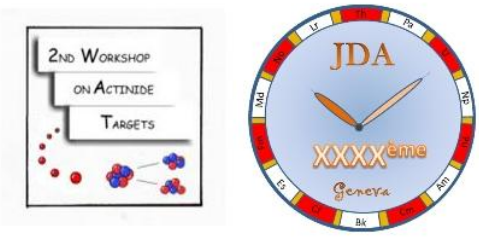

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Electronic structure theory of Pu-based alloys and compounds: Pu-Am, Pu-Ce-alloys and PuCoGa5

Tuesday, 30 March 2010 11:05 (20 minutes)

In the present work, we study the electron correlation effects in the electronic structure and spectra of Pu-Am, Pu-Ce alloys and PuCoGa5. We make use of the "local density matrix"approximation (LDMA) to DMFT, that combines the Hubbard-I approximation with the full-potential linearized augmented plane wave (FP-LAPW) method , including self-consistency over the charge density. Calculated PE spectra and electronic specific heat coefficient are in good agreement with avaliable experimental data.

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