Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Electronic Structure and Correlation Effects in $PuCoIn_5$ as Compared to $PuCoGa_5$[1] JIAN-XIN ZHU, P.H. TOBASH, E.D. BAUER, F. RONNING, B.L. SCOTT, Los Alamos National Laboratory, K. HAULE, G. KOTLIAR, Rutgers University, R.C. ALBERS, J.M. WILLS, Los Alamos National Laboratory — Since their discovery nearly a decade ago, plutonium-based superconductors have attracted considerable interest, which is now heightened by the latest discovery of superconductivity in $PuCoIn_5$. In the framework of density functional theory (DFT) within the generalized gradient approximation (GGA) together with dynamical mean-field theory (DMFT), we present a comparative study of the electronic structure of superconducting $PuCoIn_5$ with an expanded unit cell volume relative to its $PuCoGa_5$ cousin. Overall, a similar GGA-based electronic structure, including the density of states, energy dispersion, and Fermi surface topology, was found for both compounds. The GGA Pu $5f$ band was narrower in $PuCoIn_5$ than in $PuCoGa_5$ due to the expanded lattice, resulting in an effective reduction of Kondo screening in the former system, as also shown by our DMFT calculations.

[1]This work was supported by U. S. DOE at LANL, Office of Basic Energy Sciences, and LANL LDRD Program.

Jian-Xin Zhu
Los Alamos National Laboratory

Date submitted: 13 Dec 2011 Electronic form version 1.4