Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Computational modeling of the surface properties of uranium dioxide using hybrid DFT MEGAN HOOVER, RAYMOND ATTA-FYNN, Department of Physics, The University of Texas at Arlington — Computational modeling of processes such as corrosion and the interaction of environmental impurities with the surfaces of actinide materials are important to the understanding of remediation processes for actinide-based nuclear waste from the biosphere. However, accurate modeling of bare surfaces of actinide materials is a necessary precursor to accurate modeling of surface interactions. This talk will be focused on atomistic modeling of uranium dioxide (UO_2) surfaces. The theoretical formalism is all-electron hybrid Density Functional Theory (DFT) based on the full-potential linearized augmented plane wave plus local basis method. Specifically, we computed the surface energies, work functions, incremental energies, and electronic band gaps for periodic slab structures for the (110) and (111) surfaces of UO_2. We observed that the anti-ferromagnetic semiconducting behavior in the bulk structure is retained in the surface structures. The convergence of surface properties with respect to slab thickness will be discussed. The trends in the surface electronic structures, particularly the localized behavior of the U $5f$ electrons, in comparison with the bulk structure will also be elucidated.

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Date submitted: 15 Nov 2013 Electronic form version 1.4