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Transport properties of a high Z, low Z mixtures with varying concentration CHRISTOPHER TICKNOR, LEE COLLINS, JOEL KRESS, Los Alamos Natl Lab, JEAN CLEROUIN, GREGORY ROBERT, PHILIPPE ARNAULT, CEA, DAM, DIF, F-91297 Arpajon, France — 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 and densities 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. We examine the mass transport (diffusion, shear viscosity) properties of a mixture of light and heavy elements. We focus on Hydrogen-Silver mixtures with varying concentration at fixed pressure and temperature. These results will be fitted to simple functions of mass density and temperature, functions suitable for use in large-scale hydrodynamics simulation codes.

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