Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Quantum Size Effects in δ – Pu (111) and (110) Films* HAO-RAN GONG, ASOK KUMAR RAY, Department of Physics, the University of Texas at Arlington, Arlington, TX 76019 — First-principles full-potential linearized-augmented-plane-wave (FP-LAPW) calculations have been carried out for δ-Pu (111) and (110) films up to seven layers. The layers have been studied at the non-spin-polarized-no-spin-orbit coupling (NSP-NSO), non-spin-polarized-spin-orbit coupling (NSP-SO), spin-polarized-no-spin-orbit coupling (SP-NSO), spin-polarized-spin-orbit coupling (SP-SO), anti-ferromagnetic-no-spin-orbit coupling (AFM-NSO), and anti-ferromagnetic-spin-orbit-coupling (AFM-SO) levels of theory. The ground state of both δ-Pu (111) and (110) films is found to be at the AFM-SO level of theory and the surface energy is found to rapidly converge. The semi-infinite surface energy for δ-Pu (111) and (110) films is predicted to be 1.18 and 1.42 J/m^2, while the magnetic moments show an oscillating behavior, gradually approaching the bulk value of zero with increase in the number of layers. Work functions indicate a strong quantum size effect up to and including five layers for the (111) surface and seven layers for the (110) surface, respectively. The work functions of δ-Pu (111) and (110) films at the ground state are predicted be 3.41 and 2.99eV, respectively. *This work is supported by the Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, Office of Science, Department of Energy (Grant DE-FG02-03ER15409) and the Welch Foundation, Houston, Texas (Grant Y-1525).

Da Gao
Department of Physics, the University of Texas at Arlington,
Arlington, TX 76019

Date submitted: 23 Nov 2005 Electronic form version 1.4