An average-atom model for electron-electron correlations in dense plasmas

Nathaniel R. Shaffer, Charles E. Starrett

We present a model for the electron-electron structure factor, pair distribution function, and potential of mean force of dense plasma. The model uses an average-atom Kohn-Sham DFT calculation coupled with the quantum Ornstein-Zernike relations to define a two-component plasma of ions (nuclei plus bound electrons) and free electrons. The electron-electron structure factor is succinctly expressed as an electron-gas part plus a correction due to the ions. Comparison with PIMC results shows that the model accurately predicts the electron-gas part, while the accuracy of the ionic correction depends on how well the density of states can be approximated by that for free electrons. In addition to the usual thermodynamic applications for the pair distribution functions and structure factors, the model provides potentials of mean force, which are the key input to theory being developed for the electrical and thermal conductivity in dense plasmas.