

Abstract Submitted
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Time-dependent density functional theory of extreme environments RUDOLPH MAGYAR, LUKE SHULENBURGER, MICHAEL DESJARLAIS, Sandia National Laboratories — We describe the challenges involved when using time-dependent density functional theory (TDDFT) to describe warm dense matter (WDM) within a plane-wave, real-time formulation. WDM occurs under conditions of temperature and pressure (over 1000 K and 1 Mbar) where plasma physics meets condensed matter physics. TDDFT is especially important in this regime as it can describe ions and electrons strongly out of equilibrium. Several theoretical challenges must be overcome including assignment of initial state orbitals, choice of time-propagation scheme, treatment of PAW potentials, and inclusion of non-adiabatic effects in the potential energy surfaces. The results of these simulations are critical in several applications. For example, we will explain how the TDDFT calculation can resolve modeling inconsistencies in X-ray Thompson cross-sections, thereby improving an important temperature diagnostic in experiments. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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