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Spectral Properties of Plutonium and its Compounds[1] JIAN-XIN ZHU, Los Alamos National Laboratory, A.K. MCMAHAN, Lawrence Livermore National Laboratory, M.D. JONES, University at Buffalo, SUNY, T. DURAKIEWICZ, J.J. JOYCE, J.M. WILLS, R.C. ALBERS, Los Alamos National Laboratory — By combining the local density approximation (LDA) with dynamical mean field theory (DMFT), we analyze the spectral properties of plutonium and its compounds. The LDA Hamiltonian is extracted either from a tight-binding fit to full-potential linearized augmented plane-wave calculations, or directly from the full-potential linearized muffin tin orbitals calculations. The DMFT equations are solved by the exact quantum Monte Carlo method complemented with the Hubbard-I approximation. We compare the 5f electron behaviors in Pu elemental solid and compounds. The theoretical results will also be discussed in the context of photoemission spectroscopy data.

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