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Half-metallicity at the (001) surface of Co_2MnSi and magnetic properties of thin Co_2MnSi films on Si(001) P. KRATZER, S.J. HASHEMIFAR[1], HUA WU, M. SCHEFFLER, Fritz-Haber-Institut der MPG — Recently, films of the half-metal Co_2MnSi have been discussed as potential spin injectors for semiconductor spintronics. We have studied the stability, the electronic and magnetic properties of the $Co_2MnSi(001)$ surface for 15 different terminations using density-functional theory (DFT) calculations. The phase diagram obtained by *ab initio* atomistic thermodynamics shows that in practice the MnSi, pure Mn, or pure Si terminated surfaces can be stabilized under suitable conditions. Analyzing the surface band structure, we find that the pure Mn termination, due to its strong surface-subsurface coupling, preserves the half-metallicity of the system, while surface states appear for the other terminations. For ultra-thin Co_2MnSi films (2 or 3 double layers) on Si(001), we find that they are thermodynamically stable against decomposition, and that the magnetic moments of the Mn and Co atoms are still similar to those of bulk Co_2MnSi. While we see the incipient recovery of the half-metallic gap in the interior layer, this gap gets filled by electronic states at the interface with Si(001) for the atomic structures we have considered.

[1]permanent address: Physics Department, Isfahan University of Technology, 84156 Isfahan, Iran

Matthias Scheffler
Fritz-Haber-Institut der MPG

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