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Density-functional theory study of the Co_2MnSi/MgO interface
BJÖRN HÜLSEN, Fritz-Haber-Institut der MPG, PETER KRATZER, University Duisburg-Essen, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG — Magnetic memory devices that exploit the tunneling magneto-resistance (TMR) effect depend crucially on the spin polarization of the electrode materials. Using ferromagnetic half-metals, such as the full Heusler alloy Co_2MnSi, perfect electrodes with 100% spin polarization could possibly be realized, at least at zero temperature. Here, we use density functional theory (DFT) calculations to model an epitaxially grown Co_2MnSi/MgO(001) interface in a prospective TMR device. The stability, the 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 formation energy of the various interfaces is presented in form of a phase diagram. Both the interface Co/O (Co at O top site) with a high spin polarization of $P = 70\%$, and the interface MnSi/O with only small P form part of the thermodynamically accessible region. The MnMn/O interface preserves the half-metallicity of the bulk, but is found to be only metastable. Interface band structures are presented, and magnetic moments are compared to experimental data.

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