Ab initio study of Co2MnSi (001) surface and Co2MnSi/GaAs (001) interface

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We have studied the electronic and magnetic properties of Co2MnSi (001) surface as well as Co2MnSi/GaAs (001) interface within the frame work of density functional theory. Analyzing the surface band structure of two ideal (CoCo/MnSi and MnSi/CoCo) and several modified surfaces, we found out that the pure Mn termination (MnMn/CoCo) is the only surface that preserves the half metallicity of the system. For other terminations the surface states destroy the half metallicity.

In order to select the appropriate interface of Co2MnSi/GaAs (001), we calculated the phase diagram by ab initio atomistic thermodynamics. Considering the results obtained from phase diagram and suggestions based on the existing theoretical and experimental data, we focused our attention on the ideal MnSi/As and modified MnMn-As terminations. The ideal termination (and consequently also the modified one) has four different possible patterns that can be obtained by considering the continuation along [001] direction of one of the two GaAs fcc sub lattice (either As or Ga) with either Mn or Si. These patterns are labeled as Mn(Ga), Si(Ga), Mn(As), and Si(As). By comparison of the formation energy we further limited our study to Mn (Ga) and Mn (As) as the most favorable patterns. In the case of ideal MnSi-As termination we found out that the spin polarization at the Mn (As) interface is 100% while for Mn (Ga) this value diminishes to 67%. For modified MnMn-As termination the spin polarization for MnMn (Ga) is 100% while for MnMn (As) we found a value of 80%. By investigating the strength of Co-Mn bond in different terminations along with the effect of potential raise up on As we were able to analysis our results. Furthermore, the band alignments were extracted for the majority and minority spin channels.