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Adsorption and Dissociation of Molecular Hydrogen on the (0001) Surface of DHCP Americium[1] PRATIK DHOLABHAI[2], ASOK RAY, The University of Texas at Arlington — Hydrogen molecule adsorption on the (0001) surface of double hexagonal closed packed americium has been studied in detail within the framework of density functional theory. Weak molecular hydrogen adsorptions were observed. The most stable configuration corresponded to a Hor2 approach molecular adsorption at the one-fold top site where the molecule's approach is perpendicular to a lattice vector. Adsorption energies and adsorption geometries for different adsorption sites will be discussed. The change in work functions, magnetic moments, partial charges inside muffin-tins, difference charge density distributions and density of states for the bare Am slab and the Am slab after adsorption of the hydrogen molecule will be discussed. Reaction barrier for the dissociation of hydrogen molecule will be presented. The implications of adsorption on Am $5f$ electron localization-delocalization will be summarized.

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