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Dynamic Compression experiments on deuterium and their implications for first-principles theory

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Abstract

Recently a so-called shock-ramp platform has been developed on the Sandia Z Accelerator which generates relatively cool (1-2 kK), high pressure (>300 GPa), high compression (10 to 15-fold compression) states in liquids, allowing experimental access to the region of phase space where hydrogen is predicted to undergo a first-order phase transition from an insulating molecular-like liquid to a conducting atomic-like liquid. In this talk we will discuss the results of experiments on both deuterium and hydrogen that clearly show an abrupt transition to a metallic state [1]. We will also present recent Hugoniot and reshock data for deuterium with unprecedented precision in the vicinity of the molecular-to-atomic transition [2]. These data not only establish maximum compression along the Hugoniot at 4.5-fold, but also enable high-fidelity comparisons with first-principles theory. Finally, we present a detailed comparison of previous multiple-shock electrical conductivity measurements [3] in hydrogen and deuterium near the molecular-to-atomic (MA) transition with finite temperature density functional theory calculations employing various exchange-correlation (xc) functionals [4]. The measurement results are found to be inconsistent with the semilocal xc functional PBE and are in much better agreement with the nonlocal xc functionals vdW-DF1 and vdW-DF2. Furthermore, we show that the inconsistency with PBE likely stems from pressure errors associated with the PBE xc functional that result from premature dissociation, leading to calculated pressures that are too low at these temperature (T) and density (ρ) conditions. Together with previous comparisons at high-T, low-ρ and low-T, high-ρ, these results provide a consistent picture for the MA transition over a wide T and ρ range. This picture may also provide insight into differences in experimental observations of the metallization of liquid hydrogen and deuterium in the low-T regime.

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