

Abstract Submitted
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Theory of magnetism in Pu at high magnetic fields PER SODERLIND, Lawrence Livermore National Laboratory — Density-functional theory (DFT), in conjunction with the fixed-spin-moment (FSM) method, spin-orbit coupling (SO), and orbital polarization (OP), is shown to provide an apparent accurate picture of δ -Pu, while opening the possibility of a zero net magnetic moment due to complete spin- and orbital-moment cancellation. Calculated total energies, photoemission spectra, and magnetic form factors appear consistent with available experimental data. Calculations including SO, OP and the Zeeman term in the Hamiltonian, address Pu in high magnetic fields ~ 100 T. The Pu phase stability, as a function of applied field, is also investigated. This work was performed under the auspices of the US DOE by the UC LLNL under contract no. W-7405-Eng-48.

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