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First-principles calculations of multiple-shock conductivity measurements in hydrogen and deuterium MARCUS KNUDSON, MICHAEL DESJARLAIS, Sandia National Laboratories, MARTIN PREISING, RONALD REDMER, Institure of Physics, University of Rostock — We present a detailed comparison of previous multiple-shock electrical conductivity measurements in hydrogen and deuterium near molecular-to-atomic (MA) transition with finite temperature density functional theory (FT-DFT) calculations employing various exchange-correlation (xc) functionals. 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. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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