

Abstract Submitted
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The half-metallicity of the Co_2FeSi full Heusler alloy in bulk, clean surface and interfaces with Si ; first-principles investigation¹ MIYOUNG KIM, HANJO LIM, Division of Energy System Research, Ajou University, Korea, JAEIL LEE, Dept. of Physics, Inha University, Korea — We report the *ab-initio* calculational results on the half-metallicity of Co_2FeSi full Heusler alloys in bulk, (001) surfaces and interface with Si. Employing the +U corrections within the FLAPW[1] method, we investigate the effect of correlation interaction on half-metallicity and magnetic properties. For bulk, the +U approach reproduces experimental values of the minority spin band gap and total spin magnetic moment. The (001) surfaces and interfaces with Si are calculated to be metallic by both LDA and GGA due to the surface and interface states developed at E_F . Upon +U correction, the Co-terminated clean surface recovers half-metallicity with a reduced band gap (0.40 eV) from the bulk value while the rest of the systems are still metallic, which can be explained by the correlation and hybridization effects. [1] E. Wimmer, H. Krakauer, M. Weinert, and A. J. Freeman, PRB **24**, 864 (1981).

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