SYMD 1: AI-driven Materials Design: Recent Developments, Challenges and Perspectives

Time: Monday 15:00–17:45 Location: H1

Invited Talk SYMD 1.1 Mon 15:00 H1

Learning physically constrained microscopic interaction models of functional materials — •Boris Kozinsky — Harvard University, Cambridge MA, USA — Bosch Research, Watertown MA, uSA

Discovery and understanding of next-generation materials requires a challenging combination of the high accuracy of first-principles calculations with the ability to reach large size and time scales. We pursue a multi-tier development strategy in which machine learning algorithms are combined with exact physical symmetries and constraints to significantly accelerate computations of electronic structure and atomistic dynamics. First, current DFT approximations fall short of the required accuracy and efficiency for predictive calculations of defect properties, band gaps, stability and electrochemical potentials of materials for energy storage and conversion. To advance the capability of DFT we introduce non-local charge density descriptors that satisfy exact scaling constraints and learn exchange functionals called CIDER. These models are orders of magnitude faster in self-consistent calculations for solids than hybrid functionals but similar in accuracy. On a different level, we accelerate MD simulations by using machine learning to construct generalized potential and free energy functions with arbitrary nonlinear dependence on external fields and temperature. This framework enables learning and prediction of dielectric and vibrational response properties and coarse-grained free energies. We demonstrate these methods via first principles ML MD simulations of dynamics of phase transformations, heterogeneous reactions, ferroelectric transitions, nuclear quantum effects, and soft materials.

Invited Talk SYMD 1.2 Mon 15:30 H1

GRACE universal interatomic potential for materials discovery and design — •Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

Universal interatomic potentials parameterize the interaction between all chemical elements in the periodic table simultaneously. In my talk I will introduce the Graph Atomic Cluster Expansion (GRACE). GRACE builds on a complete set of graph basis functions and generalizes equivariant message passing neural networks and other machine learning interatomic potentials. Next, I will discuss the parameterization of GRACE across the periodic table and compare the performance of universal GRACE to element-specific potentials.

The ability to simulate thousands or millions of atoms with complex chemistries for extended time scales opens completely new routes for materials discovery and design. I will demonstrate usage scenarios for widely different materials, chemistries and applications.

Finally, I will focus on limitations of current universal interatomic potentials and suggest steps to overcome these.

Invited Talk SYMD 1.3 Mon 16:00 H1

Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction — •Nong Artrith — Debye Institute for Nanomaterials Science, Utrecht University, NL

Machine learning (ML) has emerged as a powerful tool to accelerate the discovery of catalytic materials by integrating information from computation and experiment. While ML excels at pattern detection in large, uniform datasets, many catalyst studies rely on small, experimentally measured datasets. Our approach combines ML and first-principles calculations to extract insights from such small experimental datasets by training a complex ML model on a large computational library of transition-state energies and combining it with simple linear regression models fitted to experimental data. We use this approach to explore the catalytic activity of monolayer bimetallic catalysts for ethanol reforming, identifying key reactions and predicting promising catalyst compositions. For the explicit modeling of catalytic reactions, we performed ML-driven molecular dynamics and metadynamics simulations of the oxygen evolution reaction (OER) over oxide materials. Using a neural network potential, trained using transfer learning, we captured the dynamic mechanistic details of OER, elucidating the impact of nickel doping on the catalytic activity of $BaTiO_3$, a perovskite oxide synthesized from earth-abundant precursors. The combined insights from these case studies illustrate the versatility of ML in guiding the design of efficient and sustainable catalysts, ranging from ethanol reforming to water-splitting reactions.

15 min. break

Invited Talk SYMD 1.4 Mon 16:45 H1

Inverse Design of Materials — •Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

Machine learning has been widely applied to obtain statistical understanding and rational design of advanced materials to map out the processing-(micro-)structure-property-performance relationships, mostly in the forward manner. In this work, focusing on the structure-property relationships, I am going to introduce the concept of inverse design and to showcase how it can be carried out based on Bayesian optimization and generative deep learning. To explore a well-defined and possibly vast design space efficiently, Bayesian optimization can be applied for reliable recommendations, either based on ranking schemas balancing exploration and exploitation or by using proper sampling strategies. This leads to a closed loop adaptive design strategy, which can be integrated with theoretical scale-bridging simulations and experimental synthesis and characterization, resulting in a domain expertise- and physics-informed active learning paradigm. Furthermore, to go beyond the known design space, generative deep learning (such as GAN, VAE, and diffusion models) can be applied. I will demonstrate such a strategy for the polycrystalline microstructure-property mapping, with the physical properties constrained based on an integrated ControlNet in stable diffusion models.

Invited Talk SYMD 1.5 Mon 17:15 H1

Data-Driven Materials Science — •Miguel Marques — Ruhr University Bochum, Germany

We summarize our recent attempts to discover, characterize, and understand inorganic compounds using novel machine learning approaches. We start by motivating why the search for new materials is nowadays one of the most pressing technological problems. Then we summarize our recent work in using crystal-graph attention neural networks for the prediction of materials properties. To train these networks, we developed a dataset of over 5 million density-functional calculations with consistent calculation parameters. Combining the data and the newly developed networks we have already scanned thousands of structural prototypes spanning a space of several billion materials and identified tens of thousands of theoretically stable compounds. We then discuss how these techniques can be used to discover new materials with tailored properties, using as an example the transition temperature of conventional superconductors. Finally, we speculate which role data-driven research will have in the future of materials science.