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Orbital-Free Molecular Dynamics Simulations at Extreme Conditions J.D. KRESS, L.A. COLLINS, C. TICKNOR, Los Alamos National Laboratory
— Large-scale molecular dynamics (MD) simulations in an orbital-free (OF) density-functional theory (DFT) formulation have been performed for pure and mixed species over a broad range of temperatures (T) and densities (ρ) that includes the warm, dense matter and high-energy density physics regimes. A finite-temperature Thomas-Fermi-Dirac form with a local-density exchange-correlation potential and a regularized electron-ion interaction represents the quantum nature of the electrons. In particular, we examine the efficacy of the OFMD approach as an effective bridge between Kohn-Sham DFT MD at low temperatures and simple, fully-ionized plasma models at high temperatures. Comparisons against intermediate-range constructions such as the Yukawa and one-component plasmas are also made. We examine the mass transport (diffusion, viscosity) properties of various systems, ranging from light to heavy elements, including lithium hydride (LiH), mixtures of LiH with uranium, mixtures of deuterium-tritium (DT) with plutonium and mixtures of DT with plastic (CH). The OFMD mass transport results have been fitted to simple functions of ρ and T suitable for use in hydrodynamics simulation codes.

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