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

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

Topical Talk MM 9.1 Mon 15:45 SCH/A251

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

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

MM 9.2 Mon 16:15 SCH/A251

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

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

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

MM 9.3 Mon 16:30 SCH/A251

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

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

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

MM 9.4 Mon 16:45 SCH/A251

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

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

15 min. break

MM 9.5 Mon 17:15 SCH/A251

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

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

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

MM 9.6 Mon 17:30 SCH/A251

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

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

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

MM 9.7 Mon 17:45 SCH/A251

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

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

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

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

MM 9.8 Mon 18:00 SCH/A251

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

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

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

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

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

MM 9.9 Mon 18:15 SCH/A251

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

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

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