Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Adsorption and Dissociation of Molecular Oxygen on the (0001) Surface of Double Hexagonal Close Packed Americium[1] PRATIK DHOLABHAI, RAYMOND ATTA-FYNN, ASOK RAY, The University of Texas at Arlington — Oxygen molecule adsorption on (0001) surface of double hexagonal packed americium has been studied in detail within the framework of density functional theory using a full-potential all-electron linearized augmented plane wave plus local orbitals method. The most stable configuration corresponded to molecular dissociation with the oxygen atoms occupying neighboring three-fold hollow h3 sites. Chemisorption energies and adsorption geometries for the adsorbed species, and change in work functions, magnetic moments, partial charges inside muffin-tins, difference charge density distributions and density of states for the bare Am slab and the Am slab after adsorption of the oxygen molecule will be discussed. The effects of chemisorption on Am $5f$ electron localization-delocalization in the vicinity of the Fermi level and the reaction barrier calculation for the dissociation of oxygen molecule to the most stable h3 sites will be discussed.

[1]This work is supported by the U. S. Department of Energy and the Welch Foundation, Houston, Texas.

Pratik Dholabhai
The University of Texas at Arlington

Date submitted: 13 Nov 2007 Electronic form version 1.4