Calculation of structural, electronic and magnetic properties of MnSi and $Co_2MnSi(001)$ thin films

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9.7 cm

We investigate thin films of Mn intermetallic compounds using density-functional calculations and the FP-LAPW or APW+lo method, with the goal to identify materials systems of possible use as spin injectors on Si(001). We find that the surface electronic structure of the ferromagnetic half-metal Co_2MnSi is strongly affected by the type of surface termination. In particular, an ad-layer of Mn atoms preserves the half-metallic gap, whereas surface states occur for other terminations. From calculated surface energies for $Co_2MnSi(001)$ we conclude that terminations either by a layer of only Mn atoms, only Si atoms, or a mixture of both are thermodynamically stable, depending on chemical environment. Next, we investigate the properties of ultra-thin films (1-3 monolayers) on Si(001), focussing on MnSi and Co_2MnSi. From our total-energy calculations, we conclude that a novel, CsCl-like crystalline phase of MnSi should be producible as a metastable epitaxial structure on Si(001). Thin films with CsCl-like sandwich structure of alternating Mn and Si layers have sizeable magnetic moments of 1–2 μ_B at Mn, and show a layered magnetic ground state, with pronounced ferromagnetic coupling between the Mn spins within the layers, and weak interlayer coupling. For ultrathin Co_2MnSi films on Si(001), we find Mn magnetic moments of 2.7–3.5 μ_B, and strong ferromagnetic coupling both within the same layer and between layers.
Both for the MnSi and the Co_2MnSi films, our calculations predict values of 20% to 50% for the spin polarization at the Fermi level.

13.4 cm

Subject category :

7. Computations of Electronic Structures

Presentation mode :
oral

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