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**Computational study of the Hydrogen equation of state 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. Recently, we incorporated backflow corrections to the orbitals obtained from DFT. This results in a much improved wavefunction over the entire crossover regime. We report preliminary results using this new wavefunction. We also compare our results with recent calculations obtained using Born-Oppenheimer Molecular Dynamics.

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