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An LAPW Study of d - Plutonium and the (001) Surface A. K RAY, X. WU, The University of Texas at Arlington — The electronic structure properties of bulk fcc δ-Plutonium and the quantum size effects in the surface energies and the work functions of the (001) ultra thin films (UTF) up to 7 layers have been investigated with periodic density functional theory calculations within the full-potential linearized augmented-plane wave approach.[1] Several levels of theory, namely NSP-NSO, NSP-SO, SP-NSO, and SP-SO, have been examined and our calculated equilibrium atomic volume of 178.3 a.u.^{3} and bulk modulus of 24.9 GPa at the fully relativistic level of theory are in good agreement with experimental results. The energy difference brought by spin-orbit coupling, about 7-8 eV, is dominant, but the energy difference brought by spin-polarization, from a few tenths to 2 eV, has a stronger dependence on the atomic volume. Density of states show that 5f electrons are more itinerant when the volume of δ-plutonium is compressed and they are more localized when the volume is expanded. The surface energy converges rapidly and the semi-infinite surface energy is predicted to be 0.692eV. Quantum size effects for the work function is not pronounced for (001) surface. *Work supported by the Department of Energy (Grant No. DE-FG02-03ER15409) and the Welch Foundation (Grant No. Y-1525). [1]P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka and J. Luitz, *WIEN2k* (Technische Universitat Wien, Austria, 2001)

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