

Abstract Submitted
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Mass Transport in the Warm, Dense Matter and High-Energy Density Regimes J.D. KRESS, L. BURAKOVSKY, C. TICKNOR, L.A. COLLINS, Los Alamos National Laboratory, F. LAMBERT, CEA/DAM/DIF — Large-scale hydrodynamical simulations of fluids and plasmas under extreme conditions require knowledge of certain microscopic properties such as diffusion and viscosity in addition to the equation-of-state. To determine these dynamical properties, we employ quantum molecular dynamical (MD) simulations on large samples of atoms. The method has several advantages: 1) static, dynamical, and optical properties are produced consistently from the same simulations, and 2) mixture properties arise in a natural way since all intra- and inter-particle interactions are properly represented. We utilize two forms of density functional theory: 1) Kohn-Sham (KS-DFT) and 2) orbital-free (OF-DFT). KS-DFT is computationally intense due to its reliance on an orbital representation. As the temperature rises, the Thomas-Fermi approximation in OF-DFT begins to represent accurately the density functional, and provides an efficient and systematic means for extending the quantum simulations to very hot conditions. We have performed KS-DFT and OF-DFT calculations of the self-diffusion, mutual diffusion and shear viscosity for Al, Li, H, and LiH. We examine trends in these quantities and compare to more approximate forms such as the one-component plasma model. We also determine the validity of mixing rules that combine the properties of pure species into a composite result.

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