Contribution ID: **43** Type: **Poster**

Quantum-accurate interatomic potentials for warm dense matter

Warm dense matter has been the subject of many studies due to its importance in various applications such as the interior of gas giants and exoplanets, inertial confinement fusion, and ablation of metals. Ongoing and upcoming experimental campaigns in large-scale facilities around the globe rely on numerical simulations on the electronic structure level. In that regard, density functional theory molecular dynamics (DFT-MD) simulations have been widely used to compute dynamical and thermodynamical properties of warm dense matter. However, there are two obstacles that impede further progress: (1) with increasing temperature, DFT-MD becomes computational infeasible making it difficult to perform large-scale simulations; (2) finite-size effects render many computational observables inaccurate because these calculations are limited to a few hundred atoms on the currently available HPC platforms. Recently, molecular dynamics simulations using machine learning-based interatomic potentials (ML-IAP) could overcome the computational limitations of DFT-based approaches. Here, we present our method to construct ML-IAPs based on SNAP descriptors [1]. We demonstrate our workflow for aluminum by the training data sets obtained from DFT-MD calculations. In particular, we investigate the transferability of ML-IAP over a large range of temperatures and pressures, which currently is a topic of active research.

[1] Thompson, Aidan P., et al. "Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials." Journal of Computational Physics, 285, 316 (2015).

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Session Classification: Poster session