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An *Ab Initio* Study of FCC $\mathbf{Pu_{1-x}Ga_x}$[1] KINJAL GANDHA, ASOK RAY, Department of Physics, University of Texas at Arlington — As is known, the addition of a few atomic percent of Ga stabilizes the fcc δ – phase of Pu at room temperature. In this work, conventional and hybrid density functional theory have been used to study the electronic, geometric, and magnetic structure properties of $Pu_{1-X}Ga_x$with varying Ga concentrations in the fcc δ phase. The calculations have been performed using the all-electron full-potential linearized augmented plane wave plus local orbitals basis method and the *WIEN2k* software. Each compound has been studied at the non-magnetic, ferromagnetic, and anti-ferromagnetic configurations with and without spin-orbit coupling (SOC) and full geometry optimizations. The ground state structures are found to be anti-ferromagnetic with a contraction of the lattice constants from pure δ-Pu. The obtained lattice parameters are in satisfactory agreement with experimental data.

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