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Multi-Fidelity Machine Learning for Extending the Range of High-Fidelity Molecular Dynamics Data[1] LUCAS J. STANEK, SHAUNAK D. BOPARDIKAR, MICHAEL S. MURILLO, Michigan State University — Macroscopic models of non-ideal plasmas rely on closure information in the form of equations of state and transport coefficients. Unfortunately, our highest-fidelity models (e.g. Kohn-Sham molecular dynamics) remain very expensive to compute, especially at elevated temperatures where transport is most important. Lower fidelity models such as pair-potential molecular dynamics and analytic theories are orders of magnitude faster but lack the accuracy of the high-fidelity models. By using machine learning tools, we combine data at the various levels of fidelity to make high-fidelity predictions where it is impossible for the high-fidelity codes to operate. Here, we examine both multi-fidelity Gaussian process regression (GPR) and deep learning to predict transport coefficients (i.e., diffusion and viscosity) at high temperatures using calculations done at low temperature with Kohn-Sham molecular dynamics. We find excellent predictions, as measured through a cross validation procedure. Moreover, GPR adds additional value in that it "suggests" the most important new high-fidelity calculations by reporting confidence intervals throughout the extent of the prediction.

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