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Improved Structure Factors for Modeling XRTS Experiments[1]
LIAM STANTON, LLNL, MICHAEL MURILLO, JOHN BENAGE, LANL, FRANK GRAZIANI, LLNL — Characterizing warm dense matter (WDM) has gained renewed interest due to advances in powerful lasers and next generation light sources. Because WDM is strongly coupled and moderately degenerate, we must often rely on simulations, which are necessarily based on ions interacting through a screened potential that must be determined. Given such a potential, ionic radial distribution functions (RDFs) and structure factors (SFs) can be calculated and related to XRTS data and EOS quantities. While many screening models are available, such as the Debye- (Yukawa-) potential, they are known to over-screen and are unable capture accurate bound state effects, which have been shown to contribute to both scattering data from XRTS as well as the short-range repulsion in the RDF. Here, we present a model which incorporates an improvement to the screening length in addition to a consistent treatment of the core electrons. This new potential improves the accuracy of both bound state and screening effects without contributing to the computational complexity of Debye-like models. Calculations of ionic RDFs and SFs are compared to experimental data and quantum molecular dynamics simulations for Be, Na, Mg and Al in the WDM and liquid metal regime.

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