

Abstract Submitted
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Hydrogen adsorption on the (020) surface of α -Pu – A computational Study¹ ASOK RAY, MD ISLAM, University of Texas at Arlington, TX 76019 — We have studied the hydrogen adsorption on (020) surface of α -Pu and the effect of surface relaxation on chemisorption using relativistic full-potential augmented plane wave with local orbital basis method. The surface is modeled with four-layer slab consisting of 32 atoms with layer by layer anti-ferromagnetic arrangements. We have investigated the adsorption properties for four different adsorption sites, namely the top, the hollow, the short bridge and the long bridge sites. All the computations are carried out both at scalar relativistic level where spin-orbit interaction is ignored and where it is included, to study the effect of SO interaction on the adsorption properties. The effect of relaxation is also studied by calculating adsorption properties both on the relaxed and the non-relaxed surfaces. Our studies show that the short bridge is the most favorable site for hydrogen adsorption with chemisorption energy of 2.75 eV. Our study also shows that the spin-orbit coupling and the surface relaxation have very little impact on adsorption.

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