Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Predictive equation of state method for heavy materials based on the Dirac equation and density functional theory JOHN M. WILLS, Los Alamos National Laboratory, ANN E. MATTSSON, Sandia National Laboratories — Density functional theory (DFT) provides a formally predictive base for equation of state properties. Available approximations to the exchange/correlation functional provide accurate predictions for many materials in the periodic table. For heavy materials however, DFT calculations, using available functionals, fail to provide quantitative predictions, and often fail to be even qualitative. This deficiency is due both to the lack of the appropriate confinement physics in the exchange/correlation functional and to approximations used to evaluate the underlying equations. In order to assess and develop accurate functionals, it is essential to eliminate all other sources of error. In this talk we describe an efficient first-principles electronic structure method based on the Dirac equation and compare the results obtained with this method with other methods generally used. Implications for high-pressure equation of state of relativistic materials are demonstrated in application to Ce and the light actinides. Sandia National Laboratories is a multi-program laboratory managed andoperated 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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Date submitted: 08 Dec 2011 Electronic form version 1.4