INVESTIGATIONS OF THE Co_2MnSi/MgO(001) INTERFACE - LOOKING FOR HALF-METALLICITY

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9.7 cm

Magnetic memory devices that exploit the tunneling magneto-resistance (TMR) effect depend crucially on the spin polarization of the electrode materials. Ferromagnetic half-metals make perfect electrodes leading to a (theoretically) infinite TMR ratio. The full Heusler alloy Co_2MnSi is predicted to be half-metallic and has recently been integrated in a magnetic tunnel junction[1] where a high TMR value and huge spin polarization have been measured.
Here, we use density functional theory (DFT) calculations to model an epitaxially grown Co_2MnSi/MgO(001) interface as potential TMR device. The stability and electronic and magnetic properties of different terminations of Co_2MnSi (stoichiometric Co- and MnSi- and non-stoichiometric Mn- and Si- planes) and different registry with respect to the insulating barrier (Mg-top, O-top, bridge and hollow site) are investigated. We find that the electronic and magnetic properties (including the existence of the spin gap) depend strongly on the termination. The largest parts of the phase diagram consist of the interface Co/O (Co at O top site) which still has a high spin polarization ($P = 70\%$) and the interface MnSi/O with only small P. The MnMn/O interface that preserves the half-metallicity lies outside the region accessible in thermodynamic equilibrium.
[1] M. Oogane *et. al.*, J. Phys. D: Appl. Phys. **39**, 834 (2006)

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