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Equation of state and electronic structure of liquid Helium at high pressure LARS STIXRUDE, University of Michigan, RAYMOND JEAN-LOZ, 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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