Abstract Submitted
for the TSF15 Meeting of
The American Physical Society

PuO_2 (111) surface study of electronic and magnetic properties using hybrid density functional theory[1] SHAFAQ MOTEN, RAYMOND ATTA-FYNN, ASOK RAY, MUHAMMAD HUDA, None — PuO_2 (111) surface have been investigated using an all-electron hybrid density functional theory. The periodic slab models of the surface, from one to six molecular layers, were examined to find surface properties and slab size effects. Both ferromagnetic (FM) and antiferromagnetic (AFM) configurations were considered with and without spin-orbit coupling for the 1x1 slab. The effect of periodicity was explored between AFM configured 11 and 22 super cell. Results based on surface energies, work function, band gaps and density of states will be presented. It will be shown that except for the top layer, the surface in general retains the Mott-insulator property.

[1]PuO2 (111) surface study of electronic and magnetic properties using hybrid density functional theory

Shafaq Moten
None

Date submitted: 01 Oct 2015 Electronic form version 1.4