Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

An Ab Initio Study of Molecular Oxygen Adsorption on Pu (111) Surface[1] M. N. HUDA, A. K. RAY, Department of Physics, University of Texas at Arlington, Arlington, Texas 76019 — We will present a study of oxygen molecule adsorption on a Pu (111) surface using the generalized gradient approximation to density functional theory using the DMol3 suite of programs [1]. Horizontal approaches on center site, with and without spin polarization, were found to be the highest chemisorbed sites among all the cases studied here with chemisorption energies of 8.365eV and 7.897eV, respectively. The second highest chemisorption energy occurs at the vertical approach on bridge site with chemisorption energy of 8.294eV (non-spin-polarized) and 7.859eV (spin-polarized). In general, with spin polarization, dissociative adsorption with a layer by layer alternate spin arrangement of the plutonium layer is found to be energetically more favorable compared to molecular adsorption. Non-spin-polarized chemisorption energies are usually higher than the spin-polarized energies. We also find that 5f electrons are more localized in spin polarized case, than the non-spin polarized counterparts. The ionic part of O-Pu bonding plays a significant role along with the Pu 5f-O 2p hybridization. [1] B. Delley, J. Chem. Phys. **92**, 508 (1990); J. Chem. Phys. **113**, 7756 (2000).

[1]Work supported by the Department of Energy (Grant No. DE-FG02-03ER15409) and Welch Foundation (Grant No. Y-1525).

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Date submitted: 30 Nov 2004 Electronic form version 1.4