

Abstract Submitted
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Strongly correlated state in δ -Pu and Am A. SHICK, Institute of Physics AS CR, Prague, J. KOLORENC, North Carolina State University, Raleigh, L. HAVELA, Charles University, Prague, V. DRCHAL, Institute of Physics AS CR, Prague — We investigate the electron-electron correlation effects in the vicinity of the localization threshold of the 5f series, which is crossed between Pu and Am. The ground state electronic and magnetic properties are calculated making use of static *around-mean-field* LDA+U approximation. We obtain non-magnetic δ -Pu with 5f occupation $n_f = 5.4$, and non-magnetic *fcc*-Am with $n_f=6.0$. The equilibrium volumes and bulk moduli are obtained in a good agreement with experiment. For Pu-Am alloys, neither tendency to a 5f localization nor formation of Pu local magnetic moments was found despite a lattice expansion caused by the Am atoms. The excitation spectra of δ -Pu and *fcc*-Am are calculated on the basis of the Dynamical Mean-Field theory (DMFT). Starting from LDA+U ground state we included multiplet transitions using the Hubbard-I approximation [1], which gives a good agreement with experimental photoelectron spectra of δ -Pu, Am, and their selected compounds. The spectral density at Fermi level explains the high γ -coefficient of the electronic specific heat found experimentally in δ -Pu. The calculations show that atomic-like excitations can be observed in a solid-state environment even if the 5f states are not fully localized as in δ -Pu. [1] A. Shick, J. Kolorenc, L. Havela *et al.*, arXiv: cond- mat/0610794 (2006).

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