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An *Ab Initio* Full Potential Fully Relativistic Study of Atomic Carbon, Nitrogen, and Oxygen Chemisorption on the (111) Surface of δ-Pu[1] RAYMOND ATTA-FYNN, ASOK RAY, Physics Department, University of Texas at Arlington, Arlington, Texas 76019 — Fully-relativistic full potential density functional calculations have been performed to investigate atomic carbon, nitrogen, and oxygen chemisorption on the (111) surface of δ-Pu using the all-electron linearized augmented plane wave plus local orbitals code WIEN2k and the generalized gradient approximation to density functional theory. The surface was modeled by a three-layer periodic slab separated by 60 Bohr vacuum with two atoms per surface unit cell. The hollow fcc adsorption site was found to be the most preferred site with chemisorption energies of 6.539 eV, 6.714 eV, and 8.2 eV for the C, N, and O adatoms, respectively. The respective distances of the C, N, and O adatoms from the surface were found to be 1.16 Å, 1.08 Å, and 1.25 Å. Analysis of the partial charges inside the atomic spheres, charge density distributions, and the local density of states indicate hybridizations between Pu 5f and the 2p states of the adatoms.

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