

Abstract Submitted  
for the MAR08 Meeting of  
The American Physical Society

**Electronic Structure of Actinide Materials**<sup>1</sup> J.J. JOYCE, Los Alamos National Laboratory, T. DURAKIEWICZ, K.S. GRAHAM, D.P. MOORE, L.A. MORALES, J.M. WILLS, R.L. MARTIN, J.-X. ZHU, L.E. ROY, C.G. OLSON, Ames Laboratory, USDOE, G.E. SCUSERIA, I.D. PRODAN, Rice University — Photoelectron spectroscopy results for both metallic and insulating actinide materials are reviewed and compared against model calculations. The dual nature of 5f electron characteristics is discussed for photoemission results and three different electronic structure calculations. Magnetic configurations as a means of f-electron localization are discussed for metallic materials. The photoemission results for U and Pu intermetallics are compared against mixed-level-model and dynamical-mean-field-theory calculations. The experimental results for the actinide oxide Mott insulators are compared against screened hybrid functional calculations.

<sup>1</sup>Work supported by the US DOE, Office of Science, Campaign II, and the LANL LDRD program.

John Joyce  
Los Alamos National Laboratory

Date submitted: 24 Jan 2008

Electronic form version 1.4