Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

An *Ab Initio* Study of α –Pu[1] SARAH C. HERNANDEZ, ASOK K. RAY, University of Texas at Arlington — Hybrid density functionals, which replace a fraction of density functional theory exchange with exact Hartree-Fock exchange has been used to study the electronic, geometric, and magnetic properties of α – Pu. Different fractions of Hartree-Fock exchange have been used and the computations have been performed using the all-electron full-potential linearized augmented plane wave plus local orbitals basis method. Pu has been studied at the non-magnetic, ferromagnetic and anti-ferromagnetic configurations with spin-orbit coupling, orbital polarization, and *full* geometry optimizations. The variations of the optimized lattice constants, magnetic moments, bulk moduli, density of states, and the degree of $5f$electron localization with the amount of Hartree – Fock exchange will be reported. Results will be compared with those of δ – Pu for which the performance of the hybrid functionals did *not* seem superior to that of the pure density functionals.[2]

[1]This work is partially supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525) and by the LSAMP-BD Program.
[2]R. Atta-Fynn and A. K. Ray, Europhys. Lett. 85, 27008 (2009).

Sarah C. Hernandez
University of Texas at Arlington

Date submitted: 18 Nov 2010 Electronic form version 1.4