FM 6: Focus Session: Materials Discovery I – Material informatics

chairs: Anna E. Böhmer (Ruhr Universität Bochum, DE), Suguru Yoshida (Kyoto University, JP)

Discovering new functional materials is crucial to advance today's technologies, ranging from caloric cooling via catalysis to next-generation energy conversion and storage, such as thermoelectric, ferroelectric, and ionic conductor materials. New materials also form the basis for potential applications in quantum information technologies. This session provides a platform to highlight functional materials discoveries and how they come about. Notably, systematic searches with high-throughput synthesis approaches, as well as predictions from materials informatics, have helped to go beyond serendipitous discoveries in recent years. However, intuition guided by general principles remains an important factor. In this session, we particularly welcome contributions that showcase the discovery of new functional materials with original approaches. Diverse material systems - from well-established to emerging and niche classes across condensed-matter and materials physics - will be featured. Bringing together diverse discoveries in a single session will help delineate general principles and inspire future work.

Time: Tuesday 9:30–12:45 Location: BEY/0138

Invited Talk FM 6.1 Tue 9:30 BEY/0138

Robust Data Generation, Heuristics and Machine Learning for Materials Design — •Janine George — BAM Berlin, Germany — University of Jena

Machine learning (ML) offers new routes to overcome the limitations of density functional theory (DFT) for advanced materials. We present data-generation strategies and workflows for ML interatomic potentials, including large-scale quantum-chemical bonding analysis.[1,2,3] Incorporating bonding descriptors into ML models enables prediction of phononic properties and validation of correlations between bonding strength, force constants, and thermal conductivity.[3] We introduce autoplex, an automated framework for training ML potentials, supporting general-purpose and phonon-focused workflows.[4] These developments provide a basis for fine-tuning foundation models for thermal transport at reduced cost.[5] For properties such as magnetism or synthesizability, we discuss complementary approaches, comparing ab initio methods with chemical heuristics and experimental data-driven ML models.[6,7] Our work advances scalable, accurate simulations for materials discovery.

References: [1] M. K. Horton, et al. Nat. Mater. 2025, 24, 1522*1532. [2] A. M. Ganose, et al., Digit. Discov. 2025, 4, 1944*1973. [3] A. A. Naik, et al. Sci. Data 2023, 10, 610. [4] Y. Liu, et al. Nat. Commun. 2025, 16, 7666. [5] J. Bustamante, et al. 2025, DOI 10.48550/arXiv.2510.23133. [6] S. Amariamir, et al. Digit. Discov. 2025, 4, 1437*1448. [7] K. Ueltzen, et al. 2025, DOI 10.26434/chemrxiv-2025-xj84d.

FM 6.2 Tue 10:00 BEY/0138

Data-driven Discovery of 2D Non-van der Waals Materials and Design of Their Heterostructures — Anastasiia Nihei[1,2], Tom Barnowsky[1,2], and •Rico Friedrich[1,2] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf

Two-dimensional (2D) materials and their heterostructures are a platform to realize advanced electronic and magnetic functionalities at the nanoscale. With traditional 2D systems extracted from weakly van der Waals (vdW) bonded bulk layered compounds, the experimental fabrication of semiconducting non-vdW 2D materials obtained from non-layered crystals [1] came as a surprise.

In our recent data-driven investigations [2], we discover several dozens of new candidates exhibiting appealing electronic, optical, and magnetic properties owing to the (magnetic) cations at their active surfaces. The electronic and magnetic properties of these next generation 2D compounds are also demonstrated to be controllable by a surface chemistry approach employing for instance hydrogen passivation [3]. Eventually, their chemically bonded interfaces in non-vdW heterostructures [4] give rise to qualitatively new properties and potential functionalities including hybrid interface bands, strong magnetic coupling, and characteristic strong moiré property variations upon twisting.

[1] A. Puthirath Balan *et al.*, Nat. Nanotechnol. **13**, 602 (2018).
[2] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[3] T. Barnowsky *et al.*, Nano Lett. **24**, 3974 (2024).
[4] A. Nihei *et al.*, submitted, arXiv:2503.12209 (2025).

FM 6.3 Tue 10:15 BEY/0138

Exfoliation and Cleavage of Crystals from a Universal Potential — •Tom Barnowsky[1,2], Carsten Timm[3], and Rico Friedrich[1,2] — [1]Theoretical Chemistry, TU Dresden — [2]Institute of Ion Beam Physics and Materials Research, HZDR — [3]Institute of Theoretical Physics, TU Dresden

Two-dimensional (2D) materials display unique electronic, optical, and mechanical features that differ from their three-dimensional bulk counterparts. Most known 2D materials are derived from layered crystals but recent experiments reveal that even non-layered compounds can give rise to stable so called non-van der Waals (vdW) 2D sheets [1]. Current models, however, provide limited guidance for such materials: existing descriptors and computational approaches are largely tailored to vdW layered systems [2].

We present a computational framework that predicts crystal cleavage and exfoliable 2D sheets directly from arbitrary bulk structures [3]. At its core is a universal interatomic potential enabling rapid, large-scale screening of diverse materials. Two complementary algorithms detect weakly bonded planes and iteratively isolate connected 2D subunits. Applying this approach, we identify several thousand candidate 2D materials from non-layered bulk crystals, opening a systematic route to explore and design new low-dimensional materials with unprecedented chemical and structural diversity.

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022)
[2] N. Mounet *et al.*, Nat. Nanotechnol. **13**, 246 (2018)
[3] T. Barnowsky, C. Timm, & R. Friedrich, Submitted (2025)

FM 6.4 Tue 10:30 BEY/0138

Research data management for high-throughput DFT calculations using NOMAD Oasis — •Vikrant Chaudhary[1,2], Fu Li[2], Yue Zhao[2], Joseph F. Rudzinski[1], Nathan Daelman[1], and Hongbin Zhang[2] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany — [2]Institute of Materials Science, Technical University of Darmstadt, Darmstadt, Germany

NOMAD Oasis is an open-source, locally installable version of the central NOMAD software [nomad-lab.eu] [1]. Importantly, it allows users to add custom extensions such as data schemas and workflows. In this work, we showcase two representative cases implemented in our local NOMAD Oasis: (I) high-throughput spin Hall conductivity calculations for 4486 2D materials [2], and (II) medium-throughput bulk-photovoltaic effect in 549 experimentally available two-dimensional hybrid perovskites. In both cases, data generation relies on complex computational workflows involving multiple software packages, including VASP, Wannier90, and WannierBerri. We implement a customized parser for Wannier90, and a locally developed parser for WannierBerri, with the resulting data organized based on NOMAD's built-in workflow functionalities. These examples show how NOMAD Oasis can simplify large-scale computational data management with custom parsers, automated workflows, unrestricted storage and uploads, and enhanced privacy. It also ensures compliance with the FAIR principles, making data Findable, Accessible, Interoperable, and Reusable.

[1] M. Scheidgen et al., JOSS 8, 5388 (2023).
[2] Li, F. et al., arXiv:2509.13204 (2025).

FM 6.5 Tue 10:45 BEY/0138

Finding interoperable datasets in diverse databases via provenance and similarity analysis — •Martin Kuban, Alvin Noe Ladines, Thea Denell, Lauri Himanen, Joseph F. Rudzinski,

Claudia Draxl, and FAIRmat team — Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany

Collecting data from different sources has the potential to significantly increase the amount of available data for data-driven discovery. However, different producers of data use distinct methods and setups, e.g., approximations and parameters used in computational data, to achieve the best data quality for the properties that are studied in a specific project. Bringing these data together requires to understand the impact of the method and setup on the accuracy and precision of the produced data. In order to do so, two key requirements must be fulfilled: First, the provenance and metadata of each data point need to be recorded. This can be achieved by leveraging the NOMAD infrastructure[1, 2], an ecosystem of parsers, schemas, and workflow tools, to extract rich metadata and provenance information. Second, using this information, similarity metrics can be used to identify data that achieve similar precision besides distinct computational setups[3]. We showcase our approach on different examples using data from NOMAD.

[1] Draxl and Scheffler, MRS Bulletin **9** (2018), 676-682.
[2] Scheidgen *et al.*, Journal of Open Source Software **8** (2023), 5388.
[3] Kuban *et al.*, MRS Bulletin **47** (2022), 991-999.

Coffee break

FM 6.6 Tue 11:15 BEY/0138

Search for thermodynamically stable ambient-pressure superconducting hydrides in GNoME database — Antonio Sanna[1,2], Tiago F. T. Cerqueira[3], Ekin Dogus Cubuk[4], Ion Errea[5,6,7], and •Yue-Wen Fang[6] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]nstitut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal — [4]Periodic Labs, San Francisco, CA, USA — [5]Fisika Aplikatua Saila, Gipuzkoako Ingeniaritza Eskola, University of the Basque Country (UPV/EHU), Europa Plaza 1, 20018 Donostia/San Sebastián, Spain — [6]Centro de Física de Materiales (CFM-MPC), CSIC-UPV/EHU, Manuel de Lardizabal Pasealekua 5, 20018 Donostia/San Sebastián, Spain — [7]Donostia International Physics Center (DIPC), Manuel de Lardizabal Pasealekua 4, 20018 Donostia/San Sebastián, Spain

There are very few ambient-pressure hydride superconductors in experiment, and their critical temperatures (T_c) are typically < 10 K. Herein, by combining machine learning techniques with ab initio methods, we have identified 25 cubic thermodynamically stable hydrides with T_c beyond the boiling point of liquid helium (4.2 K) from the GNoME database. These cubic hydrides all crystallize in double-perovskite-like or fluorite-like structures, and most of them demonstrate T_c lower than 10 K. Our study provide more candidates for the study of ambient-pressure superconductivity in the hydrides that can be very likely to be synthesized in experiment despite the low T_c.

FM 6.7 Tue 11:30 BEY/0138

Exploration of high-entropy alloys for key electrochemical reactions: a comparative study for the solid solution systems X-Pd-Pt-Ru (X=Cu, Ir, Ni) — •Jan Lukas Bürgel[1], Rico Zehl[1], Felix Thelen[1], Ridha Zerdoumi[1,2], Olga A. Krysiak[2], Benedikt Kohnen[1], Ellen Suhr[1], Wolfgang Schuhmann[2], and Alfred Ludwig[1] — [1]Chair for Materials Discovery and Interfaces, Institute for Materials, Faculty of Mechanical Engineering, Ruhr University Bochum, Bochum, Germany — [2]Analytical Chemistry - Center for Electrochemical Sciences (CES), Faculty of Chemistry and Biochemistry, Ruhr University Bochum, Bochum, Germany

Developing new electrocatalysts is essential for green energy technologies such as hydrogen production, fuel cells, and environmental remediation. Compositionally complex solid solutions offer vast opportunities for catalyst discovery due to their tunable surface sites, but exploring their large compositional spaces requires optimised strategies. Using a high-throughput approach, the electrocatalytic activity of the three quaternary systems X-Pd-Pt-Ru (X = Cu, Ir, Ni) was screened for four reactions in alkaline media: oxygen evolution, oxygen reduction, hydrogen evolution, and nitrate reduction reaction. Thin-film materials libraries were synthesised and characterised to identify composition-activity relationships, while also considering relevant information on crystal structure and surface morphology. The resulting multidimensional dataset reveals clear trends, similarities, and distinct activity maxima, demonstrating the effectiveness of this approach for navigating complex multinary systems.

FM 6.8 Tue 11:45 BEY/0138

Phase formation and stability of transition-metal solid solutions containing volatile elements — Martin Kostka[1], Luqman Mustafa[1], Jill Fortmann[2], Aurelija Mockute[2], Alan Savan[2], Susanne Kunzmann[3], Anna Grünebohm[3], Alfred Ludwig[2], Andreas Kreyssig[1], and •Anna E. Böhmer[1] — [1]Experimental physics IV, Ruhr University Bochum, 44801 Bochum, Germany — [2]Materials Discovery and Interfaces, Institute for Materials, Ruhr University Bochum, 44801 Bochum, Germany — [3]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, 44801 Bochum, Germany

In the combinatorial synthesis of thin films, multiple elements are simultaneously deposited to achieve well-defined composition gradients and create a materials library. However, including volatile elements directly into the combinatorial synthesis is a challenge. Here, we use instead a two-step synthesis process combining combinatorial cosputtering with a separate ex-situ reaction step with the volatile elements Se and Sb. In particular, we investigate the phase formation and stability of the (Fe,Ni)Sb_2 and (Fe,Cr)Sb_2 solid solutions in the orthorhombic marcasite structure. Further, we study the (Fe,Co)Se_2 solid solution, which is on the brink of transformation from orthorhombic marcasite to cubic pyrite structure. Our preparation route with a separate low-temperature synthesis step permits detailed studies of solid solutions and phase diagrams at well-defined temperatures.

FM 6.9 Tue 12:00 BEY/0138

AI for Complex Catalytic Systems: C2 Catalysis — •Haobo Li — Nanyang Technological University, Singapore

AI-driven big data set analysis offers opportunities for theoretical research on systems that combine complex catalyst materials with intricate catalytic reactions. In this study, we explore high-entropy alloys (HEAs) as potential electrocatalysts for the electrochemical semihydrogenation of acetylene. HEAs provide a variety of surface active sites due to the diverse combination of constituent elements, while the presence of bidentate dicarbon species further complicates surface interactions. By integrating density functional theory computations, geometric optimizer development, and graph neural network-based machine learning predictions, we efficiently compile a comprehensive database of 52,900 adsorption properties for AgAuCuNiPd HEA surfaces. Lasso regression and t-SNE projection reveal the distinct influences of the five metal components on adsorption and reaction properties. Using Cu as a reference, logistic regression assesses the potential for other components to surpass Cu in terms of catalytic activity and selectivity toward ethylene. Our findings suggest that, while HEAs can enhance the reaction, the ternary AgAuCu alloy achieves optimal results, indicating that high entropy is not essential. This research methodology can be extended to other complex catalytic systems, providing valuable insights into catalytic mechanisms and facilitating experimental endeavors.

FM 6.10 Tue 12:15 BEY/0138

Compositional and Structural Impact on the Hydrogen Evolution Reaction Activity across Noble-Metal-Based Compositionally Complex Solid Solutions Thin Film Libraries — •Natalia Pukhareva[1], Moonjoo Kim[2], Felix Thelen[1], Geovane Arruda de Oliveria[2], Rico Zehl[1], Wolfgang Schuhmann[2], and Alfred Ludwig[1] — [1]Materials Discovery & Interfaces, Ruhr University Bochum — [2]Analytical Chemistry - Center for Electrochemical Sciences (CES), Ruhr University Bochum

Compositionally complex solid solutions (CCSS) stabilize multielement alloys and allow tuning of surface chemistry for the hydrogen evolution reaction (HER). Three quinary libraries (Ir-Pd-Pt-Rh-Ru, Ag-Au-Pd-Pt-Ru, Ag-Au-Cu-Pd-Pt) were prepared by sputtering and mapped across 342 positions each. Energy-dispersive X-ray spectroscopy (EDX) confirmed smooth composition gradients, and X-ray diffraction (XRD) showed fcc solid solutions with minor hcp fractions in Rh-Ru-rich regions and no detectable phase effect on HER. X-ray photoelectron spectroscopy (XPS) with Gaussian-process regression revealed composition-dependent surface segregation and distinct surface compositions. HER activity, measured by scanning electrochemical cell microscopy (SECCM), followed Ir-Pd-Pt-Rh-Ru > Ag-Au-Pd-Pt-Ru > Ag-Au-Cu-Pd-Pt. In the Ag-containing libraries Pd-rich compositions outperformed Pt-rich ones, and in Ag-Au-Cu-Pd-Pt Ag-rich regions exceeded Cu-rich regions despite Cu's higher intrinsic activity, consistent with segregation limiting surface Pt and Pd and indicating that

HER in these CCSS is dominated by multielement interactions.

FM 6.11 Tue 12:30 BEY/0138

Soft Degradable Magnetic Microcarriers for Encapsulation and Guided Transport of Drugs and 3D Spheroids — •Lulu Song, Xinne Zhao, Xuan Peng, Željko Janićijević, Lin Guo, Denys Makarov, and Larysa Baraban — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Soft microrobots hold strong promise for next-generation biomedical applications, including targeted drug delivery, tissue engineering, and minimally invasive therapies. However, their translation remains limited by challenges in scalable fabrication, controlled biodegradation, and insufficient co-encapsulation and transport of diverse cargos. Here, we present degradable hydrogel microcarriers fabricated via droplet-based microfluidics and UV photopolymerization, enabling scalable production with tunable properties. These microcarriers can co-encapsulate therapeutic molecules, superparamagnetic particles, and living cell spheroids, supporting multifunctional delivery strategies. Their motion is precisely actuated under externally applied gradient magnetic fields, allowing guided navigation in microchannels for targeted delivery. Importantly, the microcarriers exhibit programmable degradation under physiological conditions, providing temporary mechanical integrity, controlled release, and safe post-treatment clearance, with complete degradation at 37 °C within several days. Overall, this platform offers a robust and biocompatible soft microrobotic system for targeted therapies, micro-tissue transport, and diagnostic monitoring, representing a promising step toward clinical translation.