Abstract Submitted for the MAR08 Meeting of The American Physical Society

Electrical conductivity of liquid Hydrogen¹ FEI LIN, University of Illinois at Urbana-Champaign, KRIS DELANEY, University of California, Santa Barbara, MIGUEL MORALES, University of Illinois at Urbana-Champaign, CARLO PIERLEONI, University of L'Aquila, RICHARD MARTIN, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — DC electrical conductivity of liquid Hydrogen under high pressure has been measured by shock-wave experiments a long time ago [Phys. Rev. Lett. 76, 1860 (1996)], however, an accurate theoretical calculation of electrical conductivity is still unavailable. Abinitio DFT calculations seem to overestimate the DC conductivity value by about 6 times. On the other hand, coupled electron-ion Monte Carlo (CEIMC) simulation [Phys. Rev. Lett. 97, 235702 (2006)] has predicted different high-pressure Hydrogen molecular-atomic transition than the DFT calculation. In this talk I will report our preliminary electrical conductivity results from CEIMC simulations using the Kubo formula with energies and current-current matrix elements computed with correlated quantum Monte Carlo methods.

¹Supported by DE-FG52-06NA26170 and computer resources of NCSA.

Fei Lin University of Illinois at Urbana-Champaign

Date submitted: 27 Nov 2007

Electronic form version 1.4