First-principles prediction of ferromagnetism in MnB and MnC monolayer films on nonmagnetic transition-metal surfaces

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Quasi-two-dimensional ferromagnetic nanostructures should open up new possibilities in fundamental physics as well as potential technological applications. However, since any finite-temperature magnetic order in the Heisenberg model of completely two-dimensional structures is prohibited according to the Mermin-Wagner theorem, ferromagnetism in realistic quasi-two-dimensional structures is quite rare. In addition, the stability of ferromagnetism in quasi-two-dimensional ferromagnetic structures is partially due to the surface magnetic anisotropy. Therefore, it is important not only to examine the magnetic order at zero temperature, but also to analyze the magnetic anisotropy. Even though MnN monolayer films on Cu(001) have been reported to have an antiferromagnetic order [1], Mn-compound monolayer films exhibiting the ferromagnetism have not been reported.

In this study, we explore monolayer-thick Mn-compound films on nonmagnetic transition-metal (TM) surfaces exhibiting the ferromagnetism, and propose valid interpretations on the mechanism for exhibiting the ferromagnetic state in predicted nanostructures [2]. First-principles calculations based on density functional theory were performed within the generalized gradient approximation with the OpenMX code [3]. We have found that MnB/TM(001) and MnC/TM(001) are ferromagnetic, whereas MnN/TM(001) is antiferromagnetic, irrespective of the kind of TM we studied. In Fig. 1, we show the calculated partial density of states (PDOS) of the Mn 3*d* states in MnB/Ag(001) for the nonmagnetic state as well as the ferromagnetic state plotted as the summation of the majority- and minority-spin states. The high PDOS of the nonmagnetic state at the Fermi energy ε_F is avoided by the exchange splitting in the ferromagnetic state, which is the characteristic of the itinerant ferromagnetism. With the detailed analysis, we have identified the mechanism of the ferromagnetism as the double-exchange mechanism. We also investigate the dependence on the TM substrates against the magnetic anisotropy energy (MAE) in MnC/TM(001) and MnB/TM(001). The detailed analysis of local MAE was performed using second-order perturbation theory [2,4]. We have clarified the main contributions to the in-plane anisotropy in MnB/Pd(001) as hybridization between Mn and Pd states.

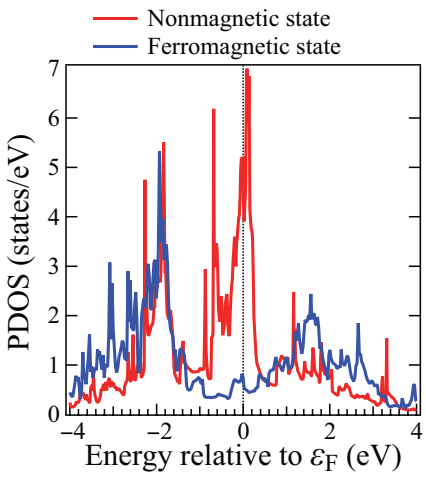

Fig. 1: The calculated PDOS of the Mn 3*d* states in MnB/Ag(001) for the nonmagnetic state as well as the ferromagnetic state plotted as the summation of the majority- and minority-spin states.

References:

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