Role of the magnetic impurities in Heusler type alloys: *ab-initio* calculations

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We have analyzed the electronic structure and magnetic properties of the group of Heusler type alloys Fe_2TiSn, $Fe_{2-x}M_xTiSn$ (M = Ni and Co), $Ni_2Ti_{1-x}Mn_xSn$, and $Ni_2MnGa_{1-x}Ge_x$ by *ab-initio* SPR-KKR-CPA [1], TB LMTO [2], FP LMTO [3], FPLO [4, 5] and SIESTA [5] methods. We have studied the role of the magnetic impurities in Heusler alloys. The influence of Fe, Co and V on the magnetic and electronic properties of Fe_2TiSn Heusler type alloy was studied by Ślebarski *et al.* [8, 9]. The transition elements strongly modified the electronic structure of Fe_2TiSn particularly near the Fermi level. We present the electronic and magnetic properties of $Ni_2Ti_{1-x}Mn_xSn$ and we find that for x=0.06 the system is magnetic. The electronic and magnetic properties of Ni_2MnGa Heusler alloy depends strongly on the atomic disorder in the fcc sublattices and the tetragonal distortion. We report the electronic structure of Ni_2MnGa obtained by SIESTA [8, 9] method. Using the SIESTA code we have shown that the shape of the density of states strongly depended on the form of the pseudopotentials and on the form of the exchange-correlation potentials.

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