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Optical Response of Warm Dense Matter Using Real-Time Electron Dynamics ANDREW BACZEWSKI, LUKE SHULENBURGER, MICHAEL DESJARLAIS, RUDOLPH MAGYAR, Sandia National Laboratories — The extreme temperatures and solid-like densities in warm dense matter present a unique challenge for theory, wherein neither conventional models from condensed matter nor plasma physics capture all of the relevant phenomenology. While Kubo-Greenwood DFT calculations have proven capable of reproducing optical properties of WDM, they require a significant number of virtual orbitals to reach convergence due to their perturbative nature. Real-time TDDFT presents a complementary framework with a number of computationally favorable properties, including reduced cost complexity and better scalability, and has been used to reproduce the optical response of finite and ordered extended systems. We will describe the use of Ehrenfest-TDDFT to evolve coupled electron-nuclear dynamics in WDM systems, and the subsequent evaluation of optical response functions from the real-time electron dynamics. The advantages and disadvantages of this approach will be discussed relative to the current state-of-the-art. 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 Security Administration under contract DE-AC04-94AL85000.

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