Electronic structure of ytterbium ternary compounds: *ab-initio* calculations

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The electronic and magnetic properties of ternary YbTM (T = transition metal (Pd, Cu, Au, Pt, Rh, Zn, Ag), M=Sn and Bi) compounds were studied experimentally by Kaczorowski *et al.* [1] and Szytuła *et al.* [2]. Ytterbium compounds show a wealth of anomalous physical properties due to the different character of the *f* electrons. In the atomic ground state Yb is divalent (f^{14}), but in the solid state the f electrons play an active role in bounding giving rise to intermediate valent . The aim of this work was a *ab-initio* study of the electronic structure of YbAuSn, YbAuBi, YbPdBi, YbRhSn and YbPtSn compounds by using the fully relativistic (including spin-orbit coupling) and full potential methods (FPLO-4 [3] and FP-LMTO [4]). The spin-orbit coupling gives the splitting of the *4f* Yb states and this effect was observed in the XPS spectra for YbAuSn, YbAuBi and YbPdBi compounds [2]. In Fig. 1 we present the XPS spectra and the total density of states for YbAudBi (FP LMTO) is plotted in Fig. 2.

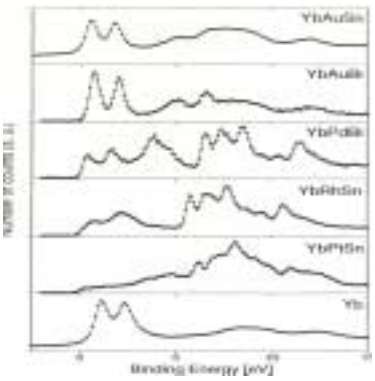

Fig. 1.

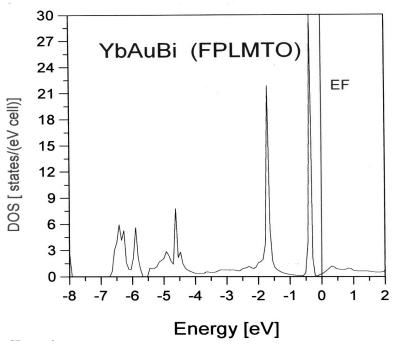

Fig. 2.

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