Abstract Submitted for the SHOCK11 Meeting of The American Physical Society

The Effects of Relativity on First-Principles Calculations T. SEMI, Colorado School of Mines, A.E. MATTSSON, Sandia National Laboratories, J.M. WILLS, Los Alamos National Laboratory — The construction of the equation of state for a given material is of central importance to its characterization. Hugoniots can be calculated using Density Functional Theory (DFT), and DFT points compared to available experimental results. By evaluating the accuracy in a relevant phase space, confidence is gained in the DFT method. This bolsters the dependability of DFT data in phase spaces in which experiment may be difficult or impossible to perform, and verifies its usefulness. The equation of state is comprised of the cold curve and thermal electronic and ionic terms. We discuss differences in the cold curve of Ce produced by first principles calculations using the Scalar Dirac equation with variational spin-orbit coupling treatment and that generated by the full relativistic formulation, both with the same DFT functionals. The relativistic effects of f-electrons in systems like Ce are expected to be of a magnitude substantial enough to be consequential to the description of these structures. "Sandia National Laboratories is a multi-program 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."

Date submitted: 16 Feb 2011

T. Semi Colorado School of Mines

Electronic form version 1.4