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Atomic Adsorptions on the (020) Surface of α-Pu: A Density Functional Study[1] RAYMOND ATTA-FYNN, ASOK RAY, Physics Department, The University of Texas at Arlington — Adsorptions of atomic carbon, nitrogen, and oxygen on the (020) surface of α-Pu have been investigated using the full-potential linearized augmented plane wave plus local basis method. The surface was modeled by a 4-layer periodic slab consisting of a total of 32 Pu atoms. Adsorption energies have been optimized with respect to the distance of the adatom from the Pu surface for four adsorption sites, namely the one-fold top, one-fold hollow, two-fold short bridge, and the two-fold long bridge sites. The short bridge site was the most stable adsorption site for C with chemisorption energy of 6.038. The long bridge site was the most stable adsorption site for N and O with chemisorption energies of 6.067 eV and 7.362 eV respectively. The work function and net spin magnetic moments respectively increased and decreased in all cases upon chemisorption compared to the bare surface. The density of states and difference charge density have been used to analyze the adsorbate-induced changes in the surface electronic structure.

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