Effect of the spin-orbit coupling on the topological phase of half Heusler compounds

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Abstract

Band inversion mechanisms of half Heusler compouds XMBi (X=Sc, Y, Lu, La, M=Pd, Pt) is investigated under different conditions, based on first-principles calculations with generalized gradient approximation approach. The results shown that Spin-orbit coupling, however, is not the leading cause but an account can add further fuel to the band inversion. The present finding provides an effective scheme to search for topologically nontrivial materials.

Keywords

Topological insulators, Half Heusler compounds, spin-orbit coupling.

1. Introduction

Topological insulators (TIs) are the latest phases to be discovered in condensed matter physics whereas one of the current hot topics because of their unique properties and potential applications[1-8]. They are distinguished from ordinary insulators due to their supports in metallic edge or surface states inside the bulk insulating gap. The surface states of topological insulators, however, were predicted to be inherently robust to external perturbations. The reason for this uniqueness is acknowledged to be largely contributed by the protection originated from time-reversal symmetry. Owing to these exotic surface electronic properties, topological insulators are highly believed to open up innovative directions for future technological applications in spintronics as well as quantum computing [1,2]. Two-dimensional (2D) TI was first predicted theoretically followed by an experimental confirmation in HgTe/CdTe quantum wells [3,4]. After that, TI family received remarkable recognition with the discoveries of over 50 three-dimensional topologically nontrivial materials [5-8] and some of them have been confirmed experimentally.

A band inversion is needed to change the topological order. The band inversion is previously assumed to result from the band splitting caused by spin-orbit coupling (SOC). Consequently, the search for new topological insulators is focused on materials composed of heavy elements with strong SOC. However, the band inversion can also be induced by lattice distortions and the external potential in a quantum well structure, without any SOC. Therefore, further investigation of the mechanism leading to the band inversion is required.

In this work we perform a systematic investigation of the band topology of 8 ternary half Heusler compounds XMBi (X=Sc, Y, Lu, La, M=Pd, Pt) of MgAgAs type. The influence of SOC on the band inversion is analyzed in detail.

2. Methodology

Band structure calculations with both SR (without SOC) and fully relativistic (with SOC) effects are conducted using a full-potential linearized augmented plane-wave method, which is implemented in the WIEN2K package. A converged ground state was obtained using 10 000 k points in the first Brillouin zone with K_{max}* R_{MT} = 9.0, where R_{MT} represents the muffin-tin radius and K_{max} is the

maximum size of the reciprocal-lattice vectors. Wave functions and potentials inside the atomic sphere are expanded in spherical harmonics up to l=10 and 4, respectively.The spin orbit coupling (SOC) is included by means of the second-variational method with the SR orbitals as the basis, where states up to 9 Ry above EF are taken into account in the basis expansion. In Fig. 1, we show the crystal structure of the half-Heusler compounds and also plot all the high symmetry points in the Brillouin zone. Atoms from groups X, Y and Z occupy the following three crystal sites of the cubic lattice: A (0 , 0 , 0) , B (1/4 , 1/4 , 1/4) and C (1/2 , 1/2 , 1/2) , respectively in Wyckoff coordinates.

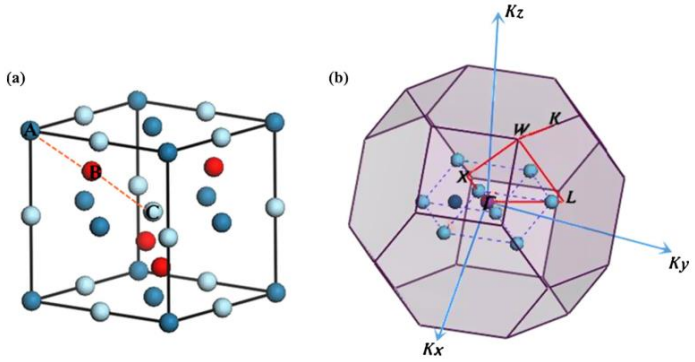

Fig 1.(a) Crystal structure of half-Heusler compound XYZ with the F-43m space group. (b) The high-symmetry points in the Brillouin zone.

3. Results and discussions

The band inversion can be achieved exclude the SOC, but about the alloys in our work, the strong effect of SOC can not be ignored due to heavy elements. Away to investigate the role of SOC played in band inversion mechanisms for the alloys contain heavy elements.

We take LaPtBi as an example, the band inversion strength under different hydrostatic strain have been shown in Fig.2(a). To explore the effect of SOC, the conditions of band inversion strength with (E_{BIS}^{SOC}) and without SOC (E_{BIS}^{noSOC}) have also been shown. Both the E_{BIS}^{noSOC} and E_{BIS}^{SOC} curves keep gradually falling with the increasing the hydrostatic expansion $\frac{a-a_0}{a_0}$ ratio. When the $\frac{a-a_0}{a_0}$ is up to -5.8% and -3.6%, E_{BIS}^{noSOC} and E_{BIS}^{SOC} change their sign and become negative, respectively. This indicates a fact that the LaPtBi, whether the SOC is taken into account or not, E_{BIS} always falls from positive to negative and the LaPtBi always can transform from the trivial phase to topological phase when the lattice is expanded. Further, we should pay more attention to the yellow covered area (the $\frac{a-a_0}{a_0}$ from -5.8% to -3.6%), where the E_{BIS}^{SOC} is negative and the E_{BIS}^{noSOC} is positive. In other words, only in this range, the SOC effect can drive an ordinary band order to convert into inversed band order. So, it indicates that the SOC is not the root cause but can narrow the energy difference EBIS and add further fuel to the band inversion.

It should be noted that, aim at different alloys, the effort of SOC is not the same. The E_{BIS}^{noSOC} and E_{BIS}^{SOC} of XMBi (X=Sc, Y, Lu, La, M=Pd, Pt) at their equilibrium lattice constants have been shown in Fig.2(b). For LuPdBi and ScPdBi alloys, the effect of SOC can be thought to be negligible. However, under the effect of SOC, the previously YPdBi alloy with ordinary band order (E_{BIS}^{noSOC}>0) can be converted into inversed band order (E_{BIS}^{SOC} <0). For YPdBi alloy, the shift will be large enough that it should be taken into account.

Finally, we should point out that, compounds with tetrahedral hybridization dominant structure are inclined to form TIs naturally, while the degree of SR effects, hydrostatic strain and the effect of SOC may be needed to process the band structures near the Fermi level further to get topological insulating states under different conditions. For example, although ScPdBi and YPdBi alloys with tetrahedral hybridization, the additional factors (hypostatic strain, SR effect and the effect of SOC) must be

added to inverting the normal band order into inverted. As discussed above, for ScPdBi alloys, hydrostatic stain can be applied to achieving the inverted band order. For YPdBi alloys, the effect of SOC or SR effect can also be applied to achieving the inverted band order.

4. Conclusion

We have shown by the first-principle calculations that Heusler compounds $Lu_2Fe/RuPb$ exhibit an inverted band order naturally. With the example of half Heusler compouds XMBi (X=Sc, Y, Lu, La, M=Pd, Pt) , we have argue that the major account for the band inversion in the half Heusler compounds is not the spin-orbit coupling. But the effect of spin-orbit coupling can narrow the energy difference so that maintain the phenomenon of band inversion further and regulating the topological electronic structure. We further pointed out that although lattice distortion play an significant role for the band inversion, more than the spin-orbit coupling. Spin-orbit coupling, however, is not the leading cause but an account can add further fuel to the band inversion.

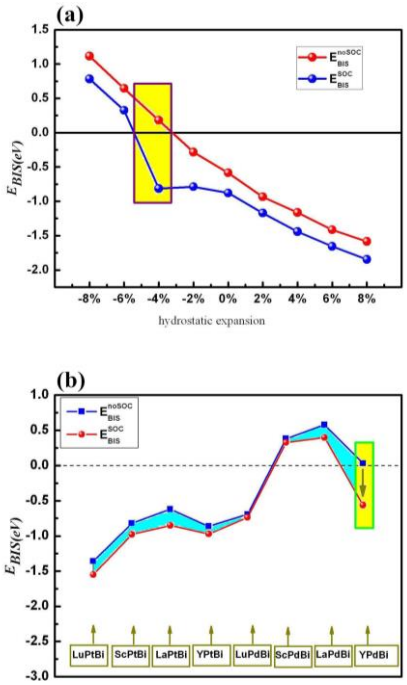

Fig 2 (a) The EBIS as a function of the hydrostatic expansion ratio $\frac{a-a_0}{a_0}$ for LaPtBi alloy. E_{BIS}^{noSOC} and E_{BIS}^{SOC} are represent the calculated EBIS without and with SOC respectively.

(b) E_{BIS}^{noSOC} and E_{BIS}^{SOC} of XMBi (X=Sc, Y, Lu, La, M=Pd, Pt) at their equilibrium lattice constant.

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