Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Equation of state and electronic structure of liquid Helium at high pressure LARS STIXRUDE, University of Michigan, RAYMOND JEANLOZ, University of California at Berkeley — As the second most abundant element, the properties of fluid Helium form an important part of our understanding of stellar and giant planetary structure. Yet the physics of Helium at pressure-temperature conditions characteristic of these bodies is uncertain. We perform first principles molecular dynamics simulations of fluid Helium over a wide range of pressure (< 1 Gbar) and temperature (< 5 eV). The simulations are based on finite-temperature density functional theory in the generalized gradient approximation, and are performed in the canonical ensemble with a Nose thermostat. We find that both temperature and compression have a strong influence on the electronic structure as revealed by the band gap. At a density of 1 g cm^{-3} the band gap varies from 20 eV for the static crystal to 0 for the fluid at 4 eV. The gap is closed at all temperatures for density greater than 20 g cm^{-3}. We find that the equation of state varies smoothly through the band gap closure transition with no indication of a high-order phase transformation. The decrease in band gap with increasing temperature at constant density results from enhanced mixing of 1s- and 2s-like states with increasing disorder (i.e., enhanced vibrational amplitudes and melting) that has profound implications for understanding the deep interiors of planets.

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Date submitted: 30 Nov 2005 Electronic form version 1.4