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Machine learning-based quantum accurate interatomic potentials for warm dense aluminum

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Modeling warm dense matter is relevant for various applications including the interior of gas giants and exoplanets, inertial confinement fusion, and ablation of metals. Ongoing and upcoming experimental campaigns in photon sources around the globe rely on numerical simulations which are accurate on the level of electronic structures. In that regard, density functional theory molecular dynamics (DFT-MD) simulations [1] have been widely used to compute the dynamical and thermodynamical properties of warm dense matter. However, two challenges impede further progress: (1) DFT-MD becomes computationally infeasible with increasing temperature (2) finite-size effects render many computational observables inaccurate, because DFT-MD is limited to a few hundred atoms on current HPC platforms. Recently, molecular dynamics simulations using machine learning-based interatomic potentials (ML-IAP) could overcome these computational limitations. Here, we propose a method to construct ML-IAPs from DFT data based on SNAP descriptors [2]. We present our results for aluminum. In particular, we investigate the transferability of ML-IAPs over a large range of temperatures (1000 to 100000 K) and pressures (ambient to 800 GPa), which currently is a topic of active research. To test the transferability of the SNAP potential, we calculate thermal conductivity, viscosity, diffusion coefficient, and sound velocity in and out of the data training range. References:

[1]. G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993).
[2]. A. P. Thompson, L. P. Swiler, C. R. Trott, S. M. Foiles, and G. J. Tucker, J. Comput. Phys., 285, 316-330, 2015.

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