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

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

MM 17.1 Tue 14:00 SCH/A251

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

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

MM 17.2 Tue 14:15 SCH/A251

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

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

MM 17.3 Tue 14:30 SCH/A251

Simultaneous Learning of Static and Dynamic Charges — Philipp Stärk[1], •Philip Loche[2], Marcel Langer[1], Henrik Stooss[1,3], Michele Ceriotti[2], and Alexander Schlaich[1,3] — [1]Stuttgart Center for Simulation Science, University of Stuttgart, Germany — [2]Laboratory of Computational Science and Modeling, École Polytechnique Fédérale de Lausanne, Switzerland — [3]Institute for Physics of Functional Materials, Hamburg University of Technology, Germany

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

MM 17.4 Tue 14:45 SCH/A251

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

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

MM 17.5 Tue 15:00 SCH/A251

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

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

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

MM 17.6 Tue 15:15 SCH/A251

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

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

MM 17.7 Tue 15:30 SCH/A251

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

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

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