Abstract Submitted
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A Non-Born-Oppenheimer Molecular Dynamics Method for Dense Plasmas[1] DAVID MICHTA, Princeton Plasma Phys Lab, Lawrence Livermore National Lab, LIAM STANTON, MIKE SURH, FRANK GRAZIANI, MICHAEL MURILLO, Lawrence Livermore National Lab — Warm Dense Matter, characterized by partially degenerate and moderately coupled electrons, is a regime realized in laser experiments, planetary interiors, and early stages of inertial confinement fusion. "Ab initio" molecular dynamics is an extremely accurate method built upon a Born-Oppenheimer (BO), plane-wave, pseudopotential electronic structure calculation. However, these assumptions are not appropriate for several important problems in dense plasmas. We desire an electron treatment that is both dynamical and quantum mechanical. Our approach combines ion MD with an electron fluid model based on orbital-free density functional theory (OF-DFT), which ensures high-quality equation of state. We discuss theoretical predictions of collective modes (electron plasma waves, ion-acoustic waves, etc.) and density fluctuations (dynamic structure factor, etc.). We have implemented fast, conservative numerical methods based on implicit time stepping and finite volume. We apply this to charged particle stopping, providing a stringent test of non-BO dynamics. We end with an outlook toward developments in numerical methods, improved OF-DFT models, and various applications.

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