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DFT-based Analytic Pair Interactions for Rapid Molecular Dynamics Simulations of Dense Plasmas LIAM STANTON, San Jose State University, MICHAEL MURILLO, Michigan State University — Electron screening of ions is among the most fundamental properties of plasmas, determining the effective ionic interactions that impact all properties of a plasma. With the development of experimental facilities that probe high energy-density (HED) physics regimes ranging from warm to hot dense matter, an accurate and computationally efficient description of dense plasma screening has become essential. We extend our previous work [Phys. Rev. E, 91, 033104 (2015)], which provides a unified framework for screening models based on finite-temperature orbital-free density functional theory, including both gradient corrections and exchange-correlation effects. Here, we generalize the model to include leading-order core electron effects via the use of pseudo-potentials. We additionally investigate a variety of exchange-correlation models, which are rarely used in simple screening models, and quantify the impact of their contributions across the HED regime with applications such as calculating transport coefficients and equations of state. The results are compared to numerical calculations from high-fidelity physics simulations in the literature.

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