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First principles investigation of the insulator-metal transition in liquid hydrogen with a recently developed deorbitalized meta-GGA exchange-correlation functional[1] JOSHUA HINZ, VALENTIN KARASIEV, SUXING HU, MAHAMED ZAGHOO, University of Rochester, DANIEL MEJIA-RODRIGUEZ, University of Florida Quantum Theory Project — Through calculations of optical and structural properties from ab initio quantum molecular dynamic simulations we have determined the insulator- metal transition (IMT) boundary for hydrogen and deuterium using the deorbitalized meta-GGA exchange correlation functional SCAN-L with the nonlocal correlation correction rVV10. The two separate criteria of a dc conductivity of 2000 S/cm and the energy gap closure from the density of states provide a consistent IMT boundary that is in good agreement with recent static compression experiments. Furthermore, upon inclusion of nuclear quantum effects via path integral molecular dynamics our initial IMT boundary shifts toward lower pressures providing an excellent agreement with three separate experiments and indicates a clear step like feature, with a physics discussion here within, consistent with coupled electron-ion Monte Carlo predictions.

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