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Relaxation of Actinide Surfaces: An All Electron Study[1] RAYMOND ATTA-FYNN, PRATIK DHOLABHAI, ASOK RAY, Physics Department, University of Texas at Arlington, Arlington, Texas 76019 — Fully relativistic full potential density functional calculations with a linearized augmented plane wave plus local orbitals basis (LAPW + lo) have been performed to investigate the relaxations of heavy actinide surfaces, namely the (111) surface of fcc δ-Pu and the (0001) surface of dhcp Am using WIEN2k. This code uses the LAPW + lo method with the unit cell divided into non-overlapping atom-centered spheres and an interstitial region. The APW+lo basis is used to describe all s, p, d, and f states and LAPW basis to describe all higher angular momentum states. Each surface was modeled by a three-layer periodic slab separated by 60 Bohr vacuum with four atoms per surface unit cell. In general, we have found a contraction of the interlayer separations for both Pu and Am. We will report, in detail, the electronic and geometric structures of the relaxed surfaces and comparisons with the respective non-relaxed surfaces.

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