

CU Physics Department Colloquium

Monday, October 17, 2011 4:10 PM 428 Pupin Hall

The phases of Hydrogen and Helium at High Pressure as revealed by simulations

Hydrogen and helium account for much of the visible mass in the universe. Their properties are important for understanding the giant planets, Jupiter and Saturn, but experiments under the relevant conditions are challenging. Even though they are the simplest elements in the periodic table, calculating their properties is not simple since they are highly quantum systems. For example, it has long been an open question how hydrogen makes a transition from a molecular insulating state to an atomic metallic state. We have developed new simulation methods starting from “first principles” to treat such systems and using them, have studied molecular dissociation in liquid hydrogen and have observed clear evidence of an “extra” liquid-liquid phase transition for temperatures $600\text{K} < T < 1500\text{K}$. We have performed a “random structure search” to determine the ground-state crystal structures of atomic metallic hydrogen from 500 GPa to 5 TPa. We also examined hydrogen–helium mixtures at Mbar pressures and high temperatures (4000 to 10000 K) and determined the temperature, at a given pressure, when helium becomes insoluble in dense metallic hydrogen: this could explain some of the observed differences between Jupiter and Saturn.



David Ceperley, University of Illinois at Urbana-Champaign