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Hybrid Density Functional Studies of δ-Pu[1] RAYMOND ATTA-FYNN, ASOK RAY, Department of Physics, The University of Texas at Arlington — Hybrid density functionals, which replaces a fraction of a density functional theory exchange with exact Hartree-Fock (HF) exchange, have been used to study the structural, magnetic, and electronic properties of δ-Pu. The fractions of exact Hartree-Fock exchange used were 25%, 40%, and 55%. Compared to the pure PBE functional, the lattice constants expanded with respect to the experimental value when the PBE-HF hybrid functionals were applied. For pure PBE and hybrids functionals with HF exchange amounts of 25% and 40%, the ground state structure was anti-ferromagnetic, while for 55% HF contribution the ground state was non-magnetic. The $5f$ electrons tend to exhibit slight delocalization or itinerancy for the pure PBE functional and well-defined localization for the hybrid functionals, with the degree of $5f$ electron localization increasing with the amount of HF exchange. Overall, the performance of the hybrid density functionals do not seem superior to pure density functionals for δ –Pu.

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