

Abstract Submitted
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A First Principles Electronic Structure Study of Quantum Size Effects in (111) Films of FCC Plutonium A. K. RAY, The University of Texas at Arlington, J. C. BOETTGER, Los Alamos National Laboratory — First principles linear combinations of Gaussian type orbitals – fitting function (LCGTO-FF) electronic structure calculations are used to study thickness dependencies in the surface energies and work functions of ultra-thin (111) films of fcc Pu, up to five layers thick. The calculations are carried out at both the scalar- and fully-relativistic (with and without spin-orbit coupling) levels of approximation. The surface energy is shown to be rapidly convergent, while the work function exhibits a strong quantum size effect for all thicknesses considered. The surface energy and work function of the semi-infinite solid are predicted to be 1.12 J/m^2 and $2.85 \pm 0.20 \text{ eV}$, respectively, for the fully-relativistic case. These results are in substantial disagreement with results from previous electronic structure calculations. The present predictions are in fair agreement with the most recent experimental data for polycrystalline fcc Pu, namely 0.91 J/m^2 and $3.1\text{-}3.3 \text{ eV}$, for the surface energy and work function, respectively. *The work of AKR is supported by DOE (Grant No. DE-FG02-03ER15409) and the Welch Foundation (Grant No. Y-1525). The work of JCB is supported by DOE under contract W-7405-ENG-36 and the LDRD program at LANL.

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