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Relaxation of the (111) Surface of δ-Pu and Effects of Atomic Adsorption: An *Ab Initio* Study[1] RAYMOND ATTA-FYNN, ASOK RAY, Physics Department, The University of Texas at Arlington — The full-potential all-electron linearized augmented plane wave plus local orbitals (FP-L/APW+lo) method has been employed to study the relaxation of the δ-Pu (111) surface and the consequent effects for atomic adsorption of C, N and O atoms on this surface. The surface was modeled by a 5-layer slab with a (2×2) surface unit cell. Upon relaxation of the slab, the interlayer separation between the surface and the subsurface layers expanded by 7.1% with respect to the bulk interlayer separation while the separation between the subsurface and central layers expanded by 0.4%. The hollow fcc adsorption site was found to be the most stable site for C and N with chemisorption energies of 6.420 eV and 6.549 eV respectively, while the hollow hcp adsorption site was found to be the most stable site for O with a chemisorption energy of 7.858 eV. The adsorbate-induced changes in the surface properties, namely the Pu magnetic moments, work function, and electronic structure will be discussed.

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