

Abstract Submitted
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An *Ab Initio* Study of α -Pu¹ SARAH C. HERNANDEZ, ASOK K. RAY, University of Texas at Arlington — Hybrid density functionals, which replace a fraction of density functional theory exchange with exact Hartree-Fock exchange has been used to study the electronic, geometric, and magnetic properties of α -Pu. Different fractions of Hartree-Fock exchange have been used and the computations have been performed using the all-electron full-potential linearized augmented plane wave plus local orbitals basis method. Pu has been studied at the non-magnetic, ferromagnetic and anti-ferromagnetic configurations with spin-orbit coupling, orbital polarization, and *full* geometry optimizations. The variations of the optimized lattice constants, magnetic moments, bulk moduli, density of states, and the degree of *f* electron localization with the amount of Hartree – Fock exchange will be reported. Results will be compared with those of δ -Pu for which the performance of the hybrid functionals did *not* seem superior to that of the pure density functionals.²

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²R. Atta-Fynn and A. K. Ray, Europhys. Lett. 85, 27008 (2009).

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