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Adsorption and Dissociation of Water on the (0001) Surface of DHCP Americium[1] PRATIK DHOLABHAI[2], ASOK RAY, The University of Texas at Arlington — Ab initio total energy calculations within the framework of density functional theory have been performed for water molecule adsorption on the (0001) surface of double hexagonal closed packed americium. Subsequent partial dissociation (OH+H) and complete dissociation (H+O+H) of the water molecule have been examined. The completely dissociated configuration exhibits the strongest binding with the surface followed by partially dissociated species, with all molecular H2O configurations showing weak physisorption. The change in work functions and net magnetic moments before and after adsorption will be presented for all the cases studied. The adsorbate-substrate interactions will be elaborated using the difference charge density distributions and the local density of states. The effects of adsorption on Am 5f electron localization-delocalization in the vicinity of the Fermi level will be discussed.

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[2]Current affiliation: Arizona State University

Pratik Dholabhai
The University of Texas at Arlington

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