Electronic structure of $CeCu_4In$ from band structure calculations and X-ray photoelectron spectroscopy

A. Szajek,[1] G. Chełkowska,[2] T. Toliński,[1] and A. Kowalczyk[1]

[1] *Institute of Molecular Physics, Polish Academy of Sciences*
Smoluchowskiego 17, 60-179 Poznań, Poland
[2] *Institute of Physics, University of Silesia in Katowice*
75 Pułku Piechoty 1A, 41-500 Chorzów, Poland

We present a combined new experimental and theoretical study of the electronic structure for the heavy fermion $CeCu_4In$ based on X-ray photoelectron spectroscopy (XPS) data and $ab-initio$ band structure calculations. The compound crystallizes in the orthorhombic $CeCu_{4.38}In_{1.62}$ type of structure (space group $Pnnm$). Below the Fermi energy the total density of states contains mainly the $3d$ states of Cu atoms that hybridize with the Ce $4f$ electronic states. The Ce core-level XPS spectra point to a stable trivalent configuration of Ce atoms in $CeCu_4In$, consistently with the magnetic susceptibility data.

For more detailed information about electronic states the fully relativistic band structure was calculated within the density functional theory (DFT) for the first time. Based on these calculations we present calculated photoemission spectra, which very well reproduce the experimental ones. The Fermi level is located at a deep decrease in the density of electron states and reaches a value of 3.69 states/(eV f.u.), which corresponds to a Sommerfeld coefficient in the electron specific heat of 8.69 mJ/(mol K). This value is much smaller than that obtained experimentally, which indicates the importance of many-body effects, which are not properly taken into account in ab-initio calculations. The valence band is formed mainly by Cu($3d$) electrons with a small contribution of Ce($4f$) electrons in the immediate vicinity of the Fermi level.