

Electronic structure of the family of compounds $\text{Ce}_m\text{M}_n\text{In}_{2m+3n}$ ($\text{M}=\text{Co}, \text{Rh}, \text{Ir}$; $m=1, 2$; $n=0, 1$)

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The compounds belonging to the family $\text{Ce}_m\text{M}_n\text{In}_{2m+3n}$, ($\text{M}=\text{Co}, \text{Rh}, \text{Ir}$; $m=1, 2$; $n=0, 1$) have attracted great interest during the last 10 years due to their heavy fermion behavior and the ground states which can be tuned between antiferromagnetic (AFM) and superconducting (SC) by external pressure or doping. To understand better the electronic structure of these systems we have performed Full Potential Linearized Augmented Plane Wave (FP-LAPW) calculations [1] and the X-ray photoelectron spectroscopy (XPS) experiments. From the XPS Ce $3d$ spectra we have estimated the occupation of the Ce $4f$ shell and the hybridization energy between $4f$ states and conduction electrons in each compound on the basis of Gunnarson-Schönhammer [2, 3] theory. The XPS valence band spectra we compare with theoretical one calculated by LAPW method using the different values of the correlation energy for Ce $4f$ shell. We conclude, that in CeIn_3 the $4f$ states are rather localized, whereas for the other compounds these states are on the border between localization and delocalization. We have found and discussed influence of the Ce $4f$ - In $5p$ and the Ce $4f$ - M d interatomic hybridization on the localization of the $4f$ shell of cerium and the ground state properties in the whole family of compounds.

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