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

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

Topical Talk MM 5.1 Mon 10:15 SCH/A251

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

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

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

MM 5.2 Mon 10:45 SCH/A251

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

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

MM 5.3 Mon 11:00 SCH/A251

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

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

[1] Y. Tian, et al., npj Comput. Mater. 11, 209 (2025)
[2] M. R-. Kochi et al., Chem. Sci. 16, 5464 (2025)
[3] R. Ouyang et al., Physical Review. M 2, 8 (2018)

MM 5.4 Mon 11:15 SCH/A251

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

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

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

15 min. break

Topical Talk MM 5.5 Mon 11:45 SCH/A251

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

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

MM 5.6 Mon 12:15 SCH/A251

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

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

MM 5.7 Mon 12:30 SCH/A251

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

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

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

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