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Extended Thomas-Fermi Molecular Dynamics for Dense, Strongly-Coupled Plasmas[1] LIAM STANTON, Lawrence Livermore National Laboratory, MICHAEL MURILLO, LANL, JAMES GLOSLI, FRANK GRAZIANI, LLNL — The primary challenge in simulating dense plasmas is the self-consistent treatment of partial ionization. We present an orbital-free density-functional theory (OF-DFT) that includes, self-consistently, the physics of partially degenerate electrons, strongly coupled ions, and arbitrary degrees of ionization. The ions are treated dynamically according to the forces derived from the all-electron density calculation thereby allowing the computation of various transport quantities. Our variant of OF-DFT is based on extending the Thomas-Fermi functional to include gradient corrections and the exact, non-local, ideal-Fermi-gas response for weak coupling. We will describe our method and discuss various applications, such as equations of state and viscous transport in heterogeneous mixtures. Finally, we will give an outlook on extending this method to a fully dynamical model that describes the electron dynamics as well.

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Liam Stanton
Lawrence Livermore National Laboratory

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