Electronic structure of $YbFe_4Al_8$ antiferromagnet: A combined X-ray photoelectron spectroscopy and first-principles study

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Depending on their chemical composition, Yb compounds often exhibit different valence states. Here we investigate the valence state of $YbFe_4Al_8$ using X-ray photoelectron spectroscopy (XPS) and first-principles calculations. The XPS valence band of $YbFe_4Al_8$ consists of two contributions coming from divalent (Yb^{2+}) and trivalent (Yb^{3+}) configurations. The determined value of the valence at room temperature is 2.81. Divalent and trivalent contributions are also observed for core-level Yb $4d$ XPS spectra. We study several collinear antiferromagnetic models of $YbFe_4Al_8$ from the first-principles and for comparison we also consider $LuFe_4Al_8$ with a fully filled $4f$ shell. We predict that only Fe sublattices of $YbFe_4Al_8$ carry significant magnetic moments and that the most stable magnetic configuration is AFM-C with antiparallel columns of magnetic moments. We also present a Mullliken electronic population analysis describing charge transfer both within and between atoms. In addition, we also study the effect of intra-atomic Coulomb U repulsion term applied for $4f$ orbitals on Yb valence and Fe magnetic moments. The results presented were published in Ref. [1].

References:

[1] W. Marciniak, G. Chełkowska, A. Bajorek, A. Kowalczyk, A. Szajek, M. Werwiński, Electronic structure of $YbFe_4Al_8$ antiferromagnet: A combined X-ray photoelectron spectroscopy and first-principles study, J. Alloys Compd. 910 (2022) 164478.

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