Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Zero-Temperature Structures of Atomic Metallic Hydrogen JEFFREY MCMAHON, DAVID CEPERLEY, Department of Physics, University of Illinois, Urbana-Champaign, IL 61801 — Since the first prediction of an atomic metallic phase of hydrogen by Wigner and Huntington over 75 years ago, there have been many theoretical efforts aimed at determining the crystal structures of the zero-temperature phases. We present results from ab initio random structure searching with density functional theory performed to determine the ground state structures from 500 GPa to 5 TPa. We estimate that molecular hydrogen dissociates into a monatomic body-centered tetragonal structure near 500 GPa ($r_s = 1.225$), which then remains stable to 2.5 TPa ($r_s = 0.969$). At higher pressures, hydrogen stabilizes in an $...ABCABC...$ planar structure that is remarkably similar to the ground state of lithium, which compresses to the face-centered cubic lattice beyond 5 TPa ($r_s < 0.86$). Our results provide a complete ab initio description of the atomic metallic crystal structures of hydrogen, resolving one of the most fundamental and long outstanding issues concerning the structures of the elements.

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Date submitted: 18 Nov 2010 Electronic form version 1.4