9.7 cm

THEORETICAL SEARCH FOR MAGNETIC HALF-HEUSLER SEMICONDUCTOR

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We present electronic structure of half-Heusler $\mathrm{CoTi}_{1-x}T_x\mathrm{Sb}$ and $\mathrm{FeV}_{1-x}T_x\mathrm{Sb}$ with $x = 0.001, 0.005, 0.01$ and 0.05 derived from the charge and spin-selfconsistent KKR-CPA computations. Experimentally, both parent compounds were found to show semiconducting properties [1]. This was supported by the band structure calculations [2], which gives an energy gap as large as 0.95 eV (CoTiSb) and 0.46 eV (FeVSb). Among transition metal impurities doped in the aforementioned semiconductors, Cr and Mn atoms exhibit a strong polarisation of density of states, if substituting selectively on Ti- and V-site in CoTiSb and FeVSb, respectively. The calculated magnetic moment on Mn is found to be on average as large as 2.5 μ_B and 3.2 μ_B in FeVSb and CoTiSb, respectively. Inspecting total DOS near the gap in these magnetic systems we find a behavior very similar of half-metallic magnetics than of magnetic semiconductors. Moreover, if impurity concentration decreases the energy gap tends to open for both spin channels.

[1] M. A. Kouacou et al., J. Phys. Condens. Matter **7** (1995) 7373; D. P. Young et al., J. Appl. Phys. **87** (2000) 317; Y. Xia et al., J. Phys. Condens. Matter **13** (2001) 77.
[2] J. Toboła et al. J. Alloys Compd. **296** (2000) 243.

13.4 cm

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