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A FP-LAPW Study of Atomic Carbon, Nitrogen, and Oxygen Chemisorption on the (100) Surface of δ-Pu[1] RAYMOND ATTA-FYNN, ASOK RAY, Physics Department, The University of Texas at Arlington, Arlington, TX 76019 — Fully relativistic full potential density functional calculations have been performed to investigate atomic carbon, nitrogen, and oxygen chemisorption on the (100) surface of δ-Pu using the all-electron augmented plane waves plus local basis code WIEN2k. The surface was modeled by a three-layer periodic slab with two atoms per surface unit cell. The center adsorption site is found to be the most preferred site with chemisorption energies of 7.964 eV, 7.665 eV, and 8.335 eV for the C, N, and O adatoms, respectively. The corresponding optimized distances of the adatoms from the surface are found to be 0.26 Å, 0.35 Å, and 0.48 Å. The work functions and the net magnet moments respectively increased and decreased in all cases compared with the bare δ-Pu (100) surface. Analysis of partial charges inside the atomic spheres, charge density distributions, and the local density of states have been performed to investigate the nature of the interaction between the surface Pu atoms and the adatoms.

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