

Abstract Submitted  
for the 4CF06 Meeting of  
The American Physical Society

**The Equation of State of  $\alpha$ -Uranium from a First Principles Perspective** SOURAV ADAK, BORIS KIEFER, New Mexico State University — Uranium occurs in diverse environments, for example as a fuel in nuclear reactors and as a major source for the internal heating of our planet. Therefore the understanding of the electronic structure of uranium is important to develop a unified model for uranium in different bonding environments. Heavy elements at the bottom of the periodic table pose a large challenge to theory due to the often complex interplay of s-, d-, and f-electrons that are difficult to treat self-consistently in density functional theory. Here we adopt the simplest description that neglects spin-orbit coupling and any special treatment of strong electronic correlations. The calculations are based on the projected augmented wave method within the GGA approximation. We find that the equation of state is in good agreement with experiment. This suggests that our simplified electronic structure model of uranium captures most of the physics and may be used to describe bonding of this element in other environments at least to first order.

Heinrich Nakotte  
New Mexico State University

Date submitted: 11 Sep 2006

Electronic form version 1.4