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Practical methods in time-dependent density functional theory (TDDFT) at elevated temperatures RUDOLPH MAGYAR, LUKE SHULENBURGER, ANDREW BACZEWSKI, Sandia National Laboratories — There is a great need to simulate dynamic material response properties under shock conditions where experimental data is often limited due to the extreme scales involved (MBars, 1000s of K, and manifold compressed solid densities). Knowing materials properties at this scale is vital element of simulations of planetary collisions, inertial confinement fusion experiments, and the surfaces of some stars. Considerable progress has been made using density functional molecular dynamics (DFT-MD) to model thermodynamic properties of material under these conditions; however, the approach is limited to cases in which the electrons are constrained to a thermodynamic distribution within the Mermin formulation. We will explore practical schemes to generalize this method to the time-dependent case. Several challenges come up such as the role of non-adiabatic electron-electron and electron-nuclear physics and the correct choice of initial state. One of the most straightforward choices of initial state is to project the Mermin state since the original Runge-Gross proof does not make explicit choice of occupations. We will present some numerical tests of finite systems to examine this formulation. We will also explore how simple models of non-adiabatic effects might be sufficiently accurate under extreme conditions. 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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