Magnetic and electronic properties of $NiMn_{1-x}Ho_xSb$ compounds

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The structural, electronic and magnetic properties of $NiMn_{1-x}Ho_xSb$ alloys and compounds have been investigated by X-ray diffraction, X-ray photoelectron spectroscopy, magnetization and magnetic susceptibility measurements and band structure calculations.

9.7 cm

The analysis of the band structure of the doped alloy shows that the half-metallic properties are completely conserved if Ho substitute Mn atoms, this effect being determined through the coupling between the Ho(4f) spin with the Mn(3d) itinerant electron spins. We evaluate the strength of such a coupling by calculating, in an ab-initio fashion, the total energy of $Co_8Mn_7HoSi_8$ compound for a parallel and antiparallel f-d coupling. It was found that the antiparallel coupling is most favorable, the energy difference being E_F-E_{AF}=52K. The experimental magnetic moments are in rather good agreement with the calculated ones in case of ferrimagnetic ordering. In order to investigate the hybridization between the Mn and Ni 3d states and the Sb 5p states, the XPS valence band spectra were calculated and compared to the experimental spectra.

13.4 cm

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