Electronic structure of $Ce_2Co_{1-x}Au_xSi_3$ $(0 \leq x \leq 1.0)$ compounds

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9.7 cm

Properties and parameters of the electronic structure of $Ce_2Co_{1-x}Au_xSi_3$ $(0 \leq x \leq 1.0)$ compounds are presented. These compounds crystallize in a hexagonal crystal structure derived from the AlB_2-type. Macroscopic measurements suggest the change of the properties from strong Kondo regime for $x = 0$ to magnetic ordering for $x \geq 0.4$. To explain such properties of these compounds X-ray photoelectron spectroscopy (XPS) measurements were performed using a commercial LHS 10 Leybold spectrometer with non-monochromatized MgK_α ($h\nu$=1253.6 eV) radiation. The measurements were carried out at room temperature in high vacuum (10^{-9} mbar). The XPS valence bands of all the investigated compounds are formed mainly by the $3d$ Co and $5d$ Au states that was confirmed by electronic structure calculations using the ab initio self consistent tight-binding linear muffing-tin orbital (TB LMTO) method. The 4f band of Ce is well above the Fermi level and does not change with changing Au content. For both compounds the contributions of the three final states $4f^0$, $4f^1$ and $4f^2$ are observed in the Ce 3d XPS spectra. The spin-orbit splitting Δ_{SO} equal 18.7 eV for x=0.4 and 18.3 eV for x=0.6, 0.8 and 1.0. Based on the Gunnarsson-Schönhammer theoretical model the hybridization energy Δ is determined. The obtained results suggest that the hybridization energy Δ changes from 28 meV, for x=0.4 to 62 meV for x=1.0

13.4 cm

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