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Diffusivity of Mixtures in Warm Dense Matter Regime[1] TOMORR HAXHIMALI, ROBERT RUDD, JULIE JACKSON, A. BRUCE LANGDON, JAMES GLOSLI, FRANK GRAZIANI, Lawrence Livermore National Laboratory — Modeling of ionic diffusion in warm dense plasma mixtures has been of longstanding interest in astrophysics and in Inertial Confinement Fusion. In this work we employ classical Molecular Dynamics (MD) to calculate diffusion coefficients in mixed plasmas. In the MD study we make use of the Yukawa potential as an effective ion-ion interaction potential that accounts for the screening effects of the electrons. We focus in binary asymmetric mixtures between Deuterium and Argon at Temperatures from 10-100eV and ion densities from 10^{23}-10^{25} ion/cc. In uniform mixed systems we use Green-Kubo techniques to calculate self-diffusivities and Maxwell-Stefan diffusivities over a range of conditions. The new results from this study show that a simple linear relations between Maxwell-Stefan diffusivity and self-diffusivities is not always valid. The interdiffusivity that enters in Fickian equation can be related to the Maxwell-Stefan diffusivities through the thermodynamic factor. The latter requires knowledge of the equation of state of the mixture. We compare these results with classical kinetic theories that assume binary collisions. To test these Green-Kubo approaches and to estimate the activity contribution we have also employed large-scale non-equilibrium, non-uniform mixed, MD.

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