Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Does Water Adsorb Molecularly or Dissociatively on a Plutonium Surface?[1] ASOK RAY, RAYMOND ATTA-FYNN, Department of Physics, University of Texas at Arlington — DFT-GGA has been used to study adsorption of water in molecular and dissociative configurations on δ-Pu (111) surface. In molecular state, water is physisorbed in an almost flat-lying orientation at a one-fold coordinated on-top site. The interaction of the water $1b_1$ orbital and the Pu-$6d$ orbital provides the stability of water on the surface, implying that the Pu-$5f$ electrons remain chemically inert. The coadsorption cases of partially dissociated and fully dissociated products at the three-fold hollow sites yield chemisorption, coupled with rumpling of the surface layer and delocalization of the Pu-$5f$ electrons and formation of strong ionic bonds.

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

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Date submitted: 19 Nov 2008 Electronic form version 1.4