# O 18: New methods: Theory – Poster

Time: Monday 18:00–20:00 Location: P2

O 18.1 Mon 18:00 P2

**Cost-Efficient Approach for Training MACE Potentials** — •Antonia Gerstenberg[1,2], Thomas Bligaard[2], and Andreas Lynge Vishart[2] — [1]currently: Fritz-Haber-Institut der MPG, Berlin, Germany — [2]DTU, Department of Energy Conversion and Storage, Denmark

Machine learning interatomic potentials (MLIPs) such as MACE offer near DFT accuracy at a fraction of the computational cost. However, a limiting factor is the cost of generating high-quality training data. This project investigates the development of a systematic and cost-efficient approach to training robust MACE models. It is therefore explored to what extent models trained on the cheapest available structures (e.g., dimers and trimers) can extrapolate to larger structures such as nanoparticles and vice versa.

To test this, an active learning workflow was implemented, iteratively adding structures with increasing numbers of atoms. The results show that widely used training strategies, including standard active learning workflows, fail to reliably extrapolate to out-of-distribution structures. The results highlight the importance of structural diversity and weight restriction from the outset.

O 18.2 Mon 18:00 P2

**The application of classical DFT for describing small molecules diffusion in porous materials.** — •Mikhail Suetin and Michael te Vrugt — Institute of Physics, Johannes Gutenberg Universität-Mainz, Staudingerweg 9, 55128, Mainz, Germany.

Metal-Organic Frameworks (MOFs) are relatively new, but promising materials potentially suitable for separation of hydrocarbon molecules for chemical industry aiming reaching the Net-Zero targets. Thousands of MOFs have been obtained experimentally, and about a million computationally. In this study, we conducted computational screening of the CoRE MOF database. Classical molecular dynamics simulations are employed for considering separation via diffusion. More importantly, classical density functional theory (cDFT) approach was employed to dramatically accelerate calculations of diffusion coefficients.

O 18.3 Mon 18:00 P2

**Increasing the Transferability of Machine Learning Potentials by Learning Atomic Properties** — •Johann Richard Springborn[1,2], Gunnar Schmitz[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Machine Learning Potentials (MLPs) have become an established tool for describing potential energy surfaces of complex systems. While they significantly speed up the evaluation of the energy and forces in comparison to ab-initio methods, they require high-quality reference data for training. Depending on the systems to be studied, generating this training data can become the computational bottleneck. Therefore it is of high interest to reduce the number and complexity of structures to be computed. We propose to achieve this goal by training MLPs on atomic properties instead of global quantities such as the system's total energy. This approach aims to increase the transferability of the resulting MLPs to more complicated systems while still utilizing easily accessible reference data.

O 18.4 Mon 18:00 P2

**Radial Dirac-Fock solver using integral equation method** — •Ernests Lazdans, Janis Užulis, and Andris Gulans — University of Latvia, Riga, Latvia

We present a relativistic generalized Kohn-Sham solver for spherically symmetric atoms. It follows the approach introduced in a multiwavelet code [1] where the Dirac equation is represented in the integral form. The solver supports local and hybrid exchange-correlation functionals and various nuclear distributions (point-like, Gaussian, and spherical). In validation test, we find that it yields Hartree-Fock energies in full agreement for all ten digits given by Visscher *et al.* [2]. However, our numerical tests show that numerical errors in our obtained atomic energies are below 10 nHa, *i.e.*, our solver's precision exceeds that of previously published data. We use the solver for testing performance of multiple exchange-correlation functionals for predicting electron removal energies from core and valence shells in noble gas atoms. The future applications of this tool include integrating it into a linearised augmented plane wave code.

[1] Anderson J. *et al.*, J. Chem. Phys. **151**, 234112 (2019)

[2] L. Visscher *et al.*, Atomic Data and Nuclear Data Tables **67**, 207-224 (1997)

O 18.5 Mon 18:00 P2

**Towards Efficient Time-Dependent Density-Functional Theory through Hubbard On- and Inter-Site Corrections** — •Lydia Fichte, Karsten Reuter, and Matthias Kick — Fritz-Haber-Institut der MPG, Berlin

Density-functional theory (DFT) with a Hubbard correction (DFT+$U$) can mitigate self-interaction errors in a manner similar to hybrid functionals, but at significantly lower computational cost. This makes extending DFT+$U$ to the time-dependent regime particularly attractive, as it allows for accurate simulations of electron dynamics at reduced computational expense. However, the on-site subspace defined by DFT+$U$ can be too rigid to describe phenomena involving strong orbital hybridization or charge transfer between sites, necessitating a more flexible definition of the correlated subspace. To address this, we are incorporating inter-site interactions through the +$V$ correction to enable a more complete and adaptable description. We implement this as an efficient real-time time-dependent DFT+$U$+$V$ framework in the all-electron electronic-structure code FHI-aims, enabling accurate and scalable simulations of correlated electron dynamics. We discuss the current status of the implementation and highlight the pitfalls and intricacies encountered when working with a numeric atom-centered orbital basis, both in the ground state and in time-dependent simulations.

O 18.6 Mon 18:00 P2

**Calculating surface energy using machine learning interatomic potentials** — •Friedrich Neumann[1], Tom Barnowsky[2,3], Rico Friedrich[2,3], and Jens Kortus[1] — [1]TU Bergakademie Freiberg - Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg — [2]Technische Universität Dresden - Theoretische Chemie, 01062 Dresden — [3]Helmholtz-Zentrum Dresden-Rossendorf e.V., Bautzner Landstraße 400, 01328 Dresden

The surface energy of a material is a fundamental property that governs the behaviour of solid interfaces in a wide range of phenomena. While density functional theory (DFT) provides highly accurate values, its computational scaling limits its applicability for large systems and systematic surface-energy screening. In this work, a workflow was developed to estimate surface energies using machine-learning interatomic potentials (ML-IAPs). Atomic Cluster Expansion (ACE) models were fitted to DFT-based molecular-dynamics data for Al, Pt, and Au, and effective two-body contributions were extracted from the resulting potentials. These were combined with a bond-counting approach to compute surface energies and Wulff constructions. Although in our present ACE model the absolute magnitudes of the pair interactions are influenced by many-body interaction, preventing quantitative reproduction of surface energies, the approach still captures general trends and identifies the dominant facets in the Wulff constructions. In this specific formulation, the results illustrate how many-body interaction can affect the apparent pair contribution.