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Plasma phase transition in high pressure hydrogen from ab-initio simulations MIGUEL MORALES, Rice University, CARLO PIERLEONI, University of L'Aquila, Italy, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — We performed a detailed study of molecular dissociation in liquid hydrogen using Born-Oppenheimer molecular dynamics with Density Functional Theory and Coupled Electron-Ion Monte Carlo simulations. We observe a range of densities for which $(dP/d\rho)_T = 0$ and find sharp discontinuities in the electronic conductivity; both are clear evidence of the plasma phase transition for temperatures $600K \leq T \leq 1500K$. Both levels of theory exhibit the transition, although Quantum Monte Carlo predicts higher transition pressures. Based on the temperature dependence of the discontinuity in the electronic conductivity, we estimate the critical point of the transition at temperatures slightly below 2000 K. Using Path Integral Molecular Dynamics we examine the influence of zero point motion on the predicted transition, which still exhibits a first order behavior; the main effect of nuclear zero point energy is to shift the transition to smaller pressures. We calculate the melting curve of molecular hydrogen up to pressures of 200 GPa, finding a reentrant melting line in good agreement with previous calculations. The melting line crosses the metalization line at 700 K and 220 GPa with density functional theory and at 550 K and 290 GPa within Quantum Monte Carlo.

Miguel Morales
Rice University

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