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Spectral Properties of Elemental Pu Studied by LDA+DMFT
JIAN-XIN ZHU, Los Alamos National Laboratory, A.K. MCMAHAN, Lawrence Livermore National Laboratory, M.D. JONES, University at Buffalo, J.M. WILLS, R.C. ALBERS, Los Alamos National Laboratory — The merger of density functional theory in the local density approximation and the many-body dynamical mean field theory is a powerful theoretical technique for the study of strongly correlated electron materials. We present calculations of spectral properties of the δ-phase plutonium by combining for the first time the sophisticated tight-binding method with a recent implementation of quantum Monte Carlo techinque. The tight-binding parameters are determined from the fit to the full-potential linearized augmented plane-wave calculation for the face-centered-cubic crystal structure of the slightly compressed δ-phase plutonium. The computationally more expensive but rigorous quantum Monte Carlo simulation is supplemented by the more efficient but approximate Hubbard-I method. By comparing the calculations without and with spin-orbit interaction included, we discuss our results in the context of several key features observed in the photoemission spectroscopy.

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