Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

A Density Functional Study of the Americium (001) Surface[1] DA GAO, ASOK KUMAR RAY, University of Texas at Arlington — Electronic structure properties of the fcc americium (001) surface, modeled by periodically repeated fcc Am (001) surface slabs, have been studied with the full-potential linearized augmented plane wave (FP-LAPW) method. The alternative basis set APW+lo is used inside the atomic spheres for chemically important orbitals that are difficult to converge, whereas LAPW is used for others. The core states are treated fully relativistically and for valence states, two levels of treatments are implemented: (1) a scalar relativistic scheme including the mass-velocity correction and the Darwin s-shift and (2) a fully relativistic scheme with spin-orbit coupling included in a second variational treatment using the scalar-relativistic eigenfunctions as basis. Our results indicate that the ground state of Am (001) surface is anti-ferromagnetic. The quantum size effects in the surface energies and the work functions of the (001) fcc americium ultra thin films (UTF) have been examined up to seven layers. In addition, the Am (001) surface properties are compared with our earlier study of the Am (111) surface.

[1]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 (Grant No. DE-FG02-03ER15409) and the Welch Foundation, Houston, Texas (Grant No. Y-1525)

Da Gao
Department of Physics, the University of Texas at Arlington,
Arlington, TX 76019

Date submitted: 23 Nov 2005 Electronic form version 1.4