Magnetic properties of a ferromagnetic Heusler alloy Co_2MnSn

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The half-metallic materials have attracted a lot of attention due to potential importance in the development of future spin-electronic devices. In this study, the electronic and magnetic properties of the MnSn terminated (001) surfaces of the ferromagnetic full-Heusler alloy Co_2MnSn with half-metallic character are investigated theoretically by using the all-electron full-potential linearized augmented plane wave (FLAPW) method [1] within the generalized gradient approximation (GGA) [2] for exchange and correlation based on the first-principles density functional theory (DFT) calculation.
In order to take into account both bulk and surface properties, we considered a single slab with nine layers so that the center layer has bulk properties. We have used theoretical lattice constant determined by the total energy calculations which is in good agreement with the experimental values [2].
The calculated magnetic moment for surface Mn (3.75 μ_B) exhibits much enhanced value compared with the bulk moment (3.17 μ_B). We can see that the MnSn terminated surface also affects the Co magnetic moment on the (S-1) layer (1.08 μ_B) to be slightly larger than the bulk value (0.98 μ_B). The local magnetic moment on the Sn site couples antiferromagnetically to Mn moment with a very small value (less than 0.1 μ_B) for both center and surface layers same as bulk calculations for other Heusler alloys [3].
The calculated density of states (DOS) shows that there is a finite very small spin-down DOS at the Fermi level instead of a band gap for the Mn surface layer, which indicates that the half-metallicity may be destroyed by surface states for the MnSn teminated surface similar to surface calculations for another Co-based alloys [4].

References

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