Co 基ハーフメタルホイスラー合金材料の理論的探索

Ab-initio search for half-metal Co-based full Heusler alloy

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Materials with Half-metallic ferromagnetism (HMF) where electronic states are fully spin-polarized at the Fermi energy have been strongly desired for realizing high-efficiency spin-dependent transport applications. Co-based full Heusler alloy is a key material due to a high Curie temperature and a possibility to show the HMF. The *ab-initio* calculations have been expected to play a great role in search of HM materials, but most of theoretical studies have a lack of many-body interaction while dealing with the correlation effect is an essential aspect to understand electronic structure of Heusler compounds.

In present study, the density functional theory (DFT) +U calculations, in which the correlation term U is determined theoretically [1, 2], were performed to reinvestigate fundamental electronic structure of Co-based full Heusler alloys in bulk system and to explore a capability of the HMF. For Co_2MnSi, our calculations revealed that the correlation effect of Mn atom is more significant than that of Co to obtain the electronic structure and magnetic moment where in good agreement with experiments. By using the DFT+U method where only the Mn-correlation is introduced, it is concluded the HMF is appeared in Co_2MnSi with a minority band gap, E_{gap}, of 0.4 eV. Furthermore, this approach was extended to quaternary $Co_2(Y_x,Mn_{1-x})Si$, where Y is 3*d* transition metal with composition x. In Y of Ti and Fe for example, the eigenstates of conduction bottom (c.b.) and valence top (v.t.) are shifted to lower in energy with the varying E_{gap} as the x increases (see Fig. 1). This result indicates position of Fermi energy and the E_{gap} are tunable by a choice of substituting atom element and its composition, and the most promising candidates for HMF materials are the $Co_2(Ti_x,Mn_{1-x})Si$ and $Co_2(Fe_x,Mn_{1-x})Si$ with the x of 0.25 in terms of the Fermi energy locating at around the center of conduction and valence states.

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[1] M. Cococcioni *et al.*, Phys. Rev. B **71**, 035105 (2005).

[2] K. Nawa *et al.*, Phys. Rev. B **97**, 035117 (2018).

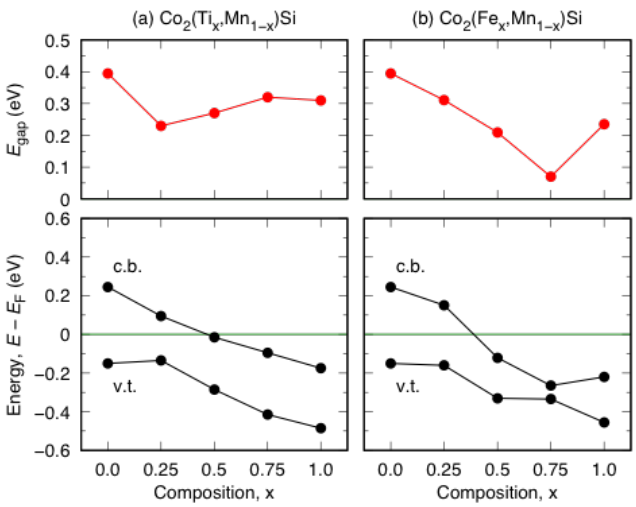

Fig. 1 Calculated E_{gap} and energies of c.b. and v.t. for (a) $Co_2(Ti_x,Mn_{1-x})Si$ and (b) $Co_2(Fe_x,Mn_{1-x})Si$.