

# Surface and Interface Effect on the Half-Metallicity of Co<sub>2</sub>FeX and Co<sub>2</sub>FeX/Si Heusler Alloys

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*Ab-initio* calculational results on the half-metallicity of Co<sub>2</sub>FeX type full Heusler alloy in the form of a free standing film as well as an overlayer on Si substrate are reported in this work. Employing the +U corrections in addition to the local density approximation (LDA) and generalized gradient approximation (GGA), the effect of correlation interaction of transition metal *3d* states on the half-metallicity and magnetic properties are investigated. While the bulk alloy demonstrates a minority spin band gap of 0.85 ~ 1.35 eV and the total spin magnetic moment of 6 $\mu_B$  in agreement with experiments, the half-metallicity is found only for the Co-terminated clean surfaces due to the surface states developed at the Fermi energy ( $E_F$ ). The +U correction enhances the  $e_g$ - $t_{2g}$  band splitting and thus pushes down the surface states below  $E_F$ , which effectively re-opens the minority spin band gap for the Co-terminated surface while not enough for the Fe-Si-terminated surface. The effect of the interface formation with (001) Si substrate is also discussed.

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