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**First-principles study of adsorption and dissociation of $CO_2$ on $\alpha$-Pu (020) surface**[1] JIANGUANG WANG, ASOK K. RAY, Department of Physics, University of Texas at Arlington, Arlington, Texas 76019, USA — The adsorption and dissociation of $CO_2$ on the $\alpha$-Pu (020) surface has been investigated using density functional theory (DFT) within generalized gradient approximation (GGA). 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. The completely dissociated configurations (C+O+O) exhibit the strongest binding with the surface, followed by the partially dissociated configurations (CO+O), with the molecular $CO_2$ adsorption having the weakest binding with the Pu surface. It is found that the SOC effect increases the adsorption energies for all considered adsorptions. For all initial vertically upright orientations, the geometry and orientation of the $CO_2$ molecule do not change after optimization. For all initial flat lying orientations, the final state of the $CO_2$ molecule corresponds to a bent geometry with a bond angle of $\sim$130°. For CO+O co-adsorption, the stable configurations corresponded to CO dipole moment orientations of $105° - 167°$ with respect to the normal surface. The local density of states and difference charge densities are also discussed.

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