

## **TDDFT for Warm Dense Matter: Theoretical Framework and Optical Response**

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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 not extreme enough to achieve an ideal plasma state, the modeling of WDM presents a significant theoretical challenge. Standard methods from quantum chemistry become cost prohibitive, as the pressured systems 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 are investigating the use of TDDFT for the characterization of its optical response. Such a theoretical predictive capability for the optical absorption and emission of WDM is of great utility to the experimental characterization of matter in these conditions. We will discuss theoretical issues including the representation of non-equilibrium dynamics that arise when perturbing hot electrons, how best to couple nuclear motion in these extreme conditions, and the extent to which non-adiabatic effects play a role in chemistry at these conditions. Optical response calculations will be discussed, illustrating the successes, open questions, and limitations of the theory as implemented. 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.