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A first principles study of water adsorption on α-Pu (020) surface[1] JIANGUANG WANG, ASOK K. RAY, Department of Physics, University of Texas at Arlington, Arlington, Texas 76019, USA — Adsorptions of water in molecular (H_2O) and dissociative (OH+H, H+O+H) configurations on the α-Pu (020) surface have been studied using *ab initio* methods. The full-potential FP/LAPW+lo method has been used to calculate the adsorption energies at the scalar relativistic with no spin-orbit coupling (NSOC) and fully relativistic with spin-orbit coupling (SOC) theoretical levels. It is found that the SOC effect increases the adsorption energies by $\sim$0.30 eV for the two dissociative adsorptions. Weak physisoprtions have been observed for the molecule H_2O on the α-Pu (020) surface with primarily a covalent bonding, while the two dissociative adsorptions are chemisorptive with ionic bonding. At the SOC level, the most stable adsorption energy is 0.58eV, the corresponding values being 5.44 eV and 5.73 eV for the partial dissociation and complete dissociation cases, respectively. Completely dissociative adsorption at a long bridge site for the dissociated O atom and two short bridge sites for the two dissociated H atoms is the most stable adsorption site. Hybridizations of O(2p)-H(1s)-Pu(5f)-Pu(6d) are observed for the two dissociative adsorptions, implying that some of the Pu-5f electrons become further delocalized and participate in chemical bonding.

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