Electronic properties of $CeNiAl_4$ based on *ab initio* calculations and XPS measurements

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The $CeNiAl_4$ compound crystallizes in an orthorhombic $YNiAl_4$-type structure with a $P6/mmm$ space group. The earlier susceptibility data and X-ray photoelectron spectroscopy (XPS), suggested a localized character of the $4f$ states in CeNiAl4 with a valence state close to a Ce^{+3} ion.

In this work we present a combined theoretical and experimental study of the electronic structure for the Kondo dense system $CeNiAl_4$ based on the XPS data and *ab initio* calculations. Based on the band structure calculations the theoretical XPS valence band spectra are evaluate. Below the Fermi energy the total density of states contains mainly $3d$ states of Ni hybridized with Ce $4f$ states.