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First principles calculations on Ga stabilized δ-Pu alloys[1] SARAH C. HERNANDEZ, University of Texas at Arlington, DANIEL S. SCHWARTZ, CHRISTOPHER D. TAYLOR, Los Alamos National Laboratory, ASOK K. RAY, Deceased — The high temperature face-centered-cubic phase (δ) of plutonium (Pu) may be stabilized at room temperature with the inclusion of impurities, such as gallium (Ga) or aluminum. The addition of Ga within the δ-phase influences the structural and electronic properties of Pu. Using the full-potential linearized augmented plane-wave density functional theory based method we present a systematic study of bulk Pu-Ga alloys. The goals of these calculations are to understand the evolution of the structural and electronic properties of Ga in a δ-Pu lattice. A 32-atom δ-Pu supercell was used to study Pu-Ga alloys at 3.125, 6.25, and 9.375 at. % Ga concentrations. We observe that regardless of the Ga concentration, the magnetic ground state predicted was anti-ferromagnetic, which is contrary to experimental results. However, the equilibrium lattice constants decrease with increasing Ga concentration, which is in agreement with experimental observations. Furthermore, when more than one Ga impurity is present within the supercell, the Ga atoms prefer to be at third nearest neighbor distance. The local effects of the bond lengths around the Ga atom, formation energies and partial density of states (PDOS) in the lowest energy structures will be discussed in detail. PDOS illustrates a Pu *6d* and Ga *4p* hybridization. Finally, we will also discuss the effects of a hydrogen-vacancy complex within a bulk Pu-Ga alloy.

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