-electron interactions as well as interactions with ions. The description of such processes has remained unclear and controversial in time-dependent density functional theory (TDDFT), given that the occupation numbers remain fixed over time and that adiabatic functionals do not include explicit dissipation. Nevertheless in the literature signs of thermalization to a Fermi-Dirac distribution have been found in effective occupations constructed by projection of the time-dependent wavefunctions onto the ground state. Key issues include whether this process is physical or an artefact, connection to the Eigenstate Thermalization Hypothesis, and the dependence on the density of states, external fields, and xc functionals. To shed light on these phenomena, we study explicit time propagation of graphene after ultrafast laser pulses, with the Octopus real-space code, with and without ionic motion in Ehrenfest molecular dynamics. We study oscillations and the approach to an effective Fermi-Dirac distribution as well as decay of off-diagonal density matrix elements. This work has implications for treatment of statistical mechanics in a TDDFT framework and the nature of time-dependence in xc functionals, as well as for practical calculations of light-matter interactions especially for strong fields as in laser fusion experiments leading to warm dense matter and plasmas

MM 37.4 Thu 16:30 SCH/A315

Bulk plasmons in elemental metals — •Claudia Cardoso[1], Dario Leon[2], and Kristian Berland[2] — [1]S3 Centre, Istituto Nanoscienze, CNR, 41125 Modena, Italy — [2]Department of Mechanical Engineering and Technology Management,
Norwegian University of Life Sciences, NO-1432 Ås, Norway

We have developed an effective analytical representation of the main collective excitations of the dielectric response of 26 elemental metals, starting from first principles calculations. Spectral band structures are then constructed , by extending our earlier model based on multipole-Padé approximants (MPA) [1,2] to incorporate both momentum and frequency dependence (MPA(q)). With this representation, we are able to identify plasmonic quasiparticle dispersions exhibiting complex features, including non-parabolic energy and intensity dispersions, discontinuities due to anisotropy, and overlapping effects that lead to band crossings and anti-crossings. We find good agreement with available experimental data. The results for elemental metals and their effective MPA(q) representation establish a reference point that can guide both fundamental studies and practical applications in plasmonics and spectroscopy.

[1] D. A. Leon, C. Cardoso, T. Chiarotti, D. Varsano, Phys. Rev. B 104, 115157 (2021).

[2] D. A. Leon, A. Ferretti, D. Varsano, E. Molinari, and C. Cardoso, Phys. Rev. B 107, 155130 (2023).

MM 37.5 Thu 16:45 SCH/A315

Probing the influence of core-hole and atomic multiplets in the final states on L2,3 edges for high-throughput studies — •Prathibha Chandrashekhar, Felix Sorgenfrei, Patrik Thunström, Olle Eriksson, and Heike C. Herper — Department of Physics and Astronomy, Uppsala University

Core level spectroscopy like X-ray absorption spectroscopy and the corresponding X-ray magnetic circular dichroic signals are powerful tools to study a wide variety of element specific properties in materials. In this work, we use ab initio density functional theory (as implemented in RSPt[1]) with multiplet ligand field theory to simulate the spectra by constructing and solving the single impurity Anderson model. We simulate the $L_{2,3}$ edges of transition metals in Heusler alloys, aiming to explore the suitability of the method for future high throughput studies, we look at $CoFeMnSi$ and Ni_2MnGa as our initial test cases. These alloys have been extensively studied for their fascinating tunable electronic and magnetic properties which find applications in spin resolved conductance devices, magnetocalorics and spintronics. We test the influence of Slater-Condon parameters on the spectra. We show that the final state effects are crucial in observing the fine structure and the branching ratio between the edges. This work is funded by Horizon Europe MSCA Doctoral Network grant n.101073486, EU-SpecLab, funded by European Union. [1] RSPt, Relativistic Spin Polarized Toolkit (2017).

MM 38: Invited Talk: Manja Krüger

Time: Friday 9:30–10:00 Location: SCH/A251

Invited Talk MM 38.1 Fri 9:30 SCH/A251
Alloy design and deformation behaviour of Mo-based silicide materials — •Manja Krueger — Otto-von-Guericke University Magdeburg

Multi-phase refractory metal-based silicide alloys are attractive candidates for high temperature structural applications. The mechanical behaviour and the oxidation response of this type of materials is significantly affected by the microstructural design, i.e. the chemical composition of the solid solution phase, the volume fraction and homogeneous distribution of the solid solution phase and the silicide phases, the grain size and orientation as well as the concentration of dissolved detrimental impurities and impurity phases. Balancing the ambient and high temperature properties requires to tailor the microstructures, which can be realized by the optimization of the chemical composition using additional alloying elements and the modification of alloying concepts with respect to the manufacturing method. However, processing of refractory metals and alloys is quite challenging due to the ultrahigh melting point above 2000°C and their strong tendency to oxidize at intermediate temperatures. This presentation will show the successful processing and tailoring of multi-phase Mo-Si-B alloys by powder metallurgical (PM) routes, directional solidification (DS) processes and laser-based additive manufacturing (AM) techniques. It will be shown that the AM materials are crack-free and the constituents are homogeneously distributed. The microstructure is very fine as can be compared to powder metallurgically processed Mo-Si-B.

MM 39: Hydrogen in Materials II

Time: Friday 10:15–12:45 Location: SCH/A215

MM 39.1 Fri 10:15 SCH/A215
Coulometric and (Magneto-)Optical Methods for Studying Hydrogen Absorption into Metals — •Felix Engelhardt, Karin Leistner, and Markus Gössler — Chemnitz University of Technology, 09107 Chemnitz, Germany

Hydrogen absorption into metals like palladium is a widely studied process with applications in hydrogen sensors, hydrogen storage systems, and recently magneto-ionics[1,2]. A major challenge in this field is to accurately quantify the hydrogen concentration within the metal. Traditionally, complex techniques such as nuclear reaction analysis or neutron scattering are used for this purpose. Alternatively, coulometric and (magneto-)optical methods are possible and offer the advantages of a simpler setup and operation under ambient conditions. We revisit the coulometric quantification of electrochemically absorbed hydrogen in metals and metallic multilayers, as well as the analysis of hydrogen absorption kinetics. Potential- and time-dependent coulometry was performed in a liquid-electrolyte flow cell designed to avoid side reactions. Complementary measurements of (magneto-)optical reflectivity of the metals upon hydrogen absorption were carried out to support findings from electrochemical methods. This presentation highlights common pitfalls in hydrogen absorption analysis and shows that, when these errors are minimized, the coulometry method yields accurate average hydrogen concentrations and reliable kinetic data. These results encourage the use of electrochemical methods in catalysis and hydrogen research. [1]M. Bischoff et al., Adv. Funct. Mater. 2024, 34, 2405323 [2]Huang, M. et al., Nat. Nanotechnol. 2021, 16, 981

MM 39.2 Fri 10:30 SCH/A215
Interfacial kinetics of hydrogen absorption in nanoporous palladium — •Seoyun Sohn[1,2], Nora Brunkhorst[2], Jürgen Markmann[2,1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

Sorption of hydrogen at metal surfaces is a key process controlling energy-conversion reactions, electrocatalysis, and battery operation. To focus on the interfacial sorption step and minimize bulk-transport contributions, we explore nanoporous (np) Pd as a model system, following the charging/discharging kinetics during electrochemical charging or exposure to H_2 gas at controlled partial pressure. Our observations point towards thermally activated transition across an internal barrier–between adsorbed and absorbed H–as the rate limiting step, and they exhibit anomalous kinetics, where absorption or desorption rates do not monotonously decrease with time. The command critiques the applicability of the Butler-Volmer equation–as a classic approach to the kinetics–and we advertise an alternative kinetic rate law that resolves the problematic issues of the classic approach. We show that the new rate law explains important features of the observations, specifically when admitting for a coherent initiation of the phase change.

MM 39.3 Fri 10:45 SCH/A215
Local hydrogenation of polycrystalline Pd nanodisks studied with in-situ TEM — •Svetlana Korneychuk[1,2], Carl Andersson[3], Stefan Wagner[1], Christoph Langhammer[3], and Astrid Pundt[1] — [1]IAM-WK, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]KNMFi, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Chalmers University of Technology, Göteborg, Sweden

Hydrogen distribution and concentration in metals is of central importance for many areas of hydrogen technology, such as hydrogen storage, detection, and hydrogen embrittlement. In particular, arrays of Pd nanodisks can serve as optical hydrogen sensors [1] at room temperature owning to fast kinetics of hydrogen absorption and desorption of Pd. Here we demonstrate hydrogen distribution and concentration in polycrystalline Pd nanodisks with the lateral resolution down to 4 nm extending our previous study on the local measurement of hydrogen concentration in Pd nanoparticles with in-situ TEM [2]. By measuring the shift of the Pd bulk plasmon peak with scanning transmission electron microscopy combined with energy electron loss spectroscopy during in-situ hydrogen gas loading and unloading, local detection of the hydrogen concentration is achieved in TEM. The method offers a way to observe hydrogen concentration at different sites: grain boundaries, surface and grains starting from early stages of hydrogenation to compete hydride formation identifying the pathways of hydrogenation of polycrystalline metals. [1] C. Wadell, et al., ACS Nano 2014 8 (12), 11925-11940 [2] S. Korneychuk, et al., Small 2025, 21, 2407092.

MM 39.4 Fri 11:00 SCH/A215
A comparative density functional theory study of hydrogen adsorption in metal organic frameworks — •Ikutaro Hamada — Department of Precision Engineering, Graduate School of Engineering, The University of Osaka , Suita, Osaka 565-0871, Japan

Metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) have attracted considerable attention due to their design and synthesis flexibility, enabling applications in catalysis, gas adsorption, and separation. Among these, hydrogen storage is one of the most extensively studied properties of MOFs. However, their hydrogen storage capacity remains low, particularly at room temperature, which limits industrial and commercial applications. To design MOFs with enhanced hydrogen storage capability, it is essential to understand the microscopic details of hydrogen adsorption and absorption within these frameworks. In this work, we assess the accuracy of dispersion-inclusive exchange-correlation functionals against the coupled cluster method using hydrogen-benzene complexes, and we investigate hydrogen adsorption in UiO-66, UiO-67, and UiO-68 as prototypical MOFs. We will present details of our systematic exploration of the geometric and electronic structures of hydrogen molecules and their stability within UiO-66, UiO-67, and UiO-68.

MM 39.5 Fri 11:15 SCH/A215
Machine Learning Potential Approach to Complex Hydrogen-Surface Interactions: GRACE Applied to the H/Sn/Ru System — •Manuel Enns and Daniel F. Urban — Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

Understanding hydrogen interactions with contaminated metal surfaces remains a challenging problem in computational materials science, requiring methods that balance accuracy with computational efficiency to capture complex multi-component dynamics. We demonstrate the application of a GRACE machine learning interatomic potential to study hydrogen behavior on tin-contaminated ruthenium surfaces - a system that exemplifies the challenges of modeling reactive adsorbates on multi-element surfaces. Data from density functional theory calculations on hydrogen penetration mechanisms through ruthenium surfaces with varying tin coverages was used to fine-tune the GRACE potential, enabling computationally efficient molecular dynamics (MD) simulations. The resulting MD simulations successfully capture key dynamic processes including hydrogen diffusion and jump mechanisms, tin growth kinetics at a prior hydrogen coverage, and low-energy hydrogen deposition. This case study demonstrates GRACE's capability to handle complex multi-component systems involving reactive species, providing atomic-level insights into how surface contamination affects hydrogen penetration pathways and adsorbate interactions.

15 min. break

MM 39.6 Fri 11:45 SCH/A215

Diffusion of hydrogen in platinum during HER catalysis — Aparna Saksena[1], Bingxin Li[1], Yujun Zhao[1], J. Manoj Prabhakar[1], Mira Todorova[1], Jörg Neugebauer[1], Dierk Raabe[1], Baptiste Gault[1,2], and •Yug Joshi[1] — [1]Max Planck Institute for Sustainable Materials (MPI-SusMat), Max Max-Planck-Straße 1, 40237 Düsseldorf — [2]Univ Rouen Normandie, CNRS, INSA Rouen Normandie, Groupe de Physique des Matériaux, UMR 6634, F-76000 Rouen, France

Platinum remains the most common electrocatalyst used for hydrogen evolution reaction (HER) in acidic conditions. It is generally believed to act as a proton-blocking catalyst with adsorption of reaction intermediates limited to its surface. In this study, we thoroughly examine how Pt interacts with hydrogen and deuterium (H/D) within the bulk by monitoring the mass change of a Pt electrode in real-time during galvanostatic heavy/water splitting, using an electrochemical quartz crystal microbalance. Surprisingly, we observe an irreversible mass increase over time along with changes in the overpotential for both HER and DER. Atom probe tomography of the Pt electrode after DER confirms that D diffuses into the bulk. The results are supported by density functional theory, showing the formation of an interstitial solid solution of H in Pt. These results challenge the conventional belief that Pt-proton interactions are only surface-limited. They suggest a need to revisit catalyst design strategies, which currently focus on surface-adsorbed species and the rate-limiting Volmer step, by also considering the bulk diffusion of H/D within the Pt matrix.

MM 39.7 Fri 12:00 SCH/A215

Hydrogen induced small polarons in iron oxides using occupation-matrix control DFT+U calculations — Ahmed Abdelkawy, •Mira Todorova, and Jörg Neugebauer — Max Planck Institute for Sustainable Materials, Max-Planck-Str.1, 40470 Düsseldorf

Over 6% of global CO_2 emissions come from using carbon-based reducing agents in iron production. Replacing these agents with hydrogen would result in water as the sole byproduct, thereby reducing harmful emissions. To understand H-based reduction of iron oxides, we focus on hydrogen interactions with bulk hematite (Fe_2O_3). Modeling transition metal oxides is challenging because conventional DFT-GGA has self-interaction errors and inadequately treats the Coulomb repulsion in partially filled d-orbitals. Corrections such as DFT+U or exchange-correlation functionals, which incorporate a fraction of the exact exchange, further complicate matters because they generate a multitude of metastable configurations that DFT cannot predict. In this study, we use DFT+U with occupation matrix control to map the energy landscape of the small electron polaron generated by H interstitials. We construct the three-dimensional potential energy surface of H interstitials using the resulting ground-state configurations. This enables us to gain detailed insight into hydrogen kinetics and rate-limiting steps.

MM 39.8 Fri 12:15 SCH/A215

An atomic-scale master-equation model study of the mobility of a dislocation core interacting with interstitial hydrogen in a metal — •Daniel Pfalzgraf[1], Daniel F. Urban[1,2], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany — [2]Freiburg Materials Research Center (FMF), University of Freiburg, Stefan-Meier-Str. 21, 79104 Freiburg, Germany

We examine the influence of interstitial hydrogen in a metal on the motion of a dislocation by means of a master equation model. This model takes as input atomic-scale information, such as material-specific defect-migration energy barriers and interatomic interaction energies, to produce the drift velocity of a mechanically driven dislocation core segment as a function of the local hydrogen concentration around it. Our approach can take detailed correlation effects into account, for example, that the dislocation core acts as a mobile hydrogen trap, resulting in an inhomogeneous distribution of hydrogen around it. The results can be used to estimate in which ranges of temperature or interaction strength the presence of hydrogen increases or decreases the mobility of the dislocation core, which is of interest in the context of hydrogen embrittlement mechanisms.

MM 39.9 Fri 12:30 SCH/A215

Hydrogen induced strain instability in Aluminum — •Ali Tehranchi[1,2], Bharathi Ganesh Ganesan Sekar[1], and Tilmann Hickel[1,2] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), D-12489, Berlin, Germany — [2]Max Planck Institute for Sustainable Materials, D-40237 Düsseldorf, Germany

Hydrogen embrittlement is a persistent form of metal degradation that arises from the complex interactions between hydrogen atoms and defects within metallic lattices. Environmental nanoindentation has become a standard experimental technique for probing these interactions, particularly the mechanisms underlying hydrogen-assisted deformation. In this work, we employ comprehensive large-scale molecular statics simulations in aluminum, complemented by ab initio calculations, to investigate the influence of hydrogen on homogeneous dislocation nucleation –the primary mechanism responsible for pop-in events observed under low-radius indenters. Our defect phase diagram analysis shows that, at hydrogen chemical potentials relevant to nanoindentation experiments, vacancy formation is significantly enhanced, leading to a substantial increase in the concentration of vacancy–hydrogen complexes. These complexes produce large local misfit strains, which in turn reduce the critical shear stress required for material instability and the onset of homogeneous dislocation nucleation.

MM 40: Transport in Materials: Diffusion, Charge, or Heat Conduction IV

Time: Friday 10:15–12:30 Location: SCH/A216

MM 40.1 Fri 10:15 SCH/A216

Quantum oscillation and tunable charge density wave of kagome metal ScV6Sn6 — •Changjiang Yi, Xiaolong Feng, Chandra Shekhar, and Claudia Felser — Max Planck Institute for Chemcial Physics of Solids

Compounds with kagome lattice structure are known to exhibit Dirac cones, flatbands, and van Hove singularities, which host versatile quantum phenomena. We investigate the magnetoelectric transports along with the theoretical calculations of, a nonmagnetic charge-density wave (CDW) metal. ScV6Sn6 exhibits Shubnikov de Haas quantum oscillations, which help to shape the Fermi-surface (FS). The Dirac band is demonstrated along with a nonzero Berry phase. In addition, the compound also shows the anomalous Hall-like behavior up to the CDW phase transition. Under Cr substitution and hydrostatic pressure, the CDW is largely suppressed. The suppression of CDW phase under pressure can be well captured by our first-principles calculations, evidenced by the lift of imaginary phonon bands. The MR and Hall resistance behave differently under Cr substitution and pressure. Our study reveals that the anomalous Hall-like behavior arises from the kagome lattice and persists as long as the lattice is maintained.

MM 40.2 Fri 10:30 SCH/A216

Investigating UAHE in layered delafossite by high-energy electron irradiation. — •Elina Zhakina[1,2], Philippa McGuinness[2], Romain Grasset[3], Seunghyun Khim[2], Marcin Konczykowski[3], and Andrew Mackenzie[2,4] — [1]Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), The University of Tokyo, Bunkyo, Tokyo, Japan — [2]Max Planck Institute for Chemical Physics of Solids — [3]Laboratoire des Solides Irradis, CEA/DRF/IRAMIS, Ecole Polytechnique, CNRS, Institut Polytechnique de Paris, Palaiseau, France — [4]Scottish Universities PhysicsAlliance, School of Physics & Astronomy, University of St. Andrews, St. Andrews, United Kingdom

PdCrO2 belongs to the delafossite family of extremely pure triangular lattice metals. While its Pd layers are metallic, the CrO2 layers are Mott insulating and order antiferromagnetically below 37 K. PdCrO2 [1]. It exhibits an unconventional anomalous Hall effect (UAHE), the origin of which has been the focus of substantial critical discussion. To investigate the origin of UAHE, we conducted a systematic study of the influence of point defects on the Hall effect of PdCrO2, the results of which are reported here. We introduced point-like defects into focused ion beam-sculpted microstructures of PdCrO2 by irradiating them with high-energy electrons. Comparing the results of UAHE as a function of disorder, we demonstrate UAHE behaviour attributed to its extrinsic origin.

MM 40.3 Fri 10:45 SCH/A216

Anisotropic anomalous Hall effect in distorted kagome GdTi3Bi4 — •Avdhesh Kumar Sharma[1], Bo Tai[1], Subhajit Roychowdhury[2], Premakumar Yanda[1], Ulrich Burkhardt[1], Xiaolong Feng[1], Claudia Felser[1], and Chandra Shekhar[1] — [1]Max Plank Institute for chemical physics of solids, Dresden, Germany — [2]Indian institute of science education and research, Bhopal, India

GdTi3Bi4 crystallizes in layered Ti-based kagome nets intertwined with zigzag Gd chains along the a-axis and orders antiferromagnetically below 15 K. Here, we present the temperature and field-dependent electrical transport of GdTi3Bi4 in different directions. The material exhibits anomalous Hall conductivity of 410 Ω-1 cm-1 at 2 K for B || c and it is completely absent for B || a, despite the similar magnetization observed in both orientations. This behavior is quite contradictory, as anomalous Hall effect (AHE) typically scales with the magnetization. Through first principles calculations, it is demonstrated that in the presence of time reversal symmetry broken by the Gd 4f sublattice and spin orbit coupling, the magnetization direction controls the orbital mixing in the Ti t_2g bands, relocating Berry curvature hot spots and producing the observed orientation selective anomalous Hall conductivity (AHC). The results establish GdTi3Bi4 as platform for investigating new avenues of AHE, such as directional AHE, and thus shed new light on the intricate coupling between magnetic and electronic structures, paving the way for exploring novel quantum phenomena.

MM 40.4 Fri 11:00 SCH/A216

Nernst effect in superconducting Weyl semimetal t-PtBi2 — Federico Caglieris[3], •Michele Ceccardi[1], Dmitriy Efremov[1], Grigory Shipunov[1], Iryna Kovalchuk[1,4], Saicharan Aswartham[1], Arthur Veyrat[1,5], Joseph Dufouleur[1,7], Daniele Marré[2,3], Bernd Büchner[1,7], and Christian Hess[1,6,7] — [1]IFW Dresden — [2]University of Genoa — [3]CNR SPIN — [4]Kyiv Academic University — [5]LPS Orsay — [6]Wüppertal University — [7]TU Dresden

Topological materials are among the most promising areas of research in Condensed Matter Physics, offering breakthroughs in dissipationless electronics or in error-free quantum computing. The combination of non-trivial topology and superconductivity opens to novel quantum devices. The discovery of intrinsic materials where such properties appear together represent a frontier in modern condensed matter physics. Trigonal PtBi2 has recently emerged as a possible candidate, being the first example of superconducting type-I Weyl semimetal. However, several aspects of this promising compound still need to be unveiled, concerning its complicated band structure, the actual role of Weyl points in determining its electronic properties and the nature of the superconducting transition. In the work, we experimentally investigated t-PtBi2 single crystals and exfoliated flakes by means of the Nernst effect, which has been demonstrated to be a powerful probe for study the fermiology of complex materials.

15 min. break

MM 40.5 Fri 11:30 SCH/A216

Negative quadratic magnetoresistance generated by spin fluctuations in the metamagnetic bilayer strontium ruthenate Sr3Ru2O7 — •Bastien Michon[1,2], Elisa Auffray[1], Amir Meddas[1], Zhiqiang Mao[3], Freek Massee[1], Pascale Senzier[1], Claude Pasquier[1], and Siham Benhabib[1] — [1]Laboratoire de Physique des Solides - University of Paris-Saclay, Orsay, France — [2]SOLEIL synchrotron, Saint Aubin, France — [3]Eberly College of Science, The Pennsylvania State University, University Park, USA

The bilayer strontium ruthenate Sr3Ru2O7 hosts a metamagnetic transition around 8T and was widely studied for its quantum criticality characterized by its linear-in-temperature resistivity. While most prior work has focused on the magnetic field evolution of the resistivity exponent α, the magnetoresistance (MR) has received less attention. Our low-temperature relative MR measurements on high-purity single crystals reveal two key features absent from the literature:

1. a well-defined negative quadratic MR between 30 and 100K, consistent with enhanced spin fluctuations, and 2. a non-monotonic MR evolution at low temperature within the 1.6-12K range.

The metamagnetic MR peak around 8T reaches nearly 90% at the lowest temperatures, broadens with increasing temperature, shifts to lower fields, and completely disappears between 20-30K. At higher temperature, the MR changes sign and follows a perfect negative H* dependence, with maximum amplitude around 30-40K. These measurements provide the first detailed mapping of the MR in Sr3Ru2O7 across a broad temperature range and up to 14T.

MM 40.6 Fri 11:45 SCH/A216

Quantum Transport in Atomic-Sized Contacts Using Break-Junction Experiments — •Guillem Pellicer and Carlos Sabater — Department of Physics, University of Alicante

The study of atomic-sized metallic contacts is fundamental to understanding the limits of electronic transport at the nanoscale. We present a comparative analysis of electronic transport in atomic-sized contacts, contrasting the behavior of noble metals with that of reactive metals under both ambient conditions and inert atmospheres. We examine how environmental interactions influence the formation and stability of these nanocontacts, employing clustering algorithms to analyze these effects.

MM 40.7 Fri 12:00 SCH/A216

Atomic Transistor-Based Implementation of Logic Gates — •Merlin Schieler[1], Florian Schieren[1], Carlotta Buchner[1], Felix Frank[1], Ida Göbel[1], Katja Marschall[1], Fanqing Xie[1], Florian Wertz[1], and Thomas Schimmel[1,2] — [1]Institute of Applied Physics, Karlsruhe Institute of Technologie (KIT), 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technologie (KIT), 76344 Eggenstein-Leopoldshafen, Germany

An atomic-scale quantum conductance switch was demonstrated in our group which allows to open and close an electrical circuit by the controlled and reproducible reconfiguration of individual silver atoms within an atomic-scale junction. The only movable parts of the switch are the contacting atoms. The device is fabricated by electrochemical deposition of silver atoms between the source and the drain electrode. It is entirely controlled by an external voltage of a few millivolts applied to an independent gate electrode. Controlled switching was performed between a quantized, electrically conducting "on-state" exhibiting a conductance of $G_0 = \frac{2e^2}{h} \approx \frac{1}{12.9\,\mathrm{k\Omega}}$ or preselectable multiples of this value and an insulating "off-state". The device, which reproducibly operates at room temperature, represents an atomic transistor or relay, opening intriguing perspectives for the emerging fields of quantum electronics and logics on the atomic scale.

Here, we show a first demonstration of logical operations such as NAND and NOR with electrical circuits consisting of two atomic-scale quantum conductance switches.

MM 40.8 Fri 12:15 SCH/A216

Quantum transport in α-Sn atomic-sized contacts tuned by strain — Francisco Guzmán[1], Wynand Dednam[2], Andres Martinez-garcia[1], Enrico Lombardi[2], Carlos Untiedt[1], and •Carlos Sabater[1] — [1]University of Alicante — [2]University of South Africa

Tin (Sn) transitions from metallic β-Sn (above 286 K) to α-Sn (diamond-cubic, zero-gap semiconductor) below this temperature. α-Sn's electronic properties are theoretically tunable under strain, potentially yielding a Dirac semimetal or topological insulator. We experimentally investigated the quantum electronic transport of α-Sn nanocontacts at 4.2 K using a Scanning Tunneling Microscopy break junction (BJ) setup. Conductance measurements revealed three distinct groups via machine-learning clustering. Supported by Molecular Dynamics (MD) simulations and Density Functional Theory (DFT) calculations with Spin-Orbit Coupling (SOC), our findings demonstrate that atomic contact geometry is crucial for quantum transport in α-Sn, providing insights for spintronics applications.

MM 41: Development of Calculation Methods II

Time: Friday 10:15–12:45 Location: SCH/A251

MM 41.1 Fri 10:15 SCH/A251

Atomistic Framework for Glassy Polymer Viscoelasticity Across 20 Frequency Decades — •Ankit Singh[1], Vinay Vaibhav[1,2], Caterina Czibula[3], Timothy W. Sirk[4], and Alessio Zaccone[1] — [1]Department of Physics "A. Pontremoli", University of Milan, Via Celoria 16, 20133 Milan, Italy — [2]Institut für Theoretische Physik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Institute of Bioproducts and Paper Technology, Graz University of Technology, Inffeldgasse 23, 8010 Graz, Austria — [4]US Army DEVCOM Army Research Laboratory, Aberdeen Proving Ground, Maryland 21005, United States

Glassy polymers are central to engineering applications, yet their viscoelastic response over broad frequency and temperature ranges remains difficult to characterize. We extend non-affine deformation theory by incorporating a time-dependent memory kernel within the Generalized Langevin Equation for atomistic non-affine motions, yielding frequency-dependent mechanical response. Applied to poly(methyl methacrylate) (PMMA), the method captures the shear modulus and relaxation spectrum across more than twenty decades in frequency, from hundreds of terahertz down to the millihertz regime, thus bridging polymer mechanics from ordinary to extreme scales. Our predictions show quantitative consistency with independent estimates from oscillatory-shear molecular dynamics, Brillouin scattering, ultrasonic spectroscopy, Split-Hopkinson testing, and dynamic mechanical analysis (DMA), demonstrating a unified theoretical computational route for multiscale characterization of polymer glasses.

MM 41.2 Fri 10:30 SCH/A251

Clarifying the existence of a miscibility gap in platinum-palladium alloys via compositional fluctuations — •Florian Groll, Sebastian Eich, and Guido Schittz — Institute of Materials Science, Stuttgart, Germany

In materials science, the Gibbs free energy is of central importance for calculating phase diagrams. CALPHAD assessments require extensive experimental measurements and data obtained from well-equilibrated samples. For alloy systems with extremely low diffusion coefficients, achieving such equilibrium can be very time-consuming or practically impossible. Because this approach relies only on nanometer-scale equilibration, it provides a significantly more efficient route to the determination of CALPHAD parameters for systems with extremely slow diffusion. The palladium-platinum system is a well-known example for those kind of systems with unknown miscibility gap. In this study, we determine the Pd*Pt phase diagram by extracting the curvature of the Gibbs free energy from local composition fluctuations in the solid state using fluctuation theory. The experimental data needed for applying the local fluctuation theory are obtained from atom probe tomography, and the phase diagram is subsequently calculated.

MM 41.3 Fri 10:45 SCH/A251

Exploring the magnetic phase behaviour of MnAl with a novel sampling method, beginning from first principles — •Georgia A Marchant[1,2], M Nur Hasan[1], Rafael Vieira[1], Julie B Staunton[2], and Heike Herper[1] — [1]Uppsala University, Uppsala, Sweden — [2]University of Warwick, Coventry, United Kingdom

The demand for powerful magnetic materials is ever-increasing, as they dominate our modern technological landscape. Addressing rare earth (RE) criticality is crucial, so the search for viable permanent magnets that are RE-free and RE-lean continues. MnAl, with around 55% Mn content, has been a popular candidate for research in this regard. It transforms from the paramagnetic epsilon phase to the ferromagnetic tau phase when annealed appropriately, but the transition rate enhances under a surprisingly modest magnetic field. To shed light on this, we have computationally predicted the magnetic properties of MnAl across the transition.

The method uses data from first-principles calculations to build efficient atomic models of the phases' magnetic interactions. Thermodynamic properties are then determined with nested sampling (NS). Recently, NS has proven to be a powerful alternative to Markhov chain Monte Carlo sampling (MCMC). While NS has been used extensively in non-magnetic physical chemistry, this work represents its first application to magnetic materials. We present these results to demonstrate the power of NS; compare its effectiveness to MCMC; and unveil previously-unknown magnetic phases of MnAl.

MM 41.4 Fri 11:00 SCH/A251

A Demonstration of the Finite-Temperature Upside-Down Adiabatic Connection with the Asymmetric Hubbard Dimer — •Vincent Martinetto[1,2,3], Juri Grossi[1], and Aurora Pribram-Jones[1] — [1]University of California, Merced, CA 95343, United States — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Center for Advanced Systems Understanding, 02826 Görlitz, Germany

The finite-temperature upside-down adiabatic connection is an integral expression for the decorrelation free energy, a quantity of interest when considering finite-temperature strictly correlated electrons. This approach smoothly connects a thermal ensemble of strictly correlated electrons to an ensemble with realistic interaction strength while requiring the density of the system to remain fixed across all interaction strengths. As the strictly correlated limit is the natural opposite of the Kohn-Sham limit, it can provide new insights into the difficult regime of strong correlation in finite-temperature systems. An exact demonstration of the upside-down finite-temperature adiabatic connection will be performed with the asymmetric Hubbard dimer, along with a discussion of strong correlation in finite-temperature systems.

MM 41.5 Fri 11:15 SCH/A251

Towards self-consistent electrostatic corrections for charged defects in periodic boundary conditions — •Ermanno Botti[1,2,3], Davide Campi[3], Nicéphore Bonnet[2], and Nicola Marzari[1,2] — [1]PSI, Switzerland — [2]EPFL, Switzerland — [3]UniMiB, Italy

Charged point defects in semiconductors and insulators play a pivotal role in determining a wide range of physical properties, significantly impacting materials behavior and device performance. First principles calculations have become an essential tool to better characterize defects properties and to speed up technological advancements. However, some key defect properties, such as formation energies in the dilute limit, are highly sensitive to finite size effects in periodic boundary conditions DFT simulations. These issues arise from long range Coulomb interactions between periodic replicas and the neutralizing background needed to prevent the divergence of the electrostatic potential. To reduce these effects, corrections are required to remove these spurious electrostatic interactions. In this work we extend an a-posteriori correction scheme to achieve self-consistency in the open access package Quantum Espresso and test it on simple systems.

15 min. break

MM 41.6 Fri 11:45 SCH/A251

Tessellation-free full charge density method for atom-centered basis sets — •Franco Moitzi[1], Andrei V. Ruban[2,3], Vsevolod I. Razumovskiy[1], and Oleg E. Peil[2] — [1]Christian Doppler Laboratory for Digital material design guidelines for mitigation of alloy embrittlement, Materials Center Leoben Forschung GmbH, Vordernberger Straße 12, A-8700 Leoben, Austria — [2]Materials Center Leoben Forschung GmbH, Vordernberger Straße 12, A-8700 Leoben, Austria — [3]Department of Materials Science and Engineering, Royal Institute of Technology, 10044 Stockholm, Sweden

Accurate Poisson solvers are essential for reliable total energies and forces in Density Functional Theory (DFT) calculations. Atom-centered basis methods, such as Korringa-Kohn-Rostoker methods, often rely on Voronoi tessellations to decompose space, which complicate Poisson solutions in the interstitial region due to the high l-cutoffs required for the nearly flat charge there and the boundary discontinuities, leading to numerical instabilities as atoms move. We introduce a tessellation-free method that avoids these issues by decomposing the charge into non-overlapping atomic spheres and an interstitial region.

Following Andersen *et al.*, the interstitial charge is expanded in screened spherical waves—Helmholtz-equation solutions with special boundary conditions—and smoothly extended from the atomic spheres, allowing the Poisson equation to be solved analytically. Their analytical properties allow accurate evaluation of the Hartree potential, electrostatic, and exchange-correlation energies, enabling precise and efficient DFT calculations with atom-centered basis sets.

MM 41.7 Fri 12:00 SCH/A251

Machine-Learning Augmented Electronic Structure Calculations via Adaptive DFTB Parameters — •Yihua Song, Christoph Scheurer, Karsten Reuter, and Chiara Panosetti — Fritz Haber Institut der MPG

As a semi-empirical DFT approximation, Density Functional Tight Binding (DFTB) combines reduced computational cost with accessible electronic structure, providing a compromise between the full physicality of *ab initio* methods and the speed of machine-learning interatomic potentials. Yet, its accuracy in realistic systems remains limited due to intrinsic approximations and dependence on parametrization quality. To this end, we propose that the precalculated Slater-Koster (SK) electronic interaction tables in DFTB should be adapted to local atomic environments and demonstrate proof-of-principle studies showing the improved electronic structure description. Building on the observed smoothness of SK integrals across chemical and spatial environments, we use machine learning based on atomic descriptors to continuously adapt the parametrization beyond discrete atomic types. As a prototype, we introduce the DFTB Orbital Verity Engine (DOVE), a machine-learning framework that learns subtle discrepancies in electronic parameters across diverse local environments from reference electronic structures. We successfully validate it against complicated systems with multiple coordination states. This machine-learning framework for environment-adaptive tight-binding parameterization enables scalable electronic structure simulations with enhanced fidelity, efficient speed, and physical interpretability.

MM 41.8 Fri 12:15 SCH/A251

Detecting topologically-protected surface states in doped systems using the coherent potential approximation — •Artem Chmeruk, Dylan Jones, and Liviu Chioncel — University of Augsburg, Augsburg, Germany

The signature of the non-trivial electronic band structure is the existence of gapless conducting states at interfaces where the topological invariant changes. This change signals a topological phase transition, which in real systems can be accomplished through doping. Modeling doping effects can be done by combining density functional theory and coherent potential approximation, which gives the possibility to model a continuous range of concentrations, and provides a sensitive probe to detect the emergent electronic states. Here, we analyse the topologically-protected surface states in $\mathrm{Bi}_{2-x}\mathrm{Sb}_x\mathrm{Se}_3$.

MM 41.9 Fri 12:30 SCH/A251

Defect-induced vibrational modes in graphene — •Iskander Mukatayev, Guillaume Radtke, and Michele Lazzeri — Sorbonne Université, CNRS UMR 7590, MNHN, IMPMC, 4 place Jussieu, 75252 Paris, France

We present a general framework for investigation of the vibrational properties of point defects in graphene, motivated by recent advances in vibrational EELS that enable phonon spectroscopy with atomic resolution. Our approach combines DFT and density-functional perturbation theory with a force-matching procedure [1-2], in which interatomic force constants (IFCs) are computed independently for pristine graphene and defect-containing supercells and then merged to dynamical matrices of very large systems(up to 20000 atoms). This strategy enables the modeling of isolated defects without defect-defect interactions while retaining full ab initio accuracy.

We investigate a wide range of point defects including substitutional dopants (B, N, Si, P), single, double vacancies and Stone-Wales reconstruction. Depending on the details of defect-induced bond reconstruction, different behaviours are observed ranging from quasi-localized (or resonant) states falling in the continuum of the bulk to high-frequency fully localised modes. From these examples we draw conclusions of the conditions of occurrence of both types vibrations.

References

1. M. Lazzeri, P. Thibaudeau, Phys. Rev. B 74, 140301 (2006)
2. G. Radtke, S. Klotz, M. Lazzeri, P. Loubeyre, M. Krisch, A. Bossak, Phys. Rev. Lett. 132, 056102 (2024)