

Abstract Submitted
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Hydrogen Molecule Adsorption and Dissociation on Plutonium (111) Surface¹ M. N. HUDA, A. K. RAY, Department of Physics, University of Texas at Arlington, Arlington, Texas 76019 — Hydrogen molecule adsorption on plutonium (111) surface has been studied in detail using the generalized gradient approximation to density functional theory. All calculations have been performed at the non-spin-polarized and spin-polarized levels of theory using the DMol3 suite of programs [1]. Weak molecular adsorptions with a layer by layer alternate spin arrangement of the plutonium atoms were observed. Horizontal approaches on the top site both with and without spin polarization were found to be the most favorable molecular adsorption sites. For dissociative adsorption, the most favorable dissociation channel needs activation energies of 0.216eV and 0.305eV at non-spin-polarized and spin-polarized levels, respectively, with considerably higher adsorption energies than those of the molecular cases. In general, adsorption of hydrogen molecule pushes the Pu 5f band away from the Fermi level. Charge transfer to the hydrogen atoms for dissociative adsorption is larger than that of molecular adsorption and the ionic part of H-Pu bonding contributes along with the covalent part due to Pu 5f - H 1s hybridization. [1] B. Delley, J. Chem. Phys. **92**, 508 (1990); J. Chem. Phys. **113**, 7756 (2000).

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