

Effect of alloying on magnetism and electronic structure of $\text{Gd}(\text{In}_{1-x}\text{Sn}_x)_3$ system – *ab initio* study

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The magnetic properties and electronic structure of $\text{Gd}(\text{In}_{1-x}\text{Sn}_x)_3$ alloys were measured recently by means of different methods. The measurements showed several intriguing properties of the alloys including multiple magnetic phase transitions and oscillatory variation of magnetic parameters (e.g. Néel temperature, effective magnetic moment, paramagnetic Curie temperature) upon the successive In/Sn substitution. The XPS valence band measurements indicated the correlation between the magnetic properties of the alloys and their electronic structure near the Fermi level.

In the contribution we present an *ab initio* study of electronic and magnetic properties of $\text{Gd}(\text{In}_{1-x}\text{Sn}_x)_3$ alloys carried out with the use of FP-LAPW method. Our *ab initio* calculations revealed that the ground state magnetic structure of the alloys is antiferromagnetic and upon the In/Sn substitution the magnetic structure undergo transition, changing the type of antiferromagnetic ordering from the *AFM-I* ($\langle\langle 001 \rangle\rangle$) for the GdSn_3 compound to *AFM-III* ($\langle\langle 111 \rangle\rangle$) for the GdIn_3 one, in agreement with the Mössbauer measurements. Moreover, calculations gave an explanation of the oscillatory variation of density of states near Fermi level, showed by XPS measurements.