Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Quantum Size Effects in the Properties of Non-Magnetic Americium-I (0001) Surface: A Hybrid DFT Study[1] RAYMOND ATTA-FYNN, ASOK RAY, Physics Department, The University of Texas at Arlington — Hybrid density functional theory (HDFT) and a periodic slab model (up to nine layers thick) have been used to study the surface properties and electronic structure of non-magnetic Americium-I (0001) surface. The work function and surface energy of the semi-infinite surface is predicted to 3.45eV and 1.09 J/m^2 respectively. The surface properties, namely the surface energy, work function, and slab incremental energy exhibit no variations after five layers. A five layer slab is thus predicted to accurately model the adsorbate-induced changes in the surface properties of Americium-I (0001). The electronic structure is in excellent agreement with recent photoemission spectroscopy data. A layer-by-layer examination $5f$ electron localization using the thickest slab clearly indicates that the $5f$ electrons are localized on each layer and the nature of the localization is independent of the local geometry indicating that there is no variation in the $5f$ electron localization at the surface and in the bulk region.

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

Raymond Atta-Fynn
Physics Department, The University of Texas at Arlington

Date submitted: 17 Nov 2009 Electronic form version 1.4