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Quantum Size Effects in α-Pu (020) Layers[1] SARAH C. HERNANDEZ, ASOK K. RAY, Physics Department, University of Texas at Arlington, Arlington, Texas 76019, CHRISTOPHER D. TAYLOR, Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545 — First principles calculations using the projector-augmented wave method and a plane wave basis set as implemented in the Vienna *Ab Initio* Simulation Package (VASP) have been performed for the α-Pu (020) layers. Because of severe demands on computational resources, scalar-relativistic computations were performed at the experimental geometry. The surface was assumed to be anti-ferromagnetic (AFM) since previous theoretical studies indicate the ground state of bulk α-Pu to be AFM. Up to ten layers have been considered in this study. Work functions and surface energies appear to converge as the number of layers increase. We predict the work function to be around 3.4eV, with the surface energy being approximately 1.6eV. While no experimental results are available for α-Pu, experimental results for δ-Pu indicate a work function of approximately 3.2eV and a surface energy of 2.0eV. We will also present results on the magnetic moments and density of states of the layers. Results will be compared with results using the full-potential linearized-augmented-plane-wave method as implemented in the WIEN2k suite of software.

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