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Performance of hybrid density functional theory for α *versus* δ-Pu[1] SARAH C. HERNANDEZ, ASOK K. RAY, University of Texas at Arlington — Hybrid density functional theory, which replaces 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 and compared with our previous results for δ–Pu. A non-magnetic (NM) ground state was realized for α=0.55 (α indicating the fraction of the HF exchange) for δ–Pu but the equilibrium atomic volume deviated from experiment by 19%, the $5f$ electron population was close to 4 and a $5f$ DOS that shows anomalous localization and failed to match experimentally obtained PES data.[2] For α-Pu, a NM ground state was obtained at 40% HF exchange. Comparing the two phases at the NM ground state, the $5f$ population is about the same, but energy differences between the different magnetic configurations for the two phases are observed. For δ-Pu NM-FM and NM-AFM ΔE are 86.33 and 82.28 mRy/atom, respectively, and for α-Pu the NM-FM and NM-AFM ΔE are 144.98 and 60.72 mRy/atom, respectively. The $5f$ DOS for δ-Pu show no DOS at the Fermi level but the presence of localized states, while for α-Pu DOS show delocalization. Though hybrid density functional theory might not perform better compared to DFT for δ-Pu, it shows promise for α-Pu.

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

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