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Merging Kohn-Sham and Orbital-Free DFT Calculations to Extend the LiH Hugoniot to Very High Pressures

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Large-scale hydrodynamic simulations of fluids and plasmas under extreme conditions require knowledge of various properties such as the equation of state (EOS), mass diffusion, and shear viscosity. While many approaches exist for the determination of these properties, one of the most accurate employs quantum molecular dynamics (QMD) simulations on large samples of atoms of the various species. Examples include the shock compression of metal hydrides and the mixing of deuterium/tritium (DT) fuel with ablator materials (such as C/H plastics and Be) in inertial confinement fusion capsules. The quantum nature of the electrons is described with two flavors of finite-temperature density functional theory (DFT), namely orbital-based Kohn-Sham (KS) and Orbital Free (OF). EOSs for Lithium Hydride and Lithium 6 Deuteride (Li6D) have been calculated with both KSMD and with OFMD. The shock Hugoniot for Li6D has been determined for temperatures up to 25 eV (5000 GPa) using a KSMD based EOS, and for T= 5 eV and above (up to 10,000 GPa) using an OFMD based EOS. KSMD simulations here have a practical upper limit of T=25 eV due to the scaling of the computational work. The OFMD simulations have a lower limit of T=5 eV since the OF DFT yields a poor description at low temperatures. The KSMD and OFMD Hugoniots agree well in the region of overlap (T=5 to 25 eV). Comparisons will be presented with experimental data and with shock Hugoniots constructed from both existing EOS tables and from a new, improved SESAME table. By utilizing the KSMD and OFMD results to guide the parameter choices, the new EOS overall is a better match to melt and shock experimental data. This work was performed in collaboration with L. A. Collins, S. Crockett, M. P. Desjarlais, and F. Lambert and under the auspices of an agreement between CEA/DAM and NNSA/DP on cooperation on fundamental science. LANL is operated by LANS, LLC for the NNSA of the USDoE under contract no. DE-AC52-06NA25396.