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Density Functional Theory (DFT) Simulations of Shocked Liquid Xenon THOMAS R. MATTSSON, RUDOLPH J. MAGYAR, Sandia National Laboratories — Xenon is not only a technologically important element used in laser technologies and jet propulsion, but it is also one of the most accessible materials in which to study the metal-insulator transition with increasing 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. 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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