Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A Hybrid Density Functional Study of Atomic Hydrogen and Oxygen Adsorptions on the (0001) Surface of Non-Magnetic DHCP Americium[1] SHAFAQ AMDANI-MOTEN, RAYMOND ATTA-FYNN, ASOK RAY, Physics Department, University of Texas at Arlington, Texas 76019 — As our group have recently shown[+], hybrid density functional theory (HDFT) which replaces a fraction (40%) of approximate DFT exchange with exact Hartree-Fock exchange yield structural, magnetic, and electronic properties for Americium-I that are in excellent agreement with experimental data. As a natural progression, *ab initio* calculations for atomic adsorptions on the (0001) surface of non-magnetic americium have been performed using HDFT. The americium surface is modeled by a seven-layer slab using inversion symmetry consisting of one atom per layer and non-magnetic ABAC stacking arrangement of these layers. Top, bridge, hcp and fcc chemisorption sites have been investigated with energies optimized with respect to the adatom distance from the surface. Details of the chemisorptions processes as well as comparisons of different sites will be presented. [+]R. Atta-Fynn and A. K. Ray, Chemical Physics Letters, **482**, 223-227 (2009).

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

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Date submitted: 22 Nov 2009 Electronic form version 1.4