MM 9: Poster

Time: Monday 18:30–20:30 Location: P1

MM 9.1 Mon 18:30 P1

Well-defined nanostructures synthesized by optimized anodic aluminum oxide template — •Linfeng Su, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The template method has unique advantages in the design and synthesis of materials with specific nanostructures but with some disadvantages. In recent years, through in-depth research and improvement of its preparation methods, the five shortcomings of the traditional anodic aluminum oxide (AAO) template method, such as short-range order and long-range disorder, insulator, single-set of pores, large dead volume, and limited capability to tune pore shape and arrangement, have been successfully addressed by our group. Large-scale control of the shape, size, spatial configuration, and combination of in-plane and out-of-plane pores of well-defined nanostructures can be achieved, thereby broadening the diversity of nanostructures[1, 2]. In addition, we have improved the mechanical strength of the prepared AAO template, so that it can maintain the stability of the nanostructure under a pressure of 10 MPa[3]. The optimized AAO template method provides practical guidance for the design and preparation of catalysts under complex application conditions. [1] Nat. Commun., 2022, 13(1), 2435; [2] Nat. Nanotechnol., 2017, 12(3), 244; [3] Nat. Commun., 2020, 11(1), 299.

MM 9.2 Mon 18:30 P1

Ferroelectric perovskite oxides: PFM investigations of (001) surface — •Andrzej Jasicki[1], Marta Macyk[1], Llorenç Albons[2], Konrad Szajna[1], Martin Setvin[2], Dominik Wrana[1], and Franciszek Krok[1] — [1]Marian Smoluchowski Institute of Physics, Jagiellonian University, Krakow, Poland — [2]Department of Surface and Plasma Science, Charles University, Prague, Czech Republic

Growing demand for energy from green sources drives development in this sector. Hydrogen, as one of the most promising fuels, is mostly produced with the use of electricity during electrolysis, what lowers the overall efficiency of whole process. To reduce energy costs, one should search for an efficient water-splitting catalyst.

Although ferroelectric perovskite oxides show great potential in photocatalysis, it can be further enhanced via piezo- and pyrocatalysis. In order to understand their role in water-splitting process, a thorough investigation of ferroelectricity manifested at surfaces is necessary. Piezoresponse Force Microscopy (PFM), a method based on inverse piezoelectric effect, provides an opportunity to have a closer look into surface domain structure of such materials.

This poster displays PFM and SEM data obtained by investigations into domain structure on surfaces of single-crystalline, ferroelectric perovskites, namely KNbO3 and BaTiO3. Measurements on both polished and cleaved (001) surfaces were conducted in room temperature and under ambient atmosphere. Influence of different poling voltages and exposure to water is also discussed.

MM 9.3 Mon 18:30 P1

Pressure-induced hybridization changes in elemental silicon at Mbar pressure — Robin Sakrowski[1], Christoph J. Sahle[2], •Gordon Scholz[1], Leonie Tipp[3], Mirco Wahab[3], Sindy Fuhrmann[3], and Christian Sternmann[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, Maria-Goeppert-Mayer-Straße 2, 44221, Dortmund, Germany — [2]ESRF, The European Synchrotron, 71 Avenue des Martyrs, CS40220, 38043 Grenoble Cedex 9, France — [3]Institut für Glas und Glastechnologie, TU Bergakademie Freiberg, Leipziger Straße 28, 09599, Freiberg, Germany

Silicon, a fundamental semiconductor material, undergoes intriguing structural and electronic transformations when subjected to high pressure [1]. These changes are investigated using X-ray Raman scattering (XRS) spectroscopy on pure Si powder loaded into a diamond anvil cell for pressures up to 108 GPa. The XRS spectra of the Si $L_{2,3}$-edge are compared with ab-initio theoretical calculations based on the Bethe-Salpeter equation. Observations include an increase in coordination number from 4-fold to 12-fold and metallization. Additionally, changes in the occupation probability of d-states under pressure are noted, as silicon valence electrons from the 3s and 3p orbitals are transferred.

This work is supported by the BMBF projects 05K22PE2 and 05K22OF1. [1] J.S.Tse et al., J. Phys. Chem. C 118, 1161 (2014)

MM 9.4 Mon 18:30 P1

THz signatures of displacive phase transformation — •Nandita Bajpai[1], Michael Dittler[1], Ahana Bhattacharya[1], Alexander Kunzmann[2], Gabi Schierning[2], and Martin Mittendorff[1] — [1]Department of Physics , University of Duisburg — [2]Institute for energy and material process, University of Duisburg

Phase Change Materials are widely applied in contemporary technological advancements such as sensors, activators, and electronic devices. The Terahertz time-domain spectroscopy (THz-TDS) reflectivity and transmissivity measurements provide valuable insights into carrier dynamics such as mobility and carrier concentration. The temperature-induced phase change results in significant changes in reflectivity and transmissivity that are linked to the presence of free electrons.

Furthermore, the change in the complex conductivity points towards the predicted formation of a charge density wave (CDW) phase, which is a manifestation of periodic modulation of the electron density. This provides more details toward understanding the role of electrons in the phase transformation.

MM 9.5 Mon 18:30 P1

Impact of hyperthermal oxygen on alumina surfaces investigated by molecular dynamics simulations — •Stephen Hocker, Hansjörg Lipp, and Johannes Roth — Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart

Oxygen atoms impinging on satellite surfaces in very low earth orbit (VLEO) transfer momentum and energy leading to material degradation as well as drag forces which result in orbital decay of the satellite. The first step in finding solutions to counteract significant drag is to gain understanding of the interaction of atomic oxygen (AO) with material surfaces. We investigate the adsorption rate and the angular distribution of reflected AO on crystalline and amorphous alumina surfaces using molecular dynamics simulations. It is found that the angular distribution depends strongly on the surface structure and the incidence angle. A higher ratio of specular reflection is found in case of smooth surfaces and large incidence angles.

MM 9.6 Mon 18:30 P1

Ultrafast phonon-mediated dephasing of color centers in hexagonal boron nitride probed by electron beams — •Masoud Taleb[1], Mario Hentschel[3], Harald Giessen[3], and Nahid Talebi[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany — [3]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany

Defect centers in hexagonal boron nitride (hBN) have gained significant interest as room-temperature single-photon sources, with strong coupling to phonons evident in their photoluminescence and cathodoluminescence spectra. Despite extensive studies, the electron-phonon coupling dynamics and phonon-mediated dephasing of these centers remain underexplored. In this study we experimentally employed an electron-driven photon source (EDPHS) to generate a coherent superposition of phonon states, with the delay between electron and photon pulses controlled to measure dephasing times. The findings reveal an ultrafast dephasing time of 200 fs and a radiative decay of 585 fs at room temperature, contradicting other optical techniques reporting a decay of a few nanoseconds. This rapid dephasing is attributed to the efficient excitation of coherent phonon-polaritons in hBN by electron beams. The research demonstrates the capability of sequential CL spectroscopy for probing the ultrafast dynamics of single emitters in quantum materials, facilitating future applications in quantum networks and devices.

MM 9.7 Mon 18:30 P1

Raman spectroscopic studies on $NiFe_2O_4$-NiO-Ni and MgO-Steel composites as inert anode materials for aluminium molten salt electrolysis — •Felix Drechsler[1], Ulziikhuu Otgonbayar[2], Cameliu Himcinschi[1], and Jens Kortus[1] — [1]TU

Bergakademie Freiberg, Institute of Theoretical Physics, D-09599 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Nonferrous Metallurgy and Purest Materials, D-09599 Freiberg, Germany

The use of inert anodes in aluminium molten salt electrolysis offers positive environmental effects compared to the commercially used graphite anode, especially by avoiding CO, CO_2 and perfluorocarbon (PFC) emissions. Cermet anodes consisting of $NiFe_2O_4$, NiO, and Ni were manufactured by powder metallurgy and sintered at different conditions using the Spark Plasma Sintering (SPS) technique. Furthermore, another type of anode was produced using MgO and steel powder mixture to form metalloceramic composites. These anode materials were investigated by micro-Raman spectroscopy to identify phases formed during the sintering process, such as nickel ferrite spinels. Temperature-dependent Raman measurements were performed to examine the micro-structure behaviour of the anode materials at elevated temperatures.

MM 9.8 Mon 18:30 P1

Influence of the alloying elements on microchemistry and nanostructure of Sm-Co based permanent magnets — •Burçak Ekitli[1], Alex Aubert[1], Fernando Maccari[1], Nikita Polin[2], Xinren Chen[2], Esmaeil Adabifiroozjaei[3], Leopoldo Molina-Luna[3], Baptiste Gault[2], Konstantin Skokov[1], and Oliver Gutfleisch[1] — [1]Functional Materials, TU Darmstadt, 64287 Darmstadt, Germany — [2]Max-Planck-Institut for Sustainable Materials, Düsseldorf 40237, Germany — [3]Advanced Electron Microscopy, TU Darmstadt, 64287 Darmstadt, Germany

Sm-Co 2:17 magnets are high-temperature, high-performance magnets that are commercially available. Their hard magnetic properties are driven by a pinning mechanism, where the complex microstructure and microchemistry play an important role [1]. Since commercial 2:17 magnets consist of five alloying elements and three coherent phases, it is difficult to establish a common understanding of their intrinsic and extrinsic properties. In this study, we continue to investigate the 2:17 magnet system, focusing on a simplified alloy system that we initially introduced [2] by adding Cu to the alloy. Our study focuses on the quaternary Sm(Co,Cu,Zr)6.7 alloy, with four different compositions chosen based on varying Cu concentrations. We investigate the microstructural properties and their influence on the hysteresis of the Sm-Co 2:17 magnet in detail, using advanced characterization techniques such as MOKE, MFM, TEM, and APT. We reveal how Cu concentration influences the microstructure and phase formation, ultimately affecting the magnetic properties.

MM 9.9 Mon 18:30 P1

Bonding changes in solid nitrogen under high pressure — Gordon Scholz[1], Robin Sakrowski[1], Johannes Niskanen[2], Christoph Sahle[3], Leonie Tipp[4], Mirco Wahab[4], Melanie White[5], •Peter Schäfer[1], Ashkan Salamat[5], Sindy Fuhrmann[4], and Christian Sternemann[1] — [1]TU Dortmund, Dortmund, Germany — [2]University of Turku, Turku, Finland — [3]ESRF, Grenoble, France — [4]TU Bergakademie Freiberg, Freiberg, Germany — [5]University of Nevada Las Vegas, Las Vegas, USA

Nitrogen has a complex phase diagram with 15 detected solid molecular phases [1]. In this study, we tracked the electronic and structural changes of nitrogen under high pressure using a novel combined set-up for X-ray Raman scattering (XRS) and X-ray diffraction (XRD) at beamline ID20 at the ESRF exploiting the diamond anvil cell method.

In the pressure regime between ambient conditions and 80 GPa we are able to confirm the δ-phase, ϵ-phase and the ζ-phase with XRD. The corresponding XRS measurements at the nitrogen K-edge show significant changes in the bonding structure. These changes are interpreted via calculated XRS spectra based on molecular dynamic simulations which reveal a hindrance of free rotations of the N_2 molecules in the ϵ-phase.

This work is supported by the BMBF via the projects 05K22PE2 and 05K22OF1.

[1] Turnbull et al. Nat. Commun., 9:4717, (2018)

MM 9.10 Mon 18:30 P1

Grain boundary transformation induced by boron segregation — Xuyang Zhou[1], •Sourabh Kumar[2], Siyuan Zhang[1], Xinren Chen[1], Baptiste Gault[1], Gerhard Dehm[1], Tilmann Hickel[1,2], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, 40237, Germany — [2]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, 12489, Germany

The segregation of solute atoms at grain boundaries (GBs) critically influences the mechanical properties of materials, including corrosion resistance and fracture toughness. This study examines structural transformations induced by minimal boron concentrations at Σ13 GBs in ferrite thin films. Two sample protocols were investigated: one with carbon as the sole solute and the other with carbon and boron co-segregation. Using ab initio calculations, we meticulously explored the competing Σ13 GB phases coexisting with defects and analyzed the energetics of solute segregation at the GB interface. A defect phase diagram was constructed to illustrate the influence of B concentration on GB structure evolution. We reveal that B segregation transforms the GB structure from flat to zigzag trigonal prisms by forming new chemical bonds, enhancing B-Fe bonding strength by 5%. This transformation doubles steel's fracture resistance and provides valuable insights into solute-driven GB phase evolution, contributing to innovative strategies for designing durable, high-performance steel.

MM 9.11 Mon 18:30 P1

Investigation of spin-crossover iron triazole complexes with carbon nanotubes — •Niloofar Azadegan[1], Marvin Dzinnik[2], Maximilian Kilic[3], Franz Renz[4], and Rolf Haug[5] — [1]Institute of solid state physics, Hannover, Germany — [2]Institute of solid state physics, Hannover, Germany — [3]Institute of inorganic chemistry, Hannover, Germany — [4]Institute of inorganic chemistry, Hannover, Germany — [5]Institute of solid state physics, Hannover, Germany

Iron triazole complexes exhibit spin-crossover (SCO) behavior, transitioning between low-spin and high-spin states under external stimuli, making them suitable for sensing and memory applications.

This study investigates carbon nanotubes (CNTs) decorated with iron triazole to enhance electronic and magnetic properties. Current-voltage measurements were performed on bare and decorated CNTs, followed by cryostat measurements under controlled conditions. Preliminary results suggest interactions between SCO behavior and CNTs, with ongoing analysis to explore their potential in advanced electronics.

MM 9.12 Mon 18:30 P1

Linking Characteristic Length Scale in Nanoporous Gold to Alloy Composition and Dealloying Parameters — •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]Hybrid Materials Systems, Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Nanoporous metals display unique material properties due to their high volume-specific surface area and characteristic sizes of pores and ligaments. Although theories of structure formation exist, the process is not yet fully understood. Investigating nanoporous gold as model system will deepen the understanding of the underlying mechanisms, enabling a more precise manipulation of nanoporous structures and their mechanical and functional properties. Therefore, a series of small-angle X-ray scattering (SAXS) data was measured, comparing AuAg alloy compositions subjected to different dealloying potentials, durations, and electrolyte concentrations. Preliminary dependencies were formulated to investigate how these parameters influence the resulting characteristic length scale. This ex-situ and future in-situ analysis of microstructural evolution can be used to identify the underlying mechanisms by validating simulated results of the same dealloying processes, such as those presented by Li et al. [Acta Mater. 222 (2022) 117424.].

MM 9.13 Mon 18:30 P1

Inhomogeneities at different length scales in nanocrystalline Pd-Au prepared by inert gas condensation — Johannes Wild[1], Fabian Andorfer[4], Svetlana Korneychuk[1,2,3], Jules M. Dake[4], Torben Boll[1], Dorothée Vinga Szabó[1,2,3], Stefan Wagner[1], Carl E. Krill III[4], and •Astrid Pundt[1,2] — [1]Institute of Applied Materials (IAM-WK), Karlsruhe Institute of Technology — [2]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology — [3]Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe Institute of Technology — [4]Institute of Functional Nanosystems, Ulm University

Inert gas condensation (IGC) is currently the only viable method to prepare bulk samples of nanocrystalline (NC) palladium-gold (Pd-Au). The raw material is thermally evaporated in a vacuum chamber with a background pressure of 10e-8 mbar that has been backfilled with low-pressure inert gas. On collision with the inert gas, the evaporated material condenses into small particles, which are then collected on

a rotating cold finger, scraped off and mechanically compacted into disk-shaped samples.

In this study, we investigate the different types of inhomogeneities in IGC Pd-Au on different length scales and compare them to samples prepared by arc melting. To this end, we apply a variety of methods to accurately characterize the composition, porosity, grain size, grain orientation and grain growth behaviour on multiple length scales. Finally, we attempt to explain the source of the inhomogeneities and verify by probing the IGC experimental setup via various experiments.

MM 9.14 Mon 18:30 P1

Development, Characterization and Catalytic Evaluation of New Nanosized metal complexes — •Tarek El-Dabea — Chemistry Department, Faculty of Science, King Salman International University, Ras Sudr, Sinai 46612, Egypt

A series of novel nano metal complexes involving Pd(II), Cu(II), Fe(III) and Ag(I) ions were synthesized using a Schiff base ligand in a bidentate coordination mode. The structural and molecular characteristics of these complexes were thoroughly characterized via an array of spectroscopic and analytical techniques, confirming molecular geometry and stoichiometry. Solution stability and stoichiometry of the complexes were systematically evaluated, demonstrating stable metal-ligand coordination. Notably, the Pd(II) complex exhibited unique electronic characteristics, identifying it as a promising candidate for catalytic applications. Based on these results, the Pd(II) complex was tested as a catalyst for synthesizing Different multicomponent reactions. This was achieved through using microwave irradiation. The selection of Pd(II) was informed by its favorable catalytic profile and theoretical insights. Optimization trials demonstrated that the Pd(II) catalyst afforded high yield and efficiency under eco-friendly (H*O/EtOH) solvent conditions. Reusability assessments showed that the catalyst retained high activity for up to five cycles, with minimal performance decline afterward. A mechanistic pathway was proposed, highlighting Pd(II)'s ability for axial coordination, supported by theoretical evidence

MM 9.15 Mon 18:30 P1

Epitaxial Stabilization of Multifunctional Oxide, Oxynitride, and Telluride Thin Films using a Hybrid Pulsed Laser Deposition Technique — Pia Henning, Anna Tschesche, Shagun Thakur, Niklas Kohlrautz, Abhishek Sharma, Laura Pflügl, and •Jasnamol Palakkal — Institute of Materials Physics, Georg-August-University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Materials science uses state-of-the-art thin film techniques, such as pulsed laser deposition (PLD) and molecular beam epitaxy (MBE), to artificially fabricate complex materials [1]. Epitaxial films with controlled defects and orientation are practical for modifying functionalities. We developed a hybrid PLD system attaching molecular beam sources (for elements with high vapor pressure) to fabricate multifunctional oxide, oxynitride, and tellurides. Additionally, gases are provided through a microplasma source. This setup makes a wide range of cation and anion engineering possible in complex materials. In this presentation, we will address challenges in the growth of thin films and how modifications in the defects and structure influence functional properties by taking examples of La_2NiMnO_6 (ordered magnetism and electrocatalysis), Cr_xTe (ferromagnetism and magnetic anisotropy), and $SrNbO_3$ (optical transparency and metallic conduction). Moreover, we will discuss how such a hybrid deposition system can be utilized to grow high-entropy materials and stabilize doping beyond the solubility limit. [1] A. Tschesche, et al., Preprint on Research Square, https://doi.org/10.21203/rs.3.rs-4861088/v1

MM 9.16 Mon 18:30 P1

EXAFS-driven Investigation of ZnO-Mn2O3 and ZnO-Mn2O3-rGO Nanocomposites: Unraveling Structural, Optical, and Electronic Properties — •Shaimaa A. Habib[1], Shehab E. Ali[2], Messaoud Harfouche[3], and Ahmed Awad[4] — [1]1.*Physics Department, Faculty of Science, Damnhour University, Damanhour 22516, Egypt — [2]Materials Science Laboratory, Physics Department, Faculty of Science, Suez Canal University, 41522, Ismailia, Egypt. — [3]SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East), Allan, Jordan — [4]Physics Department, Faculty of Science, Tanta University, Tanta 31527, Egypt

The structural, optical, and electronic properties of ZnO-Mn2O3 and ZnO-Mn2O3-rGO nanocomposites were investigated. The materials, synthesized via sol-gel and self-propagation methods, exhibited porous structures with crystallite sizes of 22-48 nm, as confirmed by XRD and SEM analyses. UV-Vis spectroscopy revealed that rGO incorporation reduced the optical bandgap from 2.63 eV to 1.86 eV and increased the Urbach energy from 1.91 eV to 2.55 eV. The Wemple-DiDomenico model showed a decrease in oscillator resonance energy from 6.64 eV to 6.15 eV and an increase in dispersion energy from 6.47 eV to 13.24 eV. EXAFS and XANES studies at SESAME synchrotron facility provided insights into the coordination environment and electronic structure of the metal centers. This comprehensive characterization establishes a foundation for applying these nanocomposites in optoelectronics, photocatalysis, and energy conversion applications, highlighting rGO's role in enhancing composite performance.

MM 9.17 Mon 18:30 P1

Electrochemical determination of the diffusion coefficient of intercalating species in host metals - conditions of applicability of potential step chronoamperometry — •Magdalena Seiler, Giorgia Guardi, Stefan Wagner, and Astrid Pundt — KIT, Karlsruhe, Deutschland

The diffusion coefficient is generally used to describe the diffusion of intercalating species such as lithium and hydrogen in host metals. It can be determined by a variety of methods, including electrochemical methods. Among these, permeation methods between front and back side of a sample are widely used. On the contrary, in potential step chronoamperometry only one side of the sample needs to be contacted, which is e.g. beneficial for thin film studies. In this work measurements using both methods are performed for hydrogen in palladium and compared to the literature. It is shown that the application of the potential step chronoamperometry approach gives correct results only under very specific restrictions regarding sample thickness and measurement period.

MM 9.18 Mon 18:30 P1

Synthesis, and Characterization of Li/Mn-Excess Cathode Materials for Li-ion Batteries. — •John Karuga[1], Mesfin Kebede[2], and Guido Schmitz[3] — [1]Institute of Materials Science, Department for Material Physics, University of Stuttgart — [2]Institute of Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa — [3]Institute of Materials Science, Department for Material Physics, University of Stuttgart

The study aims to mitigate O2 evolution, spinel phase, and unstable CEI formation common in Li/Mn-excess cathodes. The poster presents preliminary results of the pristine Li/Mn-excess cathodes, which are practical alternatives to LFP, NCA, and Ni-excess materials for high-performance Li-ion batteries. The Li2MnO3 phase in Li/Mn-excess cathodes stabilizes the crystal structure, contributes to the higher discharge capacities >250 mAh/g. Commercialization of Li/Mn-excess materials remains challenging due to undesired transformation from layered to spinel phase, O2 evolution, parasitic reactions with the LiPF6 electrolyte. The Li/Mn excess materials were prepared via solid-state synthesis. Characterization with SEM-EDS, Raman, HR-TEM, and XRD confirmed the development of a material of uniform nanocrystallites with well-layered structure and 0.472 and 0.2 nm interplanar distances, which correspond to the 003 and 104 planes. The CV analysis confirms that the redox reactions (Ni2+/Ni4+; Co3+/Co4+; Mn3+/Mn4+/5+/7+) are highly reversible. The charge transfer resistance is low, indicative of better Li+ diffusion and stable CEI.

MM 9.19 Mon 18:30 P1

Magnetic anisotropy and anomalous Nernst effect in cubic Fe4N films — •Karel Knížek[1], Jakub Vít[1], Mariia Pashchenko[1], Petr Levinský[1], Kyo-Hoon Ahn[1], Jaroslav Kohout[2], and Imants Dirba[3] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czechia — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czechia — [3]Functional Materials, Institute of Materials Science, Technical University of Darmstadt, Germany

Iron nitrides Fe(x)N are commercially important compounds because of their versatile magnetic, electrical, and mechanical properties. We have studied magnetic and transverse thermoelectric properties of Fe(4)N films prepared by magnetic sputtering. The well-known anisotropic magnetoresistance [1] and rectangular magnetization curves for thin oriented films led us to investigate magnetic anisotropy by rotating the sample in external magnetic field and measuring magnetization along the field. The signal is complex, exhibiting harmonics beyond the expected crystal symmetry. Moreover, the

magnetic-field history crucially impacts the anisotropy. The results are quite distinct below and above the metamagnetic phase transition near 50K. The results of the magnetic measurements are compared with anomalous Nernst effect experiments and DFT calculations.

[1] M. Tsunoda et al., Applied Physics Express 2, 083001 (2009).

MM 9.20 Mon 18:30 P1

Thermoelectricity in Bi-directionally Strained $CsSnI_3$ Perovskite — •Michele Reticcioli[1], Mariangela Ruggeri[2], Giovanna D'Angelo[2], and Alessandro Stroppa[1] — [1]CNR-SPIN L'Aquila, Italy — [2]Università degli Studi di Messina, Italy

Thermoelectric materials play a pivotal role in energy sustainability, converting waste heat into electricity without moving parts or emissions. Recent advances spotlight metal halide perovskites, such as $CsSnI_3$, as promising candidates for eco-friendly thermoelectric applications due to their low thermal conductivity and high electrical efficiency. In this work, we explore the influence of bidirectional strain on the orthorhombic gamma-phase of $CsSnI_3$ using density functional theory (DFT), complemented by experimental insights from our collaborators. Strain effects, ubiquitous in thin films grown on mismatched substrates, are known to modify electronic structures and transport properties. Our findings reveal a peculiar dependence of the bandgap on strain direction and intensity. These changes directly impact the thermoelectric properties, including the Seebeck coefficient and figure of merit, emphasizing the interplay between strain-induced electronic modulation and thermoelectric performance. This study contributes to the growing understanding of strain effects in perovskites, offering valuable insights into their potential for thermoelectric applications.

MM 9.21 Mon 18:30 P1

GAP vs. MACE: Efficiency evaluation in a liquid electrolyte system — •Anton Beiersdorfer[1], Lisa Hetzel[1], Carsten Staacke[2], Florian Deissenbeck[2], and Christopher Stein[1] — [1]Technische Universität München, München, Germany — [2]Cellforce Group GmbH, Tübingen, Germany

Machine learning interatomic potentials (MLIP) have transformed molecular simulations, enabling complex materials to be modeled with increasing accuracy and efficiency. As MLIP models evolve, so does the demand for advanced computing architectures, particularly graphics processing units (GPUs), which can accelerate computations compared to traditional central processing unit (CPU) based systems. However, the high cost associated with GPU resources constrain access in both academia and industry, highlighting the relevance of comparing GPU-based and CPU-based MLIPs under real-world conditions.

To this end two popular MLIPs are examined: the GPU-accelerated MACE model and the CPU-based GAP model applied to a test system of a standard battery electrolyte. The system is selected for its demanding electrostatic interactions in solution, which the MLIPs approximate by learning the local interaction patterns that contribute to the overall electrostatic behavior. Therefore, it represents a significant computational challenge and provides a rigorous benchmark for MLIP accuracy and efficiency. By focusing on these models, the study aims to reveal key differences in computational and numerical performance metrics and resource efficiency as well as in physical performance, particularly through comparisons to experimentally measured properties.

MM 9.22 Mon 18:30 P1

Navigating the Latent Space of Chemical Solid State Reactions in Hybrid Battery Interfaces — •Sina Ziegler, Christoph Scheurer, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

We explore the potential of rare earth lithium halides as a material-efficient, nanometer-thick cathode coating in contact with thiophosphate electrolytes. Traditional theoretical approaches, such as molecular dynamics (MD) and Monte Carlo (MC) simulations, are computationally intensive for larger systems, posing a challenge in simulating battery interfaces. To identify a suitable halide/thiophosphate combination, it is essential to determine an energetically feasible solid-state reaction pathway within the multidimensional phase diagram of these materials. We employ *ab initio* thermodynamics to assess the thermodynamic stabilities of the resulting solid-state electrolyte (SSE) and halide interfaces by screening the reaction-free enthalpies of potential interface reactions. An end-member analysis is then performed to evaluate possible compositions of interface products and secondary phases, using techniques such as Principal Component Analysis (PCA), t-distributed Stochastic Neighbor Embedding (t-SNE), and autoencoders to identify linked reactions within the chemical latent space.

MM 9.23 Mon 18:30 P1

Structure and transport properties of Li3MCl6 superionic conductors — •Ziyan Zhang[1,2], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]Chair for Functional Materials,School of Natural Sciences, Technical University of Munich,85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum, Technical University of Munich, 85748 Garching, Germany

Modern society permanently requires more advanced, better performant, safer, and cost-effective energy storage solutions, where the all-solid-state battery (ASSB) concept based on lithium metal is closest to commercialization. Solid electrolytes are a key component of ASSB, defining its lifetime and performance. Halide-based solid electrolytes Li3MCl6 (M = transition metals, rare-earth metals) are emerging as promising materials for all-solid-state batteries due to their high ionic conductivity, electrochemical stability, and compatibility with lithium metal anodes. The current study deals with the systematic characterization of Li3MCl6 solid conductors with M = In, Zr, and Ti transition elements. The focus will be put on the optimization of synthesis routes (between solvent-mediated and mechanochemistry), composition control as well as enhancement of ionic transport. Comprehensive structural characterization, encompassing lab X-ray diffraction (XRD) with Rietveld refinement combined with differential bond-valence estimates of lithium diffusion pathways and differential scanning calorimetry, is performed to reveal the crystallographic details, microstructure, and lithium-ion dynamics.

MM 9.24 Mon 18:30 P1

Processing of non-conductive materials by electroerosion treatment. — •Anton Bespalov — Moscow, Russia

Electroerosion processes process only conductive materials, but it is possible to process non-conductive materials by applying a thin layer of metal to their surface. In this work, based on experiments, the possibility of destruction (processing) of tungsten carbide coated with a layer of 0.01 mm copper with a copper electrode using electric erosion machines is considered. As a result of the experiments, the destruction in the samples corresponding to the shape of the electrode was revealed, which proves the possibility of processing.

MM 9.25 Mon 18:30 P1

Structure formation and phase behavior of amine-water mixtures — •Lena Friedrich[1], Michael Paulus[1], Aurélien Perera[2], Martina Požar[3], Dirk Lützenkirchen-Hecht[4], Nicola Thiering[1], Jaqueline Savelkouls[1], and Christian Sternemann[1] — [1]Fakultät Physik / DELTA, Technische Universität, 44221 Dortmund, Germany — [2]Sorbonne Université, Laboratoire de Physique Théorique de la Matière Condensée, F75252, Paris cedex 05, France; — [3]University of Split, Faculty of Science, 21000 Split, Croatia — [4]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany

Amines are associating liquids that can form transient supramolecular structures via hydrogen bonding [1]. Adding of water can significantly alter the liquids' structure [2] and amine/water mixtures show an interesting phase behavior exhibiting a lower critical solution temperature (LCST) [3]. We studied linear, primary amines mixed with various proportions of water for a variety of temperatures by X-ray diffraction at BL8 and BL9 of DELTA (TU Dortmund). The structure factor prepeak shows a peculiar concentration and temperature dependence which resembles the different phase regimes ranging from disordered nematic via single liquid to two liquid phase. We thank the BMBF for funding via DAAD in the scope of the French-German collaboration PROCOPE 2024-2025 (Project-IDs 57704875 and 50951YA). [1] A. Perera et al., JPC B 44, 128 (2024). [2] L. Almasy et al., PCCP 21, 9317 (2019); [3] J. Glinski et al., J. Colloid. Interface Sci. 162, 129-134 (1994)

MM 9.26 Mon 18:30 P1

A Phase Change Material's Journey through its Energy Landscape — •Jakob Ballmaier, Sebastian Walfort, Elias Abele, and Martin Salinga — Universität Münster, Institut für Materialphysik

The concept of energy landscapes is highly successful in explaining structural dynamics of supercooled liquids and glasses. Locally stable configurations correspond to local minima of the total potential energy of the system in the high-dimensional phase space. During physical ag-

ing a glass can evolve towards lower local minima through a series of saddle points. Experimental observation of this is challenging, since in large systems several saddle points are passed within the shortest resolvable timescales.

Here, we track paths through the energy landscape of a nanoscopic volume of germanium telluride by following the temporal evolution of its electrical resistance. Two regimes turn out to be especially instructive: fast measurements of the resistance immediately after the formation of the glass as well as slower measurements at low temperatures, where the influence of individual relaxation steps on the resistance can be resolved.

MM 9.27 Mon 18:30 P1

Graphite Composites with Titanium as a Secondary Filler - Microstructure and Electronics — •Hoang Thinh Nguyen, Maria Gaudig, and Ralf Wehrspohn — Martin Luther University Halle-Wittenberg, Institute of Physics, Group μMD, Heinrich-Damerow-Str. 4, 06120 Halle (Saale), Germany

The bipolar plate (BPP) is a crucial component in electrolyzers and fuel cell stacks, serving to separate individual electrochemical cells while ensuring electrical conductivity, water distribution, and mechanical stability. However, the high costs associated with conventional materials like titanium or stainless steel demand the exploration of novel materials and fabrication methods. Graphite-based composites have already emerged as cost-effective alternatives for BPPs. In this work, we developed and characterized an innovative composite material that combines the high electrical conductivity of titanium with the affordability and lamellar structure of graphite to create titanium-graphite composites. Microstructural analyses using scanning electron microscopy (SEM) and nano X-ray computed tomography revealed that titanium particles integrate gapless into the graphite matrix, enhancing the creation of continuous conductive pathways. Electrical conductivity measurements revealed interesting dependencies on filler composition: depending on the filler ratio, either titanium or graphite becomes the dominant contributor to the overall conductivity. These findings highlight the interrelation between particle morphology, structure, and filler ratio in optimizing the composite matrix for BPP applications.

MM 9.28 Mon 18:30 P1

Mesoporous Ti and TiCu network structures prepared by liquid metal dealloying — •Niklas Österle, Markus Ziehmer, Fabian Andorfer, and Carl E. Krill III — Institute of Functional Nanosystems, Ulm University, Germany

Metallic open-cell foams have emerged as promising functional and structural materials. The use of Ti and TiCu would extend the application of such foams into the medical field, as both materials are highly biocompatible, making them excellent choices for implants and prostheses. Combined with the porous structure of metallic foams, which facilitates the infiltration and adhesion of bone cells, the functionality and performance of prosthetic devices could be significantly improved.

In this work, we present the fabrication of mesoporous Ti and TiCu network structures via liquid metal dealloying. This technique enables the selective removal of Cu from TiCu precursor alloys within a Mg melt to form mesoporous structures. By varying the Mg-to-precursor mass ratio, we show that the chemical composition and morphology of the final network can be tailored. The network structure and morphology were investigated using 2D and 3D imaging, and EDS and XRD were employed for phase analysis. Various morphological structures can be linked to specific compounds in the TiCu phase diagram. Future investigations will focus on post-dealloying thermal coarsening.

MM 9.29 Mon 18:30 P1

Role of trace elements on the GP-Zone formation Al-Cu alloys — •Sandra Müller, Isidor Switalla, Johannes Berlin, and Ferdinand Haider — Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsbur

Both formation and dissolution of Guinier-Preston zones in Al-Cu alloys depend on the presence of excess vacancies. They are quenched in from the high temperature homogenisation treatment but will possibly disappear during the natural aging at ambient temperature. The lifetime of excess vacancies in pure Aluminium is much shorter than that in Al-Cu alloys, where vacancies presumably are trapped in GP zones. Therefore, a small increase in temperature can lead to drastic changes in the microstructure of these materials by releasing the trapped vacancies. Resistometry is a simple online method to monitor changes in the microstructure of a metallic alloy, complemented by DSC and hardness measurement.In this work we focused on natural and slightly above room temperature artificial ageing of Al-Cu samples containing 2 - 4 wt.% of Cu. DSC gives rather clear evidence that precursor cluster of only very few atoms form before the GP-zones are detected. Those precursors and the GP zones formation can be suppressed or delayed by minor addition of vacancy-binding trace elements like Tin and Indium.

MM 9.30 Mon 18:30 P1

Irradiation Induced Defects in W-Re Alloys Studied by Positron Annihilation Spectroscopy — •Lisa-Marie Krug[1], Danny 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), Technische Universität München, 85748 Garching, Germany — [2]Max Planck Institute for Plasma Physics, 85748 Garching, Germany

The plasma-facing components in a fusion reactor have to withstand the irradiation of 14 MeV neutrons, which are released in the fusion reaction of deuterium and trithium. 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 creates transmutation elements such as rhenium. In this work, the effect of rhenium on the defect characteristics in self-ion irradiated tungsten is investigated. Self-ion irradiation is used to mimic the radiation damage caused by 14 MeV neutrons. Positron annihilation spectroscopy is used to provide non destructive, atomic scale resolution measurement of the irradiation damage. Coincidence Doppler broadening spectroscopy of the 511 keV annihilation line is used to provide element sensitive measurements of vacancy type defects. This allows us to test theoretical predictions that rhenium precipitates around voids.

MM 9.31 Mon 18:30 P1

Phases of AlN by machine learning potentials — •Simon Liebing, Oliver Heymer, and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, Germany

AlN is an important wide-band gap semiconductor with e.g. applications in high power electronics. Under high pressure (about 13 GPa) the wurtzite phase transforms to the rocksalt phase. Here, we attempt to simulate this phase transition as function of temperature and pressure by means of machine learned interatomic potentials trained on accurate density functional theory molecular dynamics data. In particular we will utilize use the open-source library FitSNAP [1] for atomistic machine learning in combination with the molecular dynamics code LAMMPS [2]. FitSNAP is used to provide fast interaction potentials with accuracy inherited from DFT. It already provides interfaces for popular open-source codes such as Quantum ESPRESSO[3], PyTorch and LAMMPS and it supports the state-of-the-art atomic cluster expansion (ACE) descriptors [4]. The ACE descriptors transform structural information into machine learning models. This enables us to carry out large-scale classical MD systems of AlN with thou- sands of atoms with DFT accuracy. The results will be compared to earlier works based on small unit cells using density functional theory. [5] References [1] Rohskopf et al., Journal of Open Source Software, 8 (84), 5118 (2023). [2] A. P. Thompson et al. Comp Phys Comm, 271 10817 (2022). [3] P. Giannozzi et al. J. Chem. Phys. 152, 15 (2020). [4] Drautz, R. Physical Review B, 99 (1), 014104 (2019). [5] S.Schmerler and J. Kortus Physical Review B, 89, 6, (2014).

MM 9.32 Mon 18:30 P1

Brittle to Ductile: Elasticity and Bonding in TiVN Hard Alloys — •Santiago Gómez, Ferenc Tasnadi, Magnus Odén, and Igor A. Abrikosov — Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, 58183 Sweden

Hard alloys find extensive applications, such as in coating metal-cutting tools and turbine protective layers, among others. Despite the availability of effective alloys in the market, most remain intrinsically brittle. A critical aspect of alloy engineering is, therefore, the systematic exploration of hard but more ductile alloys with improved fracture toughness.

The low temperature dynamical instability of VN suggest an alloying pathway to improve the ductility of TiN. The idea has been realized by supporting experiments using micro-pillar fracture analysis. In this study, we are searching for novel materials descriptors to gain a better understanding of brittle and ductile behavior, all in an ideal sense suitable for modern data-driven materials science powered by Density

Functional Theory (DFT) calculations.

Our findings reveal composition-dependent variations in elastic moduli and anisotropy. Brittle to ductile behavior transition is predicted when a certain composition of Vanadium is reached. Chemical bonding analysis, employing the Quantum Theory of Atoms in Molecules (QTAIM), provide insights into the electronic structure, highlighting trends in bond critical point densities and virial ratios for first-neighbor interactions. These results are contextualized against analogous systems such as $Ti_xAl_{1-x}N$, providing a comparative framework.

MM 9.33 Mon 18:30 P1

Modeling dislocation motion in aluminium alloys by DFT — Inna Plyushchay[1,2], Anna Pliushchai[2,3], Nebahat Bulut[2], Zhengqing Wei[2], and •Sibylle Gemming[2,4] — [1]Natl. Taras Shevchenko University of Kyiv, Ukraine. — [2]Inst. Physics, TU Chemnitz, Germany — [3]Natl. TU of Ukraine, Igor Sikorsky Kyiv Polytechnic Inst., Ukraine — [4]MAIN Center, TU Chemnitz, Germany.

Measured elastic moduli of bulk metals differ from the ideal theoretical values due to the presence of point and line defects as well as grain boundaries, and their joint action has successfully been studied by atomistic simulations. For low-doped alloys with additional elements in small quantities, a plethora of further interactions is obtained, whose classical description is hampered by the lack of suitable potentials for the interaction between different elements. We therefore employ first-principles calculations to determine the dopant-induced electronic structure change in and around the core region of the Shockley partial dislocation in Aluminium as a prototype fcc metal with substitutional Mg, Zr, and Si atoms as dopants. The results indicate that the radius of the first coordination sphere changes within a range of few percent and that all discernible changes in electron density are localized within the first coordination sphere of the impurity. A tendency for the formation of aluminide precipitates is obtained, which may nucleate at 0D, 1D, or 2D defect sites and stabilize local structure motifs which would not be formed in the unperturbed bulk phase.

MM 9.34 Mon 18:30 P1

Generalized susceptibility expressed by Wannier functions — •Dominik Váňa and Jaroslav Hamrle — Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Prague

The generalized susceptibility describes the tendency (energy stability) of the cubic phase to become modulated. A typical example is the modulation of Ni_2MnGa [1] which can undergo structural transformation from austenite to a modulated structure. The generalized susceptibility is calculated using occupation probability (Fermi-Dirac distribution), however, this approach omits the dependence which the coupling coefficient of the electron-lattice interaction has on electronic states. The goal of this work is to express generalized susceptibility with calculated coupling coefficients. As the first step, we express generalized susceptibility using Wannier functions, modifying the original approach of Motizuki [2], based on a linear combination of atomic orbitals.

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MM 9.35 Mon 18:30 P1

First-principles insight into the role of electronic band filling on thermodynamic stability and mechanical properties of tantalum-diboride-based solid solutions — •Annop Ektarawong[1], Kunpot Mopoung[1], Chayanon Atthapak[1], Thiti Bovornratanaraks[1], and Björn Alling[2] — [1]Chulalongkorn University, Bangkok, Thailand — [2]Linköping University, Linköping, Sweden

Owing to their superior stabilities and mechanical behaviors at high temperature, AlB_2-type metal diborides have increasingly been considered as promising hard and protective coating materials for cutting tools. In this presentation, we theoretically demonstrate how the thermodynamic stability and mechanical properties of metal diborides can feasibly be improved either through the presence of structural defects beyond the dilute limit or through the alloying process, focusing particularly on tantalum diboride. Our first-principles studies reveal the significant enhancement of the stability, stiffness, shear strength, and hardness of the diboride can directly be interpreted in terms of electronic band filling of the bonding and antibonding states of the material.

MM 9.36 Mon 18:30 P1

Unveiling the Origin of the Yield Stress Anomaly in L12 Intermetallics via Atomistic Approaches — •Xiang Xu, Xi Zhang, and Blazej Grabowski — University of Stuttgart, Stuttgart, Germany

We present an approach to studying the yield stress anomaly (YSA) in L12 intermetallics by bridging the electronic scale with large-scale molecular dynamics simulations, using machine-learning-based interatomic potentials. An ab initio database of temperature-dependent Gibbs energy for relevant planar defects in L12 Ni3Al was developed, covering the full temperature range of the YSA. Machine-learning interatomic potentials for Ni3Al, trained through a physically informed active-learning scheme, achieved accuracy comparable to DFT data and successfully modeled key dislocation behaviors in million-atom models. These MD results enabled the development of a phenomenological model that effectively explains YSA characteristics, offering new insights into the high-temperature performance of L12-strengthened high-entropy alloys.

MM 9.37 Mon 18:30 P1

Modelling and Descriptor-based Synthesizability Analysis of High-Entropy Materials — •Chen-Chen Er[1] and Rico Friedrich[1,2,3] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [3]Duke University, Durham, USA

High-entropy materials (HEMs) are single-phase multi-component disordered systems with unique electronic 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 cation sites. There are typically five or more cation species to maximize configurational entropy.

Efficient modelling of the disordered systems is conducted based on an ensemble of supercells approach 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 results for several high-entropy ceramics, including their electronic properties and synthesizability.

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MM 9.38 Mon 18:30 P1

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

Since its introduction, the two-temperature model (TTM) has been a very powerful tool used to simulate material under strong electronic excitation following strong laser irradiation by coupled heat conduction equations for the electronic and lattice system.

Here, we present an implementation of the TTM, coupled to a molecular dynamics code, in which the heat capacity, the heat conduction, electron-phonon coupling parameter depend on the degree of excitation. We extend this model by also including an interatomic potential that depends on the degree of excitation and is capable of reproducing non-thermal effects predicted by electron temperature-dependent density functional theory calculations.

We investigate the influence and importance of each parameter in a case study applied to copper and compare our findings to experimental investigations.

MM 9.39 Mon 18:30 P1

Exploring Ionic Diffusion and Heat Transport Mechanisms in NASICON Materials: A Molecular Dynamics Study — •Insa F. de Vries and Nikos L. Doltsinis — Institute of Solid State Theory, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster

In recent years, sodium-ion batteries have emerged as both a potential replacement and a complement to traditional lithium-ion based energy storage systems [1]. However, ensuring the safety and reliabil-

ity of any future battery system requires a controlled modelling and a thorough understanding of the thermal conduction characteristics, especially with respect to preventing overheating during operation.

Our study uses molecular dynamics calculations on members of the $Na_{1+x}Zr_2Si_xP_{3-x}O_{12}$ family with different stochiometries (x=2.6, 3.4 and 3.8). For each stochiometry we use different cell geometries characterised by an order parameter. In order to reveal the influence of the sodium ion mobility on the heat transport, we calculate key transport properties, namely the sodium diffusion coefficient and the thermal conductivity. We start from a pre-established interatomic potential [2] and calculate the thermal conductivity using a Green-Kubo approach. We find that it peaks for the compounds with $x = 3.4$. Increased diffusion caused by small variations in the parameterisation of the sodium-oxygen interaction leads to simultaneous, equally directed changes in the thermal conductivity.

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MM 9.40 Mon 18:30 P1

Semiclassical transport in multiple Weyl points — •Ricardo Barbosa, Stuart Parkin, and Annika Johansson — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

We investigate transport contributions[1,2] in three-dimensional materials exhibiting multiple Weyl nodes[2,3], which are linear band touchings acting as point-like sources and sinks of Berry curvature in momentum space, often referred to as "Weyl-Berry monopoles". Specifically, we analyze the transport properties of CoSi[4,5], a chiral topologically nontrivial semimetal with band-touching points of higher-than-two-fold degeneracy and nonzero Chern numbers. Notably, at the Γ and R points, the band-touching nodes are four- and six-fold degenerate, respectively, with Chern numbers up to ±4. Using the Boltzmann transport equation[6], we investigate how these features give rise to unconventional electronic properties, focusing on the corresponding charge and node conductivities.

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MM 9.41 Mon 18:30 P1

A novel technique for measuring 3D thermal conductivity of carbon paper — •Oliver Roser[1], Achour Mahfoudi[1], Cornelius Hahn[1], and Andreas Griesinger[1,2] — [1]Center for Heat Management (ZFW), Stuttgart — [2]Baden-Wuerttemberg Cooperative State University (DHBW), Stuttgart

Gas diffusion layers based on carbon paper are used in various types of fuel cells. They make a significant contribution to dissipating the heat loss generated in the catalyst layers and homogenizing the temperature field. The material structure causes strongly direction-dependent thermal conductivities. It is not possible to determine the direction-dependent thermal conductivity under operating boundary conditions using existing methods. We present a newly developed technique with which thermal conductivity can be determined in all spatial directions. Measurements of thermal conductivity in the sample plane are carried out under steady-state boundary conditions. When measuring thermal conductivity through the sample plane, we use a transient measurement approach. The apparatus developed for this purpose and its components are presented. We show how to set and control the application-related boundary conditions such as temperature, surface pressure, moisture content and filling gas. The thermal measurements and evaluation strategies are presented, and the achievable accuracy of the method is discussed. Finally, we show initial measurement results that demonstrate a significant impact of direction, temperature and moisture content on thermal conductivity of gas diffusion layers, depending on the material structure.

MM 9.42 Mon 18:30 P1

Low-temperature thermal conductivity of $YAlO_3$ and $YbAlO_3$ — Parisa Mokhtari[1,2,3], •Ulrike Stockert[3], Stanislav Nikitin[4], Leonid Vasylechko[5], Manuel Brando[2], and Elena Hassinger[3,2] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Faculty of Physics, Technische Universität Dresden, 01062 Dresden, Germany — [4]PSI Center for Neutron and Muon Sciences, 5232 Villigen PSI, Switzerland — [5]Lviv Polytechnic National University, Lviv 79013, Ukraine

$YAlO_3$ is a popular substrate, laser, and scintillator material used at temperatures down to those of liquid helium. A good thermal conductivity is required for many applications for instance to facilitate energy release in lasers or thermal coupling via substrates.

We present for the first time thermal conductivity data on $YAlO_3$ below 80 K, covering the T range from 2 K to 300 K. In addition, we have studied the thermal conductivity of YbAlO3 in the temperature window from 50 K to 300 K. Both materials are very good thermal conductors. The thermal transport in these electrical insulators is phononic and can be fitted by the Callaway model. We discuss our results with respect to the relevance of different scattering processes, the origin of the thermal conductivity anisotropy, and the influence of Y-Yb exchange on the thermal transport. Our results on $YAlO_3$ confirm the suitability of the material for applications requiring a low thermal resistance at temperatures down to liquid He.

MM 9.43 Mon 18:30 P1

(Very) high-temperature physics of selected Planckian metals — •Zuzanna Helena Filipiak[1,2] and Andrew P. Mackenzie[1,2] — [1]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St Andrews, United Kingdom

Planckian dissipation is the mysterious phenomenon of an almost universal saturation of the electron scattering rate in many condensed matter systems despite their vastly different microscopics and strengths of electron interactions. In crystalline samples, the Planckian temperature dependence of resistivity is referred to as strange metallicity in the low-temperature regime and bad metallicity if the behaviour continues to high temperatures. Despite interest in such materials because of their unique physics, their high-temperature characteristics continues to be understudied. We 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 12 T) and atmosphere (oxygen-rich, argon, high vacuum). Our results for selected single-crystal and thin-film samples of metallic delafossites, nickelates and ruthenates, incl. ruthenium dioxide, will be presented.

MM 9.44 Mon 18:30 P1

Fitting Tensorial Properties with MACE: a Study of $Li_2Ti_5O_{12}$ Electric Field Gradient Tensors — Elena Gelzinyte[1], Karsten Reuter[1], Christian Carbogno[1], and •Johannes T. Margraf[2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

Machine learning interatomic potentials, which serve as surrogate models for predicting a structure's energy and forces, have significantly accelerated atomistic simulations. Equivalent approaches have been applied to predict other structural or atomic properties, such as charges, dipole moments, and polarisabilities. One such framework is MACE, a higher-order equivariant neural network [1]. Due to the way its internal features are constructed, the output part of the model may be readily modified to suit the symmetry of the target property. In this presentation, we discuss the required modifications for fitting atomic tensorial quantities and the resulting model's applicability, limitations, and advantages. For illustration, we focus on the prediction of electric field gradient tensors (a per-atom traceless symmetric tensor) using a $Li_2Ti_5O_{12}$ data set [2]. We consider the improvement in fitting the tensorial properties directly, rather than derived scalar properties, and compare the modified MACE's results with those of λ-SOAP [3], discussed in [2].

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MM 9.45 Mon 18:30 P1

First-Principles Analysis of Spin-Disorder Resistivity and Its Temperature Dependence — •Fabian Engelke, Felix Schug, Michael Czerner, and Christian Heiliger — Justus-Liebig-Universität, Giessen, Germany

By means of Matthiessen's rule, one can decompose the electrical resistivity of materials into contributions of separate scattering mechanisms. Here, we present ab initio calculations of the electron-magnon scattering contribution to the specific resistivity of ferromagnetic materials within the supercell method. For that purpose, we model the

spin disorder with an atomistic spin model described by a Heisenberg Hamiltonian. We then use the Landau-Lifschitz-Gilbert equation to describe the system's dynamics and introduce temperature effects utilizing Langevin dynamics. In the second step, we employ noncollinear density functional theory and the Non-equilibrium-Green's function formalism in a Koringa Kohn Rostocker (KKR) representation to calculate the conductance through slabs of varying thickness derived from the spin-configurations obtained in the first step. Subsequently, we calculate the specific resistivity by averaging over supercells and applying Ohm's Law. First results for Fe show good agreement with experimental data at high temperatures, highlighting the contribution of magnetic short-range order effects to the total temperature dependence of the specific electric resistance in the temperature regime above the Curie-Temperature.

MM 9.46 Mon 18:30 P1

Tuning intrinsic anomalous Hall effect from large to zero in two ferromagnetic states of $SmMn_2Ge_2$ — Mahima Singh[1], Jyotirmoy Sau[1], •Banik Rai[1,2], Arunanshu Panda[1], Manoranjan Kumar[1], and Nitesh Kumar[1] — [1]S N Bose National Centre for Basic Sciences, Salt Lake City, Kolkata 700106, India — [2]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Helmholtzstraße 20, 01069 Dresden

The intrinsic anomalous Hall conductivity (AHC) in a ferromagnetic metal is determined by its band structure, with spin orientation being a key band structure tuning parameter. We study a layered tetragonal room temperature metallic ferromagnet $SmMn_2Ge_2$, which gives us the opportunity to study magneto-transport properties where both the c-axis and a-axis can be magnetically easy axes depending on the temperature range we choose. We show a moderately large fully intrinsic AHC up to room temperature when the crystal is magnetized along the c-axis. Interestingly, the AHC can be tuned to completely extrinsic with extremely large values when the crystal is magnetized along the a-axis, regardless of whether the a-axis is magnetically easy or hard. First principles calculations show that nodal line states originate from Mn-d orbitals just below the Fermi energy (E_F) in the electronic band structure when the spins are oriented along the c-axis. Intrinsic AHC originates from the Berry curvature effect of the gapped nodal lines in the presence of spin-orbit coupling. AHC almost disappears when the spins are aligned along the a-axis as the nodal line states shift above E_F and become unoccupied.

MM 9.47 Mon 18:30 P1

Rapid photobleaching of Yb-doped optical fibers exposed to gamma radiation by high energy ns pulsed laser — •Esra Kendir Tekgül and Bülend Ortaç — Bilkent University UNAM, Institute of Materials Science and Nanotechnology, Ankara, 06800, TURKEY

Rare earth-doped optical fibers (OFs) have become one of the new high-power laser and sensor applications. Therefore, it is very important to protect such OFs from being exposed to external effects and to increase their reusability after these effects. Here, Radiation Induced Attenuation (RIA) and the Photo-darkening (PD) processes play an important role. The main source of the problem is the color centers formed in the OF. Preventing or recovering these formations before and after the production of OF is of great importance in both efficient and long-lasting systems.

To determine the behavior of Yb-doped OF, they are exposed to gamma radiation or PD. The important recovery process is photobleaching (PB) for defects due to the gamma radiation. In our study, a rapid and efficient PB process was achieved using a high-energy nanosecond pulse to recover existing and/or revealed color centers in OF that had been irradiated with 10 kGy of gamma radiation. The PB process was analyzed based on the wavelength and energy of the pulsed light source. The highest level was achieved with the 532 nm wavelength laser. The findings indicate that the recovery of color centers can reach up to 96% in a shorter duration (hours) compared to results from studies utilizing continuous lasers.

MM 9.48 Mon 18:30 P1

Design of a setup for conducting experiments synchronized with sample scanning — •Maksim Khasanov — Moscow, Russia

The paper focuses on designing equipment with an electronic drive for compressing samples during experiments, aimed at analyzing their internal structure using computed tomography. The manual compression system previously used prolonged the experiment due to time-consuming data processing. The new electronic system significantly reduces the time required by automating the compression process. The work includes the design of the compression apparatus and its electric drive, providing a more efficient and precise solution for experimental procedures.

MM 9.49 Mon 18:30 P1

Extreme stability of $CoCrFeMnNi_{60}$ multicomponent alloys after severe plastic deformation — •Lukas Musiol[1], Mohan Muralikrishna Garlapati[1], Shabnam Taheriniya[1], Lukasz Rogal[2], Sergiy Divinskiy[1], Harald Rösner[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institute of Metallurgy and Material Science, Polish Academy of Science, Reymonta 25 St., 30-059 Krakow, Poland

Thermal stability of a (CoCrFeMn)Ni60 multicomponent alloy is investigated using in-depth microscopic examination. The specific composition is chosen as a transition one from "high-entropy" to "concentrated alloy" behavior. Such compositional design mimics a conventional alloy design of solutes in the terminal solid solution range but in equiatomic concentrations. Along with the analyses of the homogenized samples, an analysis of compressed and rotary swaged samples was performed to investigate the influence of deformation on the phase stability. The phase stability is investigated at intermediate temperature for prolonged annealing times, which has given an in-depth understanding of the formation and growth of new phases or precipitates. Detailed microscopy analyses were performed to determine the phases and their composition. Overall, the (CoCrFeMn)Ni60 multicomponent alloy has shown a stable microstructure even after extreme deformation and after prolonged heat treatments. The phase stability results, in conjunction with deformation and microstructure, will be correlated and discussed in detail.

MM 9.50 Mon 18:30 P1

Influence of Supercell Size Effects on the Mechanical Properties and Electronic Structure of High-Entropy Transition Metal Diborides ($HETMB_2$) — Inna Plyushchay[2], •Nebahat Bulut[1], Anna Pliushchai[1,3], and Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz, Germany — [2]Institute of Physics, National Taras Shevchenko University of Kyiv, Ukraine — [3]National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"

Modeling various supercell sizes for high-entropy transition metal diborides ($HETMB_2$) holds the potential to overcome the computational challenges associated with their unique bonding configurations and complex compositions. First-principles calculations were used to predict the electronic and elastic properties of high-entropy transition-metal diborides after employing supercells with a variety of atomic configurations and complex compositions. We found that larger supercells allowed for clustering of atoms of the same metal type, as evidenced by broadening of the peaks in the histogram of interatomic distances. This, however, had no significant influence on the mechanical properties. The mechanical properties of $HETMB_2$ are determined by the number of electrons, size of atoms or polarizability. However, the average number of d-electrons per metal atom was found to be crucial because it affects the Fermi level position relative to the pseudogap, and this impacts the elastic properties strongly in comparison to the binary-TMB_2.

MM 9.51 Mon 18:30 P1

Ab initio calculations of defects in the Mg2Ge intermetallic — •Pavel Papež[1,2], Martin Friák[2], and Martin Zelený[1] — [1]Institute of Materials Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Institute of Physics of Materials, Czech Academy of Sciences, v. v. i., Brno, Czech Republic

This work is focused on ab initio calculations of different types of defects in the Mg2Ge intermetallic in order to explain a higher concentration of Mg in experimental samples. Our calculations employed VASP software and include antisite defects and vacancies on both sublattices and furthermore interstitial additions of both Mg and Ge, all in charge neutral state. The calculations were also done with the modified Becke-Johnson potentials to study their influence on the bandstructure of this semiconductor. We have calculated their formation energies in regards to Mg rich and Ge rich chemical potential limits. The phonon calculations were done to acquire the defect equillibrium concentration and the evolutiuon of defect formation energies with temperature.

MM 9.52 Mon 18:30 P1

Glass transition and physical aging studies of a gold based Bulk metallic glass by means of flash scanning calorimetry — •Klara Otto[1], Valerio Di Lisio[2], Daniele Cangialosi[2], and Isabella Gallino[1] — [1]Technische University Berlin, Chair for Metallic Materials, Berlin, Germany — [2]DIPC, San Sebastián, Spain

Flash scanning calorimetry is used to study the glass transition of metallic glasses, during direct solidification from the melt [1,2] and by reheating with rates up to thousands of K/s. This enables the access to the supercooled liquid state by avoiding crystallization during the cooling stages.

Glassy materials relax over time when held below the glass transition temperature, to minimize their excess thermodynamic properties. A new methodology to compare the relaxation times related to the atomic mobility with those determined throughout glassy aging of a gold based metallic glass, is presented. Isothermal physical aging was performed to retrieve the temperature dependent timescales of the alpha relaxation. Additionally, the characteristic time of glassy relaxation are retrieved in a wide temperature range [3] complemented with fictive temperature analysis.

The combined data were plotted on an activation diagram, that relates relaxation times to the inverse of temperature. This allowed to investigate relaxation time scales spanning 7 orders of magnitude using a single experimental technique.

[1] Di Lisio, V,(2023),Nat. Commun.,14(1),[2] Monnier, X,(2020),Sci. Adv.,6(17),[3] Gallino, I,(2018), Acta Mater.,144

MM 9.53 Mon 18:30 P1

Glass Forming Ability, Thermal and Magnetic Properties of the Multicomponent Fe-Mo-P-C-B-Si Metallic Glass for AM Applications — •Alejandro Lejtman Rotberg[1], Amirhossein Ghamivi[2], Lucas M. Ruschel[2], Izzi A. Ahmad[1], Uma Rajput[3], Purbasha Sharangi[3], Paola M. Tiberto[2], Ralf Busch[2], and Isabella Gallino[1] — [1]Technical University of Berlin, Chair for Metallic Materials, Ernst-Reuter-Platz 1, 10587 Berlin, Germany — [2]Saarland University, Chair of Metallic Materials, 66123 Saarbrücken, Germany — [3]INRIM, Strade delle Cacce 91, Torino, Italy

Efficient power-to-work conversion in electric vehicles (EVs) requires soft magnetic materials with low coercivity. Fe-based metallic glasses reduce power losses but struggle achieving casting thicknesses over 1mm due to limited glass-forming ability (GFA). Additive manufacturing (AM), like Laser Powder Bed Fusion (LPBF), provides solutions, with recent studies revisiting Fe-Si-B compositions for processability and performance [1-3]. This study evaluates the alloy Fe74Mo4P10C7.5B2.5Si2. X-ray diffraction (XRD) results of cast plates and ribbons determined the GFA. Thermal properties were analyzed via Differential Scanning Calorimetry (DSC) and Differential Thermal Analysis (DTA), while magnetic properties using Vibrating Sample Magnetometry (VSM). Results suggest the alloy's potential for AM production of soft magnetic components for EVs.[1] Thorsson, L., et al. Selective Laser Melting. Materials & Design.[2] Rodríguez-Sánchez, M., et al. Relating Laser Powder. Materialia.[3] Sadanand, S., et al. Laser Powder Bed Fusion. Journal of Laser Applications.

MM 9.54 Mon 18:30 P1

An atomistic study on the role of size and composition on the structural and thermodynamic properties of Al-Pd bimetallic nanoparticles during melting and solidification. — •Dario Gonzalo Escriba Quispe[1], Justo Alcides Rojas Tapia[1], and Gustavo Cuba Supanta[1,2] — [1]Universidad Nacional Mayor de San Marcos, Lima, Peru — [2]Universidad Privada del Norte, Lima, Peru

Bimetallic nanoparticles (NPs) of Al-Pd exhibit structurally complex phases, as well as quasicrystalline approximants to the Al-Mn-Pd system, which, combined with their controversial and complex phase diagram, makes them an interesting subject of study. In this work, using molecular dynamics, the structural and thermodynamic properties of Al(x)Pd(100-x) NPs at different sizes and compositions are calculated.

The processes of melting and solidification are simulated using the open-source LAMMPS package and a MEAM-type potential. It was found, through the calculation of heat capacity, that the melting temperature and size of AlPd, Al2Pd5, and Al1Pd4 NPs follow a linear behavior, in agreement with the scaling law. Additionally, the RDF graphs of AlPd NPs show that it is an ordered intermetallic compound, with structural parameters such as the crystal structure and lattice parameter matching those reported experimentally. The Al1Pd4 nanoalloy was explored, where it was found that the NP has an icosahedral shape. However, the atoms exhibit internal ordering with regions showing FCC and HCP crystal structures. Finally, other additional results such as MSD, common neighbor analysis (CNA), the Warren-Cowley parameter, excess energy, and phonon dispersion are presented.

MM 9.55 Mon 18:30 P1

An X-ray diffraction study of copper powder for laser-based powder bed fusion — •Eric Schneider[1], Robert Ortmann[2], Julia Frank[3], Fabienne Hellwig[3], Tobias Grimm[2], Michael Blüm[3], Lena Friedrich[1], Michael Paulus[1], Jaqueline Savelkouls[1], Jan T. Sehrt[2], Christian Sternemann[1], and Arne Röttger[3] — [1]Universität TU Dortmund, Maria-Goeppert-Mayer-Straße 2, D-44227 Dortmund — [2]Ruhr-Universität Bochum, Universitätsstraße 150, D-44801 Bochum — [3]Bergische Universität Wuppertal, Bahnhofstraße 15, D-42651 Solingen

Additive manufacturing (AM) of components using laser-based powder bed fusion of metals (PBF-LB/M) has reached market maturity. This layer-by-layer process offers advantages over casting and subtractive methods, especially for producing complex parts with internal cavities and is promising to produce topology-optimized lightweight structures. However, the use of copper powders for PBF-LB/M based AM poses challenges due to its high thermal conductivity and reflectivity. The directed oxidation and reduction of the copper particle surfaces can improve both, the powders processability and reusability. In this study we investigate the oxidation of pre-treated copper powders in air and its controlled reduction using $Ar/2\%H_2$ atmosphere at different temperature conditions up to 350°C by X-ray diffraction at beamline BL9 of DELTA synchrotron radiation source in order to reveal information about induction times and change in Cu, Cu_2O, and CuO phase composition for industrial processing. This research is funded by the DFG via projects RO 4523/9-1, SE 2935/6-1, and STE 1079/9-1.

MM 9.56 Mon 18:30 P1

Linking Process Parameters and Heat Treatment to Microstructural Properties of PBF-LBM 316L Steel for Structural Hydrogen Use — •Tim Haag, •Kai Stefan Lagemann, Stefan Wagner, and Astrid Pundt — Institut für Angewandte Materialien - Werkstoffkunde (IAM-WK), Karlsruher Institut für Technologie (KIT)

Additively manufactured (AM) 316L steel produced by powder bed-based laser melting (PBF-LBM) can be considered for sophisticated applications in hydrogen technology. This project investigates the influence of manufacturing parameters and post-processing treatments, such as heat treatment, on the resulting microstructure and its implications for material properties. The objective is to optimise the manufacturing process in order to achieve components with minimal porosity. The microstructure is comprehensively analysed using advanced techniques, which reveal hierarchical features and a complex interplay of various microstructural elements, including multiscale porosity, varying grain orientations and subgrain dislocation cells. Heat treatments are applied to alter microstructural characteristics and assess their impact on material properties.

MM 9.57 Mon 18:30 P1

Analysis of the Crack Formation in Printed Nanosilver Using In Situ Bending Technique — •Lennart Schwan[1], Michaela Klöcker[1], Michael Feige[1], Laila Bondzio[2], Thomas Kordisch[1], and Sonja Schöning[1] — [1]Bielefeld Institute for Applied Materials Research (BIfAM), Faculty of Engineering and Mathematics, Bielefeld University of Applied Sciences and Arts — [2]Thin Films & Physics of Nanostructures, Bielefeld University, Department of Physics

3D printing is an emerging technology with a wide range of applications. The modern multi-material jetting process, as used in the Nano Dimension Dragonfly Pro LDM, makes it possible to print dielectric and conductive materials in a single process. In addition to electrical circuits such as coils, capacitors, etc., strain gauges can also be printed.

The change in resistance of strain gauges is usually caused by the change in the geometric dimensions of the conductive layer when it is deformed. In the case of the printed material examined in this study, it is also known that the material is permeated by cracks which cause a directional dependence of the electrical conductivity.

The objective of this study is to investigate how these cracks develop during bending and thus also contribute to the change in resistance. For this purpose, a test specimen is loaded under a three-point bending test using a special in situ bending module. In order to investigate the propagation and formation of the cracks, the bending module is positioned in a scanning electron microscope in order to analyze the cracks under loading with a sufficient image resolution.

MM 9.58 Mon 18:30 P1

Atomistic Simulation of Laser-based Powder Bed Fusion of Metals — •Aamir Siddiqui, Simon Kümmel, and Johannes Roth — FMQ, University of Stuttgart, Germany

Additive manufacturing technology applications continue to call for increased reproducibility and quality. The goal is to study the melting and solidification of an AlTi alloy and to create a framework that allows for further studies on arbitrary alloys and metals. Molecular dynamics provides an understanding of the melting and ablation process, resulting in an understanding of different heat transfer mechanisms. The simulation framework makes it possible to see how changes in scanning speed and laser power affect the melting dynamics.

The melting process of alloys shows that a significant amount of argon gas becomes trapped inside the sample. The simulation of powder beds formed by spheres of varying sizes reveals holes that vanish under vacuum conditions, but persist when the simulation box is filled with protective gas, providing information on the creation of defects. By deforming the sample, the influence of gas pockets on the mechanical properties and the evolution of the lattice structure within the sample can be seen.

MM 9.59 Mon 18:30 P1

Nanoscale characterization of AM316L stainless steel for hydrogen application — •Gabriele Palazzo, •Felix Stierle, Kai Stefan Lagemann, Christian Kübel, Stefan Wagner, and Astrid Pundt — Karlsruhe Institute of Technology, Karlsruhe, Germany

Additive manufactured (AM) austenitic stainless steel 316L prepared by selective laser melting (SLM) is characterized by advanced nanoscale characterization techniques to examine its microstructural features. High-resolution scanning TEM (HR-STEM), selected area diffraction (SAD), and analytical methods such as energy-dispersive X-ray spectroscopy (EDX) as well as electron energy loss spectroscopy (EELS) are employed. Typical SLM printing structures (equiaxial and columnar cellular structure, nano-inclusions) are observed with atomic resolution both for as-built and tensile tested samples. The presence of silicon-manganese oxide nano-inclusions, preferential chromium and molybdenum segregation around them is revealed, as well as iron depletion and chromium enrichment along the cell boundaries. This peculiar multi-scale AM microstructure accounts for the unique mechanical properties of AM316L in terms of resistance and ductile behaviour, if compared to the conventionally manufactured counterpart, allowing to overcome the trade-off between strength and ductility.

MM 9.60 Mon 18:30 P1

Fine-tuning of machine learning interatomic potential for the prediction of phonon properties — •Jonas Grandel, Philipp Benner, and Janine George — Bundesanstalt für Materialforschung und Prüfung, Berlin

Accurate phonon predictions are critical for assessing material stability and thermal behavior, but traditional approaches based on density functional theory (DFT) are computationally expensive, motivating the need for accelerated alternatives. In this work, we investigate the performance of the machine learning interatomic potential MACE-MP-0 for predicting harmonic phonons and thermal properties. The focus is on fine-tuning MACE-MP-0 using various sets of rattled structures and different hyperparameter to identify the most effective strategy for improving model accuracy. We want to develop a general fine-tuning workflow based on the foundational model that can be used to fast and accurately generate phonons to predict both stability and thermal properties. For this purpose, a benchmark dataset was constructed using DFT consisting of a broad range of different crystal systems and mainly of phase change materials and thermoelectric materials. Each fine-tuned model targets one specific material, allowing to improve each material individually. The results demonstrate significant improvements in the prediction of phonon band structures, with a root mean square error (RMSE) reduced from 0.6 THz for the original MACE-MP-0 model to 0.3 THz for the fine-tuned models. In addition, performance in terms of computational speed was improved by up to a factor of 10 compared to traditional DFT-based phonon calculations.

MM 9.61 Mon 18:30 P1

Learning the Reduced Density Matrix Functional from Quantum Processors and Using Density Matrix Embedding Theory to Extend its Universality — •Martin Uttendorfer — Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Deutschland

The advent of quantum computing makes reduced density matrix functional theory (RDMFT) on an exact level viable. By directly applying RDMFT, derived from Levy-Lieb's constrained search, this work leverages quantum processors to overcome some of DFT*s shortcomings, enabling more accurate modeling of quantum chemical and condensed matter systems. The proposed approach incorporates quantum algorithms that utilize variational quantum eigensolvers (VQE), which is viable to be executed on near-term intermediate scale quantum devices (NISQ) in conjunction with machine learning techniques. This work examines the theory*s application to different particle types, including fermions, bosons, and hard-core bosons, highlighting the flexibility of the RDMFT framework. Additionally, density matrix embedding theory (DMET) is incorporated, allowing for a hybrid classical-quantum approach that extends the functional*s universality. This work presents a quantum algorithmic approach to obtain the functional and provides a computational strategy for studying complex many-body systems while keeping the use of limited quantum resources to a minimum.

MM 9.62 Mon 18:30 P1

Integrating Long-Range Interactions into Machine Learning Interatomic Potentials — •Tulga-Erdene Sodjargal[1,2], Egor Rumiantsev[1], Philip Loche[1], and Michele Ceriotti[1] — [1]Laboratory of Computational Science and Modeling (COSMO), Institute of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Department of Bio and Brain Engineering, Korea Advanced Institute of Science and Technology (KAIST), 34141 Daejeon, Republic of Korea

Machine learning-based interatomic potentials (MLIPs) often rely on the locality ansatz, calculating atomic energies based on a fixed cutoff radius. While effective for many systems, this nearsightedness can lead to inaccuracies when long-range interactions, such as ionic interactions, dominate. To overcome this limitation, we integrate Particle Mesh Ewald (PME) techniques into existing MLIP frameworks. Our extension is modular and plug-and-play, requiring minimal modifications to incorporate into various models. We demonstrate significant improvements in both simple architectures, such as Behler-Parrinello Neural Networks, and advanced models, including state-of-the-art graph neural networks like the Point Edge Transformer (PET).

MM 9.63 Mon 18:30 P1

pyiron - Automated Workflows for Materials Science — •Jan Janssen[1], Marvin Poul[1], Sarath Menon[1], Tilmann Hickel[2], and Joerg Neugebauer[1] — [1]MPI for Sustainable Materials, Düsseldorf, Germany — [2]BAM Federal Institute for Materials Research and Testing, Berlin, Germany

The pyiron framework, originally developed for atomistic simulations in the field of materials science, has recently been extended beyond the atomistic scale to enable data-driven materials design on all scales and including experiments. As a central interface for materials acceleration platforms (MAP), pyiron couples simulation methods ranging from ab-initio methods of the electronic scale, to the atomistic scale of machine-learned interatomic potentials and up to the continuum scale of crystal plasticity modelling with interfaces for experimental equipment and machine learning.

On our poster, we give a brief overview of the recent developments in the pyiron project and highlight a series of materials science applications. These range from pyiron_workflow, our redesigned graph-based workflow engine, to executorlib for up-scaling workflows for high-performance computing (HPC) and the python workflow definition, a joined standard developed in collaboration with AiiDA and jobflow, the workflow engine of the materials project. At the same time, the poster will provide an opportunity to meet the pyiron developers and discuss ideas and future applications.

Read more about pyiron on our website: https://pyiron.org

MM 9.64 Mon 18:30 P1

Investigating the Impact of Optimization Algorithms on Element-Substitution Based Materials Discovery — •David Greten[1], Konstantin Jakob[1], Karsten Reuter[1], and Johannes T. Margraf[2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

In this study, we investigate how different optimization algorithms affect the relaxation of inorganic structures using general-purpose machine-learned interatomic potentials (MLIPs) like MACE-MP-0. Assessing computational efficiency and relaxation quality via structural similarity and kernel distance metrics, we find that optimizer

choice significantly influences performance and can lead to different equilibrium structures. Analyzing both DFT-relaxed structures from the Materials Project and element-substitution based trial structures, we highlight the optimizer's impact in different scenarios. Our findings emphasize the critical role of optimizer selection in large-scale computational materials science workflows, particularly in the context of element-substitution based materials discovery. This can hopefully guide the community towards choosing appropriate algorithms for efficient and reliable structure relaxations.

MM 9.65 Mon 18:30 P1

The APyT Package: From Raw Data to Three-Dimensional Reconstruction — •Sebastian Eich — Department for Materials Physics, Institute for Materials Science, University of Stuttgart

The APyT package is an advanced, open-source Python framework for evaluating atom probe tomography (APT) data. It offers a suite of modules that automate key steps in APT processing, from mass spectrum calibration to three-dimensional sample reconstruction. Its modular architecture ensures seamless integration with external tools through standardized input/output interfaces, supporting both Linux and Windows environments.

Key features include high efficiency with NumPy and Numba, a low memory footprint, and extensive documentation. The modules are highly automated, requiring minimal user input to achieve accurate results. The package also integrates SQL database management for raw measurement data and corresponding metadata.

The mass spectrum module automatically calibrates and detects peaks, producing high-resolution spectra. The mass spectrum fitting module further refines this by fitting spectra with an analytical function, automatically de-convolving overlapping peaks by incorporating isotope abundances. The reconstruction module generates a 3D sample reconstruction, including automatic chemical identification and export capabilities. Future enhancements include a PyQt-based GUI to streamline access to all APyT modules in one application.

MM 9.66 Mon 18:30 P1

Relation between the electronic structure and X-ray absorption spectra discussed using multiple-scattering formalism — Hubert Ebert[1], •Sergiy Mankovsky[1], and Jan Minar[2] — [1]LMU of Munich, 81377 Munich, Germany — [2]University of West Bohemia, Pilzen, Czech Republic

Recently, the concept of crystal orbital overlap population (COOP) has been reconsidered [1] based on the finite difference method (FDM), representing the calculated x-ray absorption spectra (XAS) in terms crystal orbital overlap population functions. This allows to reveal the correlation between XAS and the formation of the bonding/antibonding states in solids. Following the idea suggested in Ref. [1], we demonstrate that this relation can be investigated in a very efficient way using the multiple scattering formalism for electronic structure calculations. In this representation, both, the density of states and the x-ray absorption function are determined by the site-diagonal scattering path operator $\tau^{00}(E)$ which can be expressed as $\tau^{00}(E) = t^0 + \sum_n \tau^{0n}(E)\, G^{n0}(E)\, t^0$, in terms of the single-site scattering matrix t^0, the site-off-diagonal operators $\tau^{0n}(E)$, and the structural Green function $G^{n0}(E)$. The second term determines in a pair-wise resolved way the fine structure of the electron density of states (DOS) $n(E)$ as well as the XAS absorption coefficient $\mu(E)$. The DOS and the normalized x-ray absorption coefficient are calculated for several representative systems and discussed in line with the idea of the COOP concept.

[1] M. Diaz-Lopez, *et al.*, J. Phys. Chem. A **124**, 6111 (2020)

MM 9.67 Mon 18:30 P1

Upgrading the Coincidence Doppler Broadening Spectrometer at FRM II — •Danny R Russell, Francesco Guatieri, Leon Chryssos, and Christoph Hugenschmidt — FRM II - Technische Universität München, München, DE

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

We present simulations and hardware design for an upgrade to the CDBS which will allow backscattered positron capture. Up to $\sim$ 40 % of the incident positrons are backscattered when they reach the sample surface. The annihilation events occurring when these backscattered positrons return to the sample or annihilate in experimental hardware contribute unwanted signal to the measured spectrum which cannot be removed in data processing.

We use an in-house particle tracking code to design a positron dump that will capture backscattered positrons at an electrode outside detector lines of sight. This will reduce the unwanted signal by up to 50 % and improve the quality of CDBS data. Additionally, we apply the same code to optimize an electrostatic focusing lens, further increasing the spatial resolution of the instrument.

MM 9.68 Mon 18:30 P1

High-entropy alloy pre-screening for lead-free halide double perovskites from material databases — •Marina S. Günthert[1,2], Bernd Meyer[1], and Christoph J. Brabec[2] — [1]Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg — [2]Materials for Electronics and Energy Technology (i-MEET), FAU Erlangen-Nürnberg

Over the last decade, lead-free halide double perovskites with composition $A_2BB'X_6$ have emerged as an interesting class of materials for optoelectronics. Furthermore, it was suggested to introduce different ion ratios on each of the double perovskite sublattices, leading to a vast space of possible compositions.

Two criteria are applied to have a first fast filtering approach to reduce the number of combinations. First, the search is limited to non-toxic and non-f elements for a green chemistry approach. Second, we estimate the thermodynamic stability of the compounds by using a criteria recently proposed by Muzzillo *et al.* [1], which focuses on the entropy stabilization by using several elements on each sublattice. This method can be easily adjusted for halide double perovskites. We applied it first to the Materials Project database but it can also be extended to other databases such as NOMAD and OQMD. In the end, this pre-screening gives an idea, which elements on the different sublattices of the double perovskite are worth further exploration.

[1] C.P. Muzzillo, C.V. Ciobanu, D.T. Moore, High-entropy alloy screening for halide perovskites, Mater. Horiz. **11** (2024) 3662-3694

MM 9.69 Mon 18:30 P1

Effect of $4f$ occupancy on L_3 edge of Cerium — •Prathibha Chandrashekhar, Patrik Thunström, Felix Sorgenfrei, and Heike Herper — Department of Physics and Astronomy, Uppsala University, Sweden

The valence $4f$ electrons in Cerium exhibit a strong itinerant tendency, allowing them to exist in a mixed-valence regime, between localized and delocalized states. This regime hosts correlated electron phenomena which has profound implications on the material's magnetic, transport, and electronic properties. The shift in $5d$ orbitals to higher energy levels, due to reduced screening from delocalized $4f$ electrons, provides critical insights into electronic properties. We study this shift by probing $2p$ to $5d$ transition using X-ray Absorption Spectra(XAS). However, accurately modeling the light-matter interaction in such systems remains challenging due to the itinerant nature of the $4f$ electrons, strong core-hole effects, multiplet interactions, and hybridization dynamics. In this work, we employ advanced theoretical approach that combines density functional theory (DFT) with multiplet ligand-field theory (MLFT). This method enables computation of $L_{2,3}$-edges by constructing and solving single-impurity Anderson model (SIAM) derived from first-principles calculations. Additionally, we investigate sensitivity of the computed spectra to Slater integrals, hybridization effects, and core-hole relaxation, offering new insights into the intricate electronic behavior of Cerium-based systems. PC acknowledges partial funding from Horizon Europe MSCA Doctoral Network grant n.101073486, EUSpecLab, funded by European Union.

MM 9.70 Mon 18:30 P1

Stability of AgI Polymorphs and the AgI(0001) Surface Reconstruction — •Angela Rittsteuer[1], Andrea Conti[2], Michael Schmid[2], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics, 1090 Vienna, Austria — [2]TU Wien, Institute of Applied Physics, 1040 Vienna, Austria

Silver iodide (AgI) is a compound widely used in cloud seeding due to its ability to act as an effective nucleating agent for cloud condensation. Under ambient conditions, AgI crystallizes in hexagonal or cubic close-packed structures, the most prominent polymorphs being the wurtzite and the zincblende structure. A comprehensive under-

standing of its groundstate structures and phase behavior is essential not only to optimize its role in cloud condensation but also to explore broader applications in solid-state chemistry and catalysis.

To investigate the stability of AgI polymorphs, we perform extensive benchmarking studies across various levels of theory. These include Density Functional Theory with different approximations for the exchange-correlation energy, hybrid Hartree-Fock Density Functionals, and the Random Phase Approximation, offering a hierarchy of accuracy. Building on recent atomic force microscopy studies of the wurtzite AgI(0001) surface, we further provide theoretical insights by developing a machine-learned force field and applying simulated annealing and parallel tempering to study the surface reconstruction.

MM 9.71 Mon 18:30 P1

Investigation of Lloyd's formula at finite electronic temperatures — •Christian Maas[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen

In DFT calculations within the Korringa-Kohn-Rostoker (KKR) Green's function formalism the integrated density of states is analytically given by Lloyd's formula. Its better l-convergence can be used for a precise determination of the Fermi energy and a charge density normalization. In the past it has been shown that for finite electronic temperatures the calculation of Lloyd's formula can in principle be done on the same energy mesh that is used for the calculation of the charge density [1]. These calculations require to numerically evaluate the derivative of Lloyd's formula. We show that it is possible to accurately determine the derivative without using additional energy mesh points. This is done by interpolating Lloyd's formula with cubic splines which in turn are used to calculate the derivative. We compare the method to calculations without electronic temperatures and show that the spline interpolation does not lead to a significant accuracy lost.

[1] R. Zeller 2005 J. Phys.: Condens. Matter 17 5367, https://dx.doi.org/10.1088/0953-8984/17/35/005

MM 9.72 Mon 18:30 P1

Fiber composite materials in construction of go-cart. — •Mikhail Brusnikin — Moscow, Russia

Lightweighting any vehicle, especially sports equipment, has always been a pertinent issue, and I aimed to determine how significantly material substitution would affect the mass of the power structure by using modern composite constructions instead of classical steel solutions, with the condition of maintaining the same torsional stiffness as the steel sample.

Fiber composite materials are currently at the forefront of technology in terms of stiffness-to-weight ratio and are sufficiently accessible for my research, which was focused on their application in a sports device such as a go-kart.

The assumptions regarding the weight of the final product, which were proposed at the beginning of the research, turned out to be erroneous. Even in the best-case scenario, the weight reduction of the construction was less than anticipated.

MM 9.73 Mon 18:30 P1

RuNNer 2.0: An Efficient and Modular Program for High-Dimensional Neural Network Potentials — •Alexander L. M. Knoll[1,2], Moritz R. Schäfer[1,2], K. Nikolas Lausch[1,2], Moritz Gubler[3], Jonas A. Finkler[3], Alea Miako Tokita[1,2], Gunnar Schmitz[1,2], Henry Wang[1,2], Richard Springborn[1,2], Marco Eckhoff[4], 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]Department of Physics, Universität Basel, Switzerland — [4]Laboratorium für Physikalische Chemie, ETH Zürich, Switzerland

Machine learning potentials (MLPs) have become an important tool for atomistic simulations in chemistry and materials science. As methods in this domain grow increasingly complex and mature, the creation of efficient and user-friendly libraries now receives a lot of attention. We introduce the second major release of RuNNer, an open-source, standalone software package designed for constructing and evaluating second-, third-, and fourth-generation high-dimensional neural network potentials (HDNNPs). RuNNer 2.0 integrates the entire workflow into a fully OpenMP- and MPI-parallel program: from generating atomistic descriptors, via training a specific machine learning model, to its application in molecular dynamics simulations.

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Hybrid soldering: Interfacial flux-doping of Cobalt nanoparticles hindering the formation and growth of intermetallic compound (IMCs) layers — •Farzad Khodabakhshi[1,2], Irina Wodak[1], Andriy Yakymovych[1], Gerhard Wilde[2], and Golta Khatibi[1] — [1]Vienna University of Technology — [2]University of Münster

The study investigated hybrid nanocomposite soldering of copper components using a lead-free tin-based solder alloy (Sn-3.5 wt% Ag). To suppress the growth of intermetallic compound (IMC) layers, specifically Cu3Sn and Cu6Sn5, at the interface between the solder alloy and the copper substrate during reflow solidification, a modified flux containing cobalt nanoparticles was applied. The research focused on the effects of incorporating cobalt nanoparticles in different fractions, up to 1.0 wt%, on the microstructural development of the soldered joints and the formation of IMC layers. Additionally, the impact of post-soldering aging treatment, conducted at approximately 180°C for extended periods (up to around 20 days), was assessed. The study analyzed how the alloying of cobalt nanoparticles affected the structure of Cu3Sn and Cu6Sn5 IMC layers, as well as the Sn-based solder alloy. This was done using energy-dispersive X-ray spectroscopy (EDS) elemental mapping in conjunction with field emission-scanning electron microscopy (FE-SEM). Furthermore, the microstructural evolutions of the soldered joints, influenced by the contribution of Co-nanoparticles and the aging treatment, were characterized and discussed using electron channeling contrast imaging (ECCI) microscopy.