Transport Properties of Asymmetric Mixtures

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ABSTRACT

We have explored a variety of warm dense matter (WDM) and hot plasma systems with a quantum molecular dynamics (QMD) approach. In the QMD, we solve the many-body Schrodinger equation for a large, representative sample of atoms, periodically replicated through space to effect the characteristics of a fluid, which may include a mix of atoms, molecules, ions, and free electrons. For the electrons, we employ density-functional theory (DFT) in two guises: an orbital-based in the Kohn-Sham (KS) form and an orbital-free (OF), usually in a Thomas-Fermi-Dirac approximation. This dual capability permits thorough coverage of these extreme conditions and provides a set of consistent static, dynamic, and optical properties such as equation of state (EOS), mass transport (viscosity/diffusion), opacity, and conductivity (thermal/electrical).

This versatility has permitted applications to a diverse range of environments including planetary interiors of ice-giant solar and exosolar planets, ICF capsules, and material interfaces, which span densities from solid to hundreds of times compressed and temperatures from a few to 1000 eV. A few examples serve to illustrate this breadth. First, the ice-giant planetary interiors comprise a complex fluid mixture of ammonia, methane, and water that can support very complex chemical reactions yielding a variety of interesting structures such as superionic states and large carbon clusters [1]. Second, simulations in the ICF regime have examined deuterium, polystyrene (CH), silicon [2], and beryllium as well as their mixtures; the resulting properties have been introduced “in-line“ within hydrodynamics programs. The third application involves highly asymmetric mixtures [3] such as H paired with several heavy components ranging from Li to Ag as well as ternary systems such as H-C-Ag and Li-D-U. We have found that certain properties, most notably viscosity, show a strong sensitive to small amounts of the heavy species. Such cases require large-scale simulations and large computational investments.

We present mass transport coefficients for a variety of binary and ternary mixtures from weakly (D-Li-C) to highly [H-C-Ag] asymmetric in the mass concentrations over a broad range of temperatures and densities from QMD simulations in both the OF and KS formulations. The results are compared with various approximations such as the Darken, with classical MD simulations using model potentials such as the Yukawa, and with integrated models such as pseudo-ion in jellium.

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