Electronic Structure and Magnetism of $YFe_{11-x}Si_xTi$ compounds

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9.7 cm

A detailed theoretical investigation on the electronic and magnetic properties of several $YFe_{11-x}Si_xTi$ systems in $ThMn_{12}$ tetragonal type of structure (S.G. I4/mmm, z=2) have been performed. All theoretical investigations of the electronic and magnetic properties have been done using the Korringa-Kohn-Rostoker (KKR) band structure method. The disorder in the system has been accounted for by means of the Coherent Potential Approximation (CPA). The spin resolved density of states (DOS) reflects the covalent nature of the interatomic bands. The Si for Fe substitution in $YFe_{11-x}Si_xTi$ induces a significant broadening of the Fe 8f, 8i and 8j bands, as a consequence of Si(p)-Fe(d) hybridization. The calculated magnetic moments decrease with Si content from 20.82 μ_B/f.u. for $YFe_{11}Ti$ to 15.05 μ_B/f.u. for YFe_9Si_2Ti. The SPR-KKR calculated magnetic moments are in good agreement with the corresponding values determined by magnetization measurements. Comparing calculated hyperfine fields with experimental results, it is found that the calculated and experimental hyperfine fields are correlated. The theoretical calculations predict a decrease of the hyperfine fields on all Fe sites (8i, 8j and 8f) induced by Si for Fe substitution.

13.4 cm

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