Density-Functional Theory Molecular Dynamics Simulations at Extreme Conditions

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Large-scale molecular dynamics (MD) simulations, using both Kohn-Sham (KS) and orbital-free (OF) density-functional theory (DFT) formulations, have been performed for pure and mixed species over a broad range of temperatures (1 to 1,000 eV) and densities (ambient to 10-fold compressed) that spans the warm, dense matter and high energy density regimes. A finite-temperature Thomas-Fermi-Dirac form with a local-density exchange-correlation potential and a regularized electron-ion interaction represents the quantum nature of the electrons. In particular, we examine the efficacy of the OFMD approach as an effective bridge between KSMD at low temperatures and simple, fully-ionized plasma models at high temperatures. We discuss the challenges encountered when applying DFT MD at these extreme conditions. Comparisons against intermediate-range average-atom constructions such as the Yukawa and one-component classical plasmas are also made. To this end, we treat a variety of systems, ranging from light to heavy elements, from which lithium hydride, including illustrations from the shock Hugoniot and mass transport properties (diffusion, viscosity), serves as a representative example. In addition, non-equilibrium simulations, both with OFMD and classical Yukawa MD, of the interpenetration of two components at an interface are presented, with relevance to such applications as inertial confinement fusion. This work, in collaboration with L. A. Collins, C. Ticknor, L. Burakovsky, S. Herring, D. Sheppard, S. Crockett, F. Lambert, J. Clerouin, and M. P. Desjarlais, was performed in part 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.