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**Time-Dependent Density Functional Theory for Extreme Environments** ANDREW BACZEWSKI, RUDOLPH MAGYAR, LUKE SHULENBURGER, Sandia National Laboratories — In recent years, DFT-MD has been shown to be a powerful tool for calculating the equation of state and constitutive properties of warm dense matter (WDM). These studies are validated through a number of experiments, including recently developed X-Ray Thomson Scattering (XRTS) techniques. Here, electronic temperatures and densities of WDM are accessible through x-ray scattering data, which is related to the system's dynamic structure factor (DSF)–a quantity that is accessible through DFT-MD calculations. Previous studies predict the DSF within the Born-Oppenheimer approximation, with the electronic state computed using Mermin DFT. A capability for including more general coupled electron-ion dynamics is desirable, to study both the effect on XRTS observables and the broader problem of electron-ion energy transfer in extreme WDM conditions. Progress towards such a capability will be presented, in the form of an Ehrenfest MD framework using TDDFT. Computational challenges and open theoretical questions will be discussed. 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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