Abstract Submitted
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Calculation of Transport Coefficients in Binary Yukawa Mixtures[1] TOMORR HAXHIMALI, ROBERT RUDD, Lwarence Livermore National Laboratory — We employ classical molecular dynamics (MD) to estimate species diffusivity and viscosity in binary Yukawa Mixtures. The Yukawa potential is used to describe the screened Coulomb interaction between the ions, providing the basis for models of dense stellar materials, inertial confined plasmas, and colloidal particles in electrolytes. We calculate transport coefficients in equilibrium simulations using the Green-Kubo relation over a range of thermodynamic conditions including the viscosity and the self-diffusivity for each component of the mixture. The inter-diffusivity (or mutual diffusivity) can then be related to the self-diffusivities by using a generalization of the Darken equation. We have also employed non-equilibrium MD to estimate inter-diffusivity during the broadening of the interface between two regions each with a high concentration of either species. The main motivation in this work is to build a model that describes the transport coefficients in binary Yukawa mixtures over a broad range of thermodynamic conditions.

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