Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Actinide electronic structure based on the Dirac equation and density functional theory JOHN M. WILLS, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, ANN E. MATTSSON, Sandia National Laboratories, Albuquerque, NM 87185, USA — Density functional theory (DFT) provides a formally predictive basis for predicting the structural properties of actinides. Although available approximations to the exchange/correlation functional provide accurate predictions for many materials, they fail qualitatively and sometimes quantitatively when applied to actinides. Major contributors to this deficiency are an inadequate treatment of confinement physics and an incomplete treatment of relativity in the underlying equations. The development of a functional correctly incorporating confinement physics with a proper treatment of relativity would provide definitive, internally consistent predictions of actinide properties. To enable the development of such a functional and quantify the predictions of currently available functionals, we have developed an efficient first-principles electronic structure method based on the Dirac equation. Results are compared with current methods, and the implications for relativistic density functionals discussed. Sandia National Laboratories is a multiprogram 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.

John Wills
Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Date submitted: 19 Dec 2012 Electronic form version 1.4