Abstract Submitted
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***Ab* initio study of the electronic and structural properties of Pu-Al alloys**[1] JAIME L. STERRETT, SARAH C. HERNANDEZ, University of Texas at Arlington — Existing only at higher temperatures, δ-plutonium (Pu) can be stabilized at room temperature when doped with the so-called δ-stabilizers, which are impurities from the IIIA group, such as gallium or aluminum (Al). This is ideal since the δ-phase is the preferred phase used for technological applications. Using density functional theory, we modeled a 32 atom Pu supercell doped with Al concentrations of 3.125, 6.25, and 9.375 atomic percent. The results to be presented will include energy versus volume curves (E-V) for fixed atomic positions performed at the non-magnetic, ferro-magnetic, and anti-ferromagnetic spin structures. Further optimizations of the internal positions of the lowest energy E-V structures will be discussed. The effects of Al within the δ-Pu lattice, particularly changes in the lattice constants, bulk modulus, preferred location of Al, and the bond lengths between Al and the first nearest neighbor Pu atoms will be discussed in detail. The electronic interactions, specifically the Pu-Al hybridizations, will also be discussed by analyzing the partial electronic density of states. Finally, we will the present relaxation and formation energies of the Pu-Al systems.

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