

Abstract Submitted
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Requirements for Predictive Density Functional Theory Methods for Heavy Materials Equation of State ANN E. MATTSSON, Sandia National Laboratories, JOHN M. WILLS, Los Alamos National Laboratory — The difficulties in experimentally determining the Equation of State of actinide and lanthanide materials has driven the development of many computational approaches with varying degree of empiricism and predictive power. While Density Functional Theory (DFT) based on the Schrödinger Equation (possibly with relativistic corrections including the scalar relativistic approach) combined with local and semi-local functionals has proven to be a successful and predictive approach for many materials, it is not giving enough accuracy, or even is a complete failure, for the actinides. To remedy this failure both an improved fundamental description based on the Dirac Equation (DE) and improved functionals are needed. Based on results obtained using the appropriate fundamental approach of DFT based on the DE we discuss the performance of available semi-local functionals, the requirements for improved functionals for actinide/lanthanide materials, and the similarities in how functionals behave in transition metal oxides. 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.

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