

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

An *Ab Initio* Full Potential Fully Relativistic Study of the (0001) Surface of Double Hexagonal Close Packed Americium* DA GAO, Idaho National Laboratory, ASOK RAY, the University of Texas at Arlington — The electronic and geometric properties of bulk dhcp Am as well as quantum size effects in the surface energies and the work functions of the dhcp Am (0001) ultra thin films up to seven layers have been examined at nonmagnetic, ferromagnetic, and anti-ferromagnetic configurations via full-potential all-electron density-functional calculations with a mixed APW+lo/LAPW basis. The anti-ferromagnetic state including spin-orbit coupling is found to be the ground state of both bulk and the (0001) surface of dhcp Am with the $5f$ electrons primarily localized. Our results show that magnetic configurations and spin-orbit coupling play important roles in determining the equilibrium lattice constant, the bulk modulus as well as the localized feature of $5f$ electrons for dhcp Am. Quantum size effects are found to be more pronounced in work functions than in surface energies. *This work is supported by the Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, Office of Science, U. S. Department of Energy and the Welch Foundation, Houston, Texas.

Da Gao
Idaho National Laboratory

Date submitted: 19 Dec 2006

Electronic form version 1.4