Abstract Submitted
for the DPP20 Meeting of
The American Physical Society

A Machine-Learned Orbital-Free Force-Correction Model: Extending the Thermodynamic Range of Affordable Kohn-Sham Level Accuracy[1] JOSHUA HINZ, VALENTIN KARASIEV, SUXING HU, Lab for Laser Energetics, University of Rochester , — Density functional theory (DFT) is an essential tool for material property predictions in warm dense matter. DFT-based molecular-dynamic (MD) predictions require a delicate balance of computational cost and desired accuracy. Orbital-based Mermin–Kohn–Sham (MKS) DFT is a widely successful branch of DFT; unfortunately, the computational cost scales cubically with the number of thermally occupied orbitals; leading to prohibitive costs at higher temperatures. Alternatively, orbital-free (OF)-DFT is orders of magnitude faster but tends to be less accurate than MKS-DFT. In this work we have developed a machine-learning–based force-correction model, using a deep neural network, to map OF-DFT forces to the corresponding MKS forces. With the use of local ion descriptors in conjunction with the less-accurate OF forces, the model is able to significantly reduce the relative error between OF and MKS forces, thereby enabling MD simulations with the best of both worlds. The success of the model is benchmarked by reproducing DFT predictions for the insulator-to-metal transition of fluid hydrogen—a system that is strongly dependent on the underlying ion configurations. The potential strengths and weaknesses of the model will be discussed.

[1]This material is supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856 and U.S. National Science Foundation PHY Grant No. 1802964.

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Date submitted: 29 Jun 2020 Electronic form version 1.4