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Adsorption and dissociation of molecular oxygen on α-Pu (020) surface: A density functional study[1] JIANGUANG WANG, ASOK RAY, University of Texas at Arlington — Molecular and dissociative oxygen adsorption on the (020) surface of α-Pu have been studied using the full-potential linearized augmented-plane-wave plus local orbitals (FP-LAPW+lo) basis method. Four adsorption sites and three approaches of O_2 molecule have been considered. Adsorption energies have been optimized according to the distance of the adsorbates from the Pu surface as well as the oxygen dimer bond length. Dissociative adsorption is found for two horizontal approaches (O_2 is parallel to the surface and parallel/perpendicular to a lattice vector) and to be more energetically favorable at the scalar and "fully" relativistic (NSOC vs. SOC) levels of theory. Hor2 approach on the top site was the preferred adsorption site among all cases studied here. Molecular adsorption occurs at the Vert (O_2 is vertical to the surface) approach. The work functions, net spin magnetic moments, and charge transfer are also calculated.

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