

Recent Developments in TDDFT of Warm Dense Matter

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Warm dense matter (WDM) is matter at the edge of chemical stability, due to intense pressures and temperatures. As the conditions are intermediate between a condensed phase and an ideal plasma, WDM presents a unique theoretical challenge that requires borrowing ideas from plasma physics and quantum chemistry. Even so, standard wave function methods from quantum chemistry become cost prohibitive, as systems of interest are best treated as extended, and the elevated temperatures require the inclusion of many virtual states. Motivated by the established success of DFT-MD in characterizing the thermodynamic properties of WDM, we have implemented finite temperature time-dependent density functional theory (TDDFT) to compute a number of quantities of relevance, including optical conductivity, stopping power, and the dynamic structure factor. We will provide details of our framework and focus on recent results in which we have performed the first calculations of the dynamic structure factor of shock-compressed beryllium independent of the widely used Chihara model. 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.