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A Density Functional Study of Atomic Hydrogen and Oxygen Chemisorptions on the (0001) Surface of Double Hexagonal Close Packed Americium[1] PRATIK DHOLABHAI, RAYMOND ATTA-FYNN, ASOK RAY, The University of Texas at Arlington — *Ab initio* total energy calculations within the framework of density functional theory have been performed for atomic hydrogen and oxygen chemisorptions on the (0001) surface of double hexagonal packed americium using a full-potential all-electron linearized augmented plane wave plus local orbitals (FLAPW+lo) method. The three-fold hollow hcp site was found to be the most stable site for H adsorption, while the two-fold bridge adsorption site was found to be the most stable site for O adsorption. Chemisorption 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 adatom will be discussed. The implications of chemisorption on Am $5f$ electron localization-delocalization will also be discussed.

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