

Abstract for an Invited Paper
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First Principles Calculations of Hydrogen-Helium Mixtures and the Structure of Jupiter¹

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Most of the over two hundred recently discovered extrasolar planets are gas giants that are primarily composed of dense fluid hydrogen and helium at megabar pressures and temperature of thousands of degrees Kelvin. The characterization of hydrogen-helium mixtures at such extreme conditions has posed a challenge to experimental and theoretical methods. Great progress has been made with recent shock wave experiments and the megabar regime has been probed. However, the temperatures were much higher and the densities were significantly lower than those present in giant planets because planetary interiors are characterized by isentropes, which rise much slower in the P-T plane than shock Hugoniot curves. In this talk, results from an extensive set of density-functional molecular dynamics simulations will be presented [J. Vorberger *et al.*, *Phys. Rev. B* **75** (2006) 024206] and an equation of state (EOS) of hydrogen-helium mixtures that spans for Jupiter's interior is derived. Going beyond the commonly assumed linear mixing approximation, the interaction effects of dense hydrogen and helium are analyzed. It will be discussed how helium affects the molecular-to-metallic transition in hydrogen and why the presence of helium stabilizes the molecular phase. Based on this first-principles EOS, an updated model for the interior of Jupiter will be introduced. Our interior model updates the suite of models that were based on the widely used Saumon-Chabrier-Van Horn (SCVH) EOS. Deviations from SCVH are up to about 5 percent depending on the pressure, and thus affect interior models at the same level. Unlike SCVH, the computed DFT-EOS does not predict any first-order thermodynamic discontinuities associated with pressure-dissociation and metallization of hydrogen. Finally, the size of a rocky core in Jupiter and the heavy elements enrichment in its mantle will be estimated. It will be discussed whether the planet was formed by core-accretion.

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