## Abstract Submitted for the MAR09 Meeting of The American Physical Society

Phase separation in hydrogen-helium mixtures at high pressure MIGUEL MORALES, University of Illinois at Urbana-Champaign, ERIC SCHWE-GLER, Lawrence Livermore National Laboratory, DAVID CEPERLEY, University of Illinois at Urbana-Champaign, CARLO PIERLEONI, University of L'Aquila, L'Aquila (Italy), SEBASTIAN HAMEL, KYLE CASPERSEN, Lawrence Livermore National Laboratory — We study the properties of hydrogen-helium mixtures at Mbar pressures and intermediate temperatures (4000 to 10000 K) using first-principles molecular dynamics simulations. Our main goal is to calculate the temperature, as a function of pressure, at which helium becomes insoluble in dense metallic hydrogen. We perform an extensive study of the equation of state of the mixture as a function of density, temperature, and composition and, together with a variety of thermodynamic integration techniques, we calculate the Gibbs free energy of mixing. We will show how to calculate the entropic contribution of the free energy using coupling constant integration methods, which allows us to directly calculate immiscibility temperatures without the need to resort to approximations of the entropy of mixing. These results are relevant to models of the interior structure and evolution of Jovian planets. We find demixing temperatures that are sufficiently high to cross the planetary adiabat of Saturn at pressures around 5 Mbar, implying the existence of partially miscible regions over a significant portion of the interior of the planet.

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