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DFT-MD simulations of shocked Xenon RUDOLPH J. MAGYAR, THOMAS R. MATTSSON, Sandia National Laboratories — Xenon is not only a technologically important element used in laser technologies, jet propulsion and dental anesthesia, but it is also arguably the simplest material in which to study the metal-insulator transition at high pressure. Because of its closed shell electronic configuration, Xenon is often assumed to be chemically inert, interacting almost entirely through the van der Waals interaction, and at liquid density, is typically modeled well using Leonard-Jones potentials. However, such modeling has a limited range of validity as Xenon is known to form compounds at normal conditions and likely exhibits considerably more chemistry at higher densities when hybridization of occupied orbitals becomes significant. In this talk, we present DFT-MD simulations of shocked liquid Xenon with the goal of developing an improved equation of state. The relative importance of the van der Waals interaction compared to other Coulomb interactions is considered, and estimates of the relative accuracy of various density functionals are quantified. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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