Abstract Submitted
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An Ab Initio Study of H2 Interaction with Pu (100) Surface[1] M. N. HUDA, A. K. RAY, Department of Physics, University of Texas at Arlington, Arlington, Texas 76019 — We present here a detailed study of hydrogen molecule adsorption on a plutonium (100) surface, using the generalized gradient approximation to density functional theory. All calculations were done 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 have been observed and the vertical approaches at the center site are found to be the most favorable molecular adsorption sites, with slightly higher adsorption energies for non-spin-polarized cases. The most favorable dissociation channel needs activation energies of 0.551eV and 0.778eV at the non-spin-polarized and spin-polarized levels, respectively, with considerably higher adsorption energies compared to molecular adsorptions. The 5f electrons are more localized in spin polarized cases than the non-spin polarized counterparts. For dissociative adsorption, the ionic part plays an important role in H-Pu bonding, and the Pu 5f - H 1s hybridization is rather weak. Also, adsorption of hydrogen pushes the top of 5f band further away from Fermi level. [1] B. Delley, J. Chem. Phys. **92**, 508 (1990); J. Chem. Phys. **113**, 7756 (2000).

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