

Abstract Submitted
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Quantifying Ab Initio Equation of State Errors for Hydrogen-Helium Mixtures RAYMOND CLAY, Sandia National Laboratory, MIGUEL MORALES, Lawrence Livermore National Laboratory — In order to produce predictive models of Jovian planets, an accurate equation of state for hydrogen-helium mixtures is needed over pressure and temperature ranges spanning multiple orders of magnitude. While extensive theoretical work has been done in this area, previous controversies regarding the equation of state of pure hydrogen have demonstrated exceptional sensitivity to approximations commonly employed in ab initio calculations. To this end, we present the results of our quantum Monte Carlo based benchmarking studies for several major classes of density functionals. Additionally, we expand upon our published results by considering the impact that ionic finite size effects and density functional errors translate to errors in the equation of state. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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