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Computational study of the equation of state of hydrogen using the Coupled Electron-Ion Monte Carlo Method MIGUEL MORALES, Department of Physics, University of Illinois at Urbana-Champaign, KRIS DELANEY, Materials Research Laboratory, UCSB, DAVID CEPERLEY, Department of Physics, University of Illinois at Urbana-Champaign, CARLO PIERLEONI, Dipartimento di Fisica, Universita del l'Aquila, l'Aquila, Italy — We study the equation of state of liquid hydrogen at Mbar pressures, in the regime of pressure dissociation/ionization, using the Coupled Electron-Ion Monte Carlo (CEIMC) method. Our aim is to accurately describe the crossover from the molecular to the atomic regime. The CEIMC method is based on the Born-Oppenheimer approximation and consists of a Monte Carlo simulation of the ionic degrees of freedom (either with path integals or classical Metropolis) using a potential energy surface obtained from a zero temperature QMC method. The electronic calculation is done using either Variational Monte Carlo or the more accurate Reptation Quantum Monte Carlo. A Slater-Jastrow wavefunction is used, with an analytical RPA Jastrow term and one-body orbitals, obtained from a fast band structure calculation, with backflow corrections. In addition to the thermodynamic and structural properties of the dense fluid, we will discuss the influence of quantum effects on the protons. We also compare our results with recent calculations obtained using Born-Oppenheimer Molecular Dynamics.

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