Abstract Submitted
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Liquid-liquid phase transition in high pressure hydrogen from ab-initio simulations[1] MIGUEL A. MORALES, ERIC SCHWEGLER, LLNL, CARLO PIERLEONI, U. of L'Aquila, IT, DAVID M. CEPERLEY, UIUC — Using Born-Oppenheimer molecular dynamics with Density Functional Theory and Coupled Electron-Ion Monte Carlo simulations, we study molecular dissociation in liquid hydrogen. We observe a range of densities for which $(dP/d?)_T = 0$ and find sharp discontinuities in the electronic conductivity; both are clear evidence of a liquid-liquid phase transition for temperatures 600K < T < 1500K. Both levels of theory exhibit the transition, although Quantum Monte Carlo predicts higher transition pressures. We estimate the critical point of the transition at temperatures slightly below 2000K using the discontinuity in the electronic conductivity. Using Path Integral Molecular Dynamics we examine the influence of zero point motion on the predicted transition, which still exhibits a first order behavior. We calculate the melting curve of molecular hydrogen up to pressures of 200GPa, finding a reentrant melting line in good agreement with previous calculations. The melting line crosses the metalization line at 700K and 220GPa with density functional theory and at 550K and 290GPa within Quantum Monte Carlo.

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