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Controllable topological quantum phase transitions in magnetic material FeBi$_2$Te$_4$

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Abstract
Here, we report a new intrinsic magnetic topological insulator FeBi$_2$Te$_4$ based on first-principles calculations and it can achieve a rich topological phase under pressure modulation. In the absence of pressure, we predict that both FeBi$_2$Te$_4$ ferromagnetic and antiferromagnetic orders are non-trivial topological insulators. Furthermore, FeBi$_2$Te$_4$ of FM-z ordering will undergo a series of phase transitions from topological insulator to semimetals and then to trivial insulator under pressure. Finally, we further clarify and verify the fact of topological phase transitions in conjunction with low-energy effective model calculations. This topological phase transition process is attributed to the synergy of the magnetic moment and the spin-orbit coupling. The unique topological properties of FeBi$_2$Te$_4$ will be of great interest in driving the development of quantum effects.

1 Introduction
The combination of magnetism and topology will obtain many topological quantum materials, such as Weyl semimetal, Chern insulator, and axion insulator[1–8]. And the effective ways to achieve topological and magnetic coupling are magnetic doping[9–12] and construction of magnetic/topological heterostructures[13–17]. However, the above two approaches will correspondingly to problems leading to inhomogeneous magnetic regions and strong dependence on interfacial properties[12, 13, 18]. Therefore, it is crucial to find a material that possesses magnetic and topological properties stoichiometrically.

Recently, an intrinsic magnetic topological insulator MnBi$_2$Te$_4$ has been reported, which possesses rich topological phases[3–7, 19]. Its ferromagnetic (FM) and antiferromagnetic (AFM) orders are Weyl semimetal and axial insulator, respectively[4, 5]. Due to its typical van der Waals layered structure, MnBi$_2$Te$_4$ will exhibit Te-Bi-Te-Mn-Te-Mn-Te septuple layers (SLs) thin films. Further studies show that multiple heptad layered films of MnBi$_2$Te$_4$ have parity number dependence and may have quantum anomalous Hall effect and topological magnetoelectric effect, respectively[7, 20]. A series of multilayer MnBi$_{2m}$Te$_{1+3n}$ materials based on the MnBi$_2$Te$_4$ parent material derived by inserting different
numbers of Bi₂Te₃ quintuple layers has also been widely investigated[21–34]. Although MnBi₂Te₄ has been a breakthrough in achieving novel physical phenomena, the experimental synthesis of the material is very demanding, slow-growing, and prone to sub-stability. In addition, the physical phenomena associated with MnBi₂Te₄ materials are hard to realize, especially the observed temperature of the quantum anomalous Hall effect (QAHE) is extremely low[35–39]. Although QAHE was observed in MnBi₂Te₄ thin film samples at 1.4 K[8], many experimental results failed to reach the quantum conductivity plateau[26, 40, 41], and no directly grown epitaxial films have been available to realize this effect[42]. Therefore, the topological magnetic community has devoted their research to enhance the temperature for realizing QAHE. The observed temperature of QAHE can increase by doping[7, 8, 43–53], building magnetic insulator/topological insulator heterostructures[38, 54–58], and applying external magnetic fields[22, 23, 28, 50, 50]. Sun et al. established a topological phase diagram for triggering QAHE by tuning slab thickness and magnetization[21]. However, the lack of stability of the MnBi₂Te₄ material has resulted in epitaxial films that are not yet directly grown[42]. In disagreement with earlier theoretical and experimental results[3], later experimental results[59–61] observed energy-gapless Dirac cones in the topological surface states of AFM MnBi₂Te₄. In addition, the dispersion relation of electrons in MnBi₂Te₄ is not consistent with the theoretical calculation[62].

Meanwhile, the magnetic order of the MnBi₂Te₄ series materials is also controversial. For example, MnSb₂Te₄ may exhibit FM phase[48], AFM phase[43, 44, 63, 64], and a Weyl semimetal with ferrimagnetic properties[35, 65]. MnBi₆Te₁₀ was reported to be in the FM[30] and AFM[28] orders. Complex competing magnetic orders greatly hinder the application of intrinsically magnetic topological insulators. The same as MnBi₂Te₄, Li et al. predicted that monolayer MBi₂Te₄ is a FM insulator for M=Ti, V, Mn, Ni, Eu, while it may present an unstable metallic state for M=Cr, Fe, Co[5]. Individual studies have also reported this series of materials one after another[54, 57, 66–68]. It has been reported that FeBi₂Te₄ single crystal has been successfully synthesised[66], which were also shown to be stable, and recent studies have also demonstrated its stability[68]. However, as a new potential intrinsic magnetic topological insulator, the magnetic ordering, electronic structure, and topological properties of FeBi₂Te₄ are still unclear.

In this work, we theoretically investigate the topological properties of different magnetic orders of FeBi₂Te₄ by first-principles calculation. Firstly, we confirm that both AFM-x and AFM-z orders of FeBi₂Te₄ are intrinsic magnetic topological insulators with gapless surface states. Then we find that modulating the in-plane to out-of-plane antiferromagnetism will break the Mirror symmetry and thus induce the (001) plane of FeBi₂Te₄ to acquire gapped surface states. Furthermore, we also demonstrate that the FM-x and FM-z orders are topological insulators with gapped surface states. The surface states of the FM-x and FM-z orders are connected and separated from the conduction band, respectively. Remarkably, we find that magnetic ground state FM-z ordering has a small bulk band gap and can be tuned to be topological Weyl semimetal and normal insulator under slight pressure, which achieves the phase transition from topological insulator to topological semimetal then to a trivial insulator. Moreover, we further construct the low-energy effective model to study the essential reasons for the series of topological phase transitions under pressure regulation. These intriguing topological states in FeBi₂Te₄ not only deepen our understanding of magnetic topology physics but also can broaden its applications in different spin quantum devices.

Results and discussion

Stability and topological properties of the intrinsic magnetic topological insulator FeBi₂Te₄

We first evaluate their stability for the different magnetic configurations of FeBi₂Te₄ (e.g. AFM-x, AFM-z, FM-x, and FM-z). Figs. 1(a), 1(b), and 1(c) show the structures and their Brillouin zone of FeBi₂Te₄ with a magnetic order in FM and AFM, respectively. The arrows in the crystal structure indicate the magnetic moments along the z-direction for FM and AFM, respectively. The FM-x and AFM-x orders only require the
magnetic moments to be along the x-direction. The schematic diagram of the magnetic moment settings in z and x directions is shown by the arrows on the left side of Fig. 1(a). All our antiferromagnetic sequences are calculated using the A-type antiferromagnetic configuration, which is the intra-layer ferromagnetic while inter-layer antiferromagnetic form. Both the magnetic configuration in the z and x directions, the interlayer exchange interaction ($\Delta E_{FM-AFM}$) is defined as the energy difference between the bulk structures of FM and AFM bulk per formula unit, respectively. As shown in Figs. 1(d) and 1(e), the band gaps unit cell energy differences between the different magnetic orders of FeBi$_2$Te$_4$ were first calculated theoretically. Figure 1(d) reveals that the band gaps of both FM and AFM orders become narrower due to spin-orbit coupling, while the non-magnetic (NM) state without SOC has the largest indirect band gap as the black arrow shown in Fig. S1(b). When considering SOC, both FM and AFM orders will behave as direct and indirect band gaps if the [100] (x-direction) and [001] (z-direction) directions are set. Combined with Figs. 1(d) and 1(e), the FM-z and AFM-x orders with lower energy in the FM and AFM orders, which are more stable, have smaller indirect band gaps (0.034 eV) and direct band gaps (0.129 eV), respectively. As shown in Fig. 1(e), compared to MBi$_2$Te$_4$ (M=Mn,V,Ni,Eu)[5] and MnX$_2$Y$_4$ (X=Sb,Bi,Y=Se,Te)[46], FeBi$_2$Te$_4$ tends to present an AFM order in the [100] direction, which is about 21.49 meV/f.u. lower than the FM order. In contrast, it prefers to form a FM order in the [001] direction. Furthermore, we find that the energy of the FM-z magnetic ordering is 1.7 meV lower than that of the AFM-x magnetic ordering base on the same unit-cell calculation. This intrinsic ferromagnetism does not appear in the remaining materials enumerated in Fig. 1(e). The intrinsic ferromagnetism of FeBi$_2$Te$_4$ might facilitate the realization of physical phenomena such as QAHE.

By investigating the electronic structure and topological properties of the bulk FeBi$_2$Te$_4$ AFM orders, we found that it exhibits physical properties similar to MnBi$_2$Te$_4$. From Figs. 2(a) and 2(b), it can be concluded that the band structure of the FeBi$_2$Te$_4$ AFM order without SOC interaction and its projected band structure has a slightly smaller direct band gap of 0.556 eV than that of the NM state shown in Fig. S1(a) and S1(b). Their conduction and valence bands can be recognized as mainly contributed by Bi-p/Fe-d and Te-p, respectively. When SOC effects are considered, as in Figs. 2(c) and 2(d), both AFM-z and AFM-x orders undergo band inversion (Bi-p and Te-p) near $\Gamma$, predicting a non-trivial topological property. AFM-z has a larger direct band gap 0.196 eV at $\Gamma$ than 0.129 eV of AFM-x (green line in the projected band structure diagrams). But due to the mutual proximity of the conduction and valence bands near the Z high-symmetry point, AFM-z presents an indirect band gap of 0.14 eV (yellow shading indicates the global band gap), different with the global direct band gap 0.16 eV at Z for MnBi$_2$Te$_4$[5].

To confirm the non-trivial surface states protected by a new symmetry $S = \Theta \tau_{1/2}$ ($\Theta$ represents time-reversal and $\tau_{1/2}$ represents a half magnetic-unit-cell translation), the Wannier Charge Centers (WCC) in the $k_z=0$ plane are computed. The WCCs of AFM-z and AFM-x in the $k_z$($k_y$ or $k_z$)=0 planes all have the topological number characteristic of $Z_2$=1, which means the AFM-z and AFM-x orders of FeBi$_2$Te$_4$ are non-trivial magnetic topological insulators. We take the $k_z=0$ planes for reference, as shown in Figs. 3(a) and 3(b). While for $k_z$($k_y$ or $k_z$)=0.5 planes all exhibit the topological trivial characteristic of $Z_2$=0. We further calculated the surface states of FeBi$_2$Te$_4$ with AFM-z and AFM-x orders using a semi-infinite (110) surface, as shown in Figs. 3(c) and 3(d). They exhibit gapless topological surface states protected by the $S$ symmetry. As for the semi-infinite (001) surface, AFM-z appears as a gapped surface state, while the surface state of AFM-x presents as a gapless feature, as shown in Fig. S2(a) and S2(b). For the FeBi$_2$Te$_4$ AFM order from in-plane and out-of-plane, the topological band gap will opening as the breaking of Mirror symmetry $M_z$. In short, we can identify FeBi$_2$Te$_4$ with AFM orders as a typical intrinsic magnetic topological insulator.

In contrast to the AFM order, the spin-polarized energy band structure of the bulk FM order exhibits a metallic state, as shown in Figs. S1(c). Comparing the spin-up and spin-down projected band structures in Fig. S3(a) and S3(b), they possess a very close direct band gap at $\Gamma$. However, a bulge at the top of the valence band of the spin-down band structure between the Z-F-$\Gamma$
paths drives the global indirect band gap down to 0.303 eV. This bulge is mainly contributed by the Fe-3d orbitals, and thus induces a spin magnetic moment of nearly 4 μB. After the introduction of the SOC effect, both FM-z (Fig. S3(c)) and FM-x (Fig. S3(d)) exhibit topological insulator characteristics with band inversion near Γ. FM-z order has an indirect band gap as small as about 0.034 eV and its Fermi level is close to the valence band at Γ, unlike AFM-z, AFM-x, and FM-x where the Fermi level is in the middle of the direct band gap at Γ. From FM-z to FM-x, the valence bands at Γ change from splitting to close to each other (black arrows at Figs. S3(c) and S3(d)), while the conduction bands change from degeneracy to splitting (purple arrows at Figs. S3(c) and S3(d)).

To further observe their topological properties, we calculated the surface states in their (110) terminals as shown in Figs. S4(c) and S4(d). The WCC calculations as shown in Figs. S4(a) and S4(b) confirm that FM-z and FM-x are topological insulators as well as the AFM orders.

Pressure-induced topological quantum phase transitions

Pressure is an effective way of regulating the band structure of the material. A series of topological phase transitions are realized in the FM-z magnetic order of FeBi2Te4 by pressure. As shown in Fig. 4(a), negative pressure induces the transformation of FeBi2Te4 with FM-z magnetic order from a nontrivial topological insulator with band inversion to an ordinary insulator. The lower panel in Fig.4(a) specifies the topological phase transition process under pressure regulation. The system undergoes five phases with increasing tension: the topological insulator, Dirac semimetal, type-II Weyl semimetal, type-I Weyl semimetal, and trivial insulator. Bi ions in FeBi2Te4 have a significant SOC effect, and the magnetic moment of Fe ion is particularly important for the electronic structure properties near the Fermi level. Figure 4(b) shows the dependence of SOC and magnetic moment on pressure. As the pressure decreases to a negative value, the magnetic moment in the z-direction of Fe ion gradually increases, inducing the system to transition from a topological insulator phase to a semimetal phase. At the same time, the SOC effect gradually weakened until the -0.85 GPa pressure applied and it transformed into a trivial insulator phase.

We transform the FM-z of narrow gaped into the gapless type-II Weyl semimetal state by applying tensile stress of 0.5 GPa, which is induced by interlayer orbital hybridizations, as shown in the band structure of Γ-Z line crossing each other in Fig. 5(a). The Weyl cone is slightly tilted along the Γ-Z line so that part of the electron pocket is below the cavity pocket, which is characteristic of type II Weyl semimetals [69]. In order to study its topological properties, we likewise performed surface state calculations for the FM-z system with -0.5 GPa action. The surface state at its (110) terminal (Fig. 5(b)) is slightly different from the one absent from the pressure in Fig. S4(c), which shows contact with the bulk band near the minimum of the conduction band. The Fermi arc exhibited by the energy contour at the Weyl point W in Fig. 5(d) is ample evidence of the fact that FM-z can be tunable into Weyl semimetal. Similar to MnBi2Te4[5], these two Weyl points (W/W') very close to the Fermi level are well separated in the momentum space, and while convenient for experimental observation its thin film may also facilitate the realization of QAHE. As the WCC in Fig. 5(c) shows, the W point is a monopole with a topological charge of +1 positioned in the momentum space, corresponding to a Berry phase of 2π, and similarly, the W' point with which it has a time-reversal relationship has the opposite topological charge, further proving that the system is a typical topological Weyl semimetal. In the absence of pressure, the FM-z order of bulk FeBi2Te4 possesses a gaped (001) terminal surface state (Fig. 6(a)) and a highly helical spin texture (Fig. 6(b)), although its Fermi level crosses the surface state (Fig. 6(a)) and presenting a metallic character. Due to the action of the tensile stress, the Fermi level evolves from crossing the surface state without applied pressure to residing in the surface band gap. At a pressure of -0.5 GPa, we achieved a phase transition of the topological surface state in the FM-z order of the FeBi2Te4. Its spin texture in Fig. 6(d) also becomes shrinked like a vortex. Moreover, FeBi2Te4 in the FM-z order with -0.5 GPa pressure has a lower enthalpy of production than the ground state FM-z.

Continuing to apply negative pressure to -0.7 GPa, the FeBi2Te4 FM-z magnetic order system will be tuned to be a type-I ideal Weyl semimetal.
As shown in Figs. S5(a) and S5(b), the motion of the WCC sum over a small sphere centered at C=-1 and C=1 in the momentum space and the existence of the Fermi arc confirm that the system is a Weyl semimetal. The surface state of the (110) plane under -0.7 GPa pressure (Fig. S5(c)) is similar to that of -0.5 GPa (Fig. 5(b)), except that the surface state is shifted more towards the conduction band. When the pressure comes to -1 GPa, the nontrivial topological property of band inversion no longer exists, and the system transforms into a trivial insulator (see Fig. 4(a)). Its (110) plane surface state is no longer connected to the valence band, and the Fermi level is in the middle of the gapped surface state (see Fig. S5(d)). We also confirmed the existence of the non-trivial topological insulator phase (Fig. S6) and trivial insulator phase (Fig. S7) by WCC calculations in various planes. Thus, we achieve multiple topological phase transitions in FeBi$_2$Te$_4$ FM-z ordering under pressure assistance.

**Low-energy effective model**

To understand the physical mechanisms embedded in the topological phase transition, we have further constructed a low-energy effective model for verification. Since the topological properties are mainly determined by the physical of the Γ point, we can construct an effective Hamiltonian to characterize the system. We use the four-band Dirac model to describe the low-energy properties. This model was presented in [4, 70] and has been well used to study the magnetoelectric properties of topological insulators. The Hamiltonian is written as Eq. (1).

$$\mathcal{H}(k) = A_2(k_x \alpha_x + k_y \alpha_y) + A_1 k_z \alpha_z + M(k) \beta ,$$

where $\alpha_i(i=x, y, z)$ and $\beta$ are the Dirac matrix. As the mass parameter $m$ varies, the Hamiltonian quantity proves the phase transition from the topological phase ($m < 0$) to the one with a non-topological (trivial) phase ($m > 0$). Set to develop boundary conditions in the $z$-direction to simulate the finite-scale model and the $k_z$ must be replaced by gradient operator $i \partial_z$. So the Hamiltonian quantity in the plane can be written as $h_z(k) = A_2(k_x \alpha_x + k_y \alpha_y) + (m + 2B_1 - B_2 k_z^2) \beta$, and the inter-plane hopping is $\Delta_z = -iA_1 \alpha_z/2 - B_1 \beta$. When we let $m$ vary from complex to positive, the system also undergoes a topological phase transition, as shown in Fig. 7(c).

**Conclusion**

In conclusion, based on first-principles calculations, we have investigated the electronic structure and topological properties of FeBi$_2$Te$_4$ in different magnetic orders. Different with A-type AFM topological insulator MnBi$_2$Te$_4$, the ground state of FeBi$_2$Te$_4$ is out-plane ferromagnetic. The AFM-x (AFM-z) and FM-x (FM-z) orders are gapless and gapped non-trivial topological insulators, respectively. A topological phase transition can be induced in the surface states of the (001) plane of the FeBi$_2$Te$_4$ AFM order by changing the direction of the magnetic moment. That is to say that Mirror symmetry breaking induces the opening of the (001) surface band gap during the change of antiferromagnetism from in-plane to out-of-plane. When the pressure is absent, the FM-z order has a Fermi level across the conduction band in the (001) terminal surface state, while the Fermi level under higher negative pressure will be between the gapped surface states, like -0.5 GPa. Notably, application of pressure induces a series topological phase transitions of the FM-z ordering,
$$\mathcal{H}(k) = \varepsilon_0(k) + \begin{pmatrix}
M(k) + M_1 & A_1 k_z & 0 & -A_2 k_z \\
A_1 k_z & -M(k) + M_2 & -A_2 k_z & 0 \\
0 & A_2 k_z & M(k) - M_1 & -A_1 k_z \\
A_2 k_z & 0 & -A_1 k_z & -M(k) - M_2
\end{pmatrix}, \quad (1)$$

from non-trivial topological insulators to Dirac semimetals, type-II Weyl semimetal and type-I Weyl semimetal to ordinary insulators. Combined with low-energy effective model calculations, we find that the phase transition from topological insulators to Weyl semimetals is mainly due to the enhancement of the magnetic moment of the system. In addition, the phase transition from non-trivial topological insulators to trivial insulators critically depends on the weakening of the SOC effect. Our results will not only provide opportunities for further research into quantum effects such as QAHE but also advance the design and application of magnetism topological quantum devices.

Methods

First-principles calculations are performed in Vienna ab initio simulation package (VASP) [71, 72] via using all-electron projected augmented wave (PAW) [73] method and Perdew-Burke-Ernzerhof (PBE) type generalized gradient approximation (GGA) [74] exchange-correlation function. The valence wave functions are expanded on the plane-wave basis with a cut-off energy of 350 eV. Our calculations, except for the nonmagnetic state, all take into account spin-orbit coupling (SOC). FeBi$_2$Te$_4$ has the same space group R$\overline{3}$m as MnBi$_2$Te$_4$, but the optimized lattice constant is slightly smaller ($a = 4.325$ Å). For the 3$d$ orbit of Fe, the on-site coulombic is chosen to be 4 eV and the magnetic moment is set to 4 $\mu_B$. The structures are relaxed with a conjugate-gradient algorithm till the energy on atoms is less than $1 \times 10^{-5}$ eV in our all calculations. The $\Gamma$-centered Monkhorst-Pack $k$-point mesh is chosen to $11 \times 11 \times 5$ and the force on each atom is set to $1 \times 10^{-4}$ for the energy difference calculation. We reproduce band structure obtained by constructing a tight-binding model based on Maximum Local Wannier Functions (MLWFs) [75, 76]. Based on the surface Green’s function approach [77–80], our calculations of Wannier Charge Center (WCC), surface states, spin-texture, and Fermi surfaces (FS) of the semi-infinite surfaces are performed via WannierTools package [81].

Supplementary information. Please see the attachment for detailed supplementary information.

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Author contributions. J.-M. Zhang conceived and supervised this work. W.-T. Guo and N. Yang performed the calculations. W.-T. Guo and J.-M. Zhang wrote the manuscript. Y. Yang and Z. Huang analyzed the datas and provided valuable and constructive suggestions.

Conflict of interest. The authors declare no conflict of interest.

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Fig. 1 Crystal structures and energies of FeBi$_2$Te$_4$ in different orders. Crystal structures of bulk FeBi$_2$Te$_4$ (a) FM ordering and (b) A-type AFM ordering. (c) The First Brillouin zone with (001) and (110) planes. (d) Comparison of the global band gap of the bulk FeBi$_2$Te$_4$ for different magnetic orders (FM, AFM and NM) with and without SOC, where the magnetic moment orientations [001] and [100] are calculated when SOC effects are considered. The direct band gap and indirect band gap are marked with D and I respectively in parentheses. (e) The relative energies of FM and AFM magnetic orders $\Delta E_{FM-AFM}$, where positive values indicate lower energy in the AFM order. To visualize the energy difference values close to 0 (like EuBi$_2$Te$_4$), we break the axes at certain positions. We considered AFM orders in both [100] and [001] directions, while the AFM states of the cited references a[5] and b[46] are along the [001] direction.

Fig. 2 Band structures of FeBi$_2$Te$_4$ in AFM order. (a) Bulk band structure and (b) projected band structure of AFM order FeBi$_2$Te$_4$ without SOC. Projected band structures of (c) AFM-z and (d) AFM-x orders. The black and green lines in the projected band structure indicate the global band gap and the local band gap at $\Gamma$, respectively, and in addition, the global band gap size is visualized by the yellow shading.

Fig. 3 Topological properties of AFM-z and AFM-x orders FeBi$_2$Te$_4$. WCC calculation results for two configurations considering SOC for (a) AFM-z and (b) AFM-x. Topological surface states in (110) termination of (c) AFM-z and (d) AFM-x orders.

Fig. 4 Pressure induced a series of topological phase transitions in FM-z order FeBi$_2$Te$_4$. (a) FeBi$_2$Te$_4$ of the FM order undergoes multiple phase transitions under pressure: topological insulators, Dirac semimetal, type-I Weyl semimetals, type-II Weyl semimetals, and ordinary insulators. The upper panel shows the band structure of each phase at different pressures, and the lower panel shows the corresponding phase transition results. Where $\delta_{DSM}^C = -0.34$ GPa, $\delta_{Weyl} = -0.6$ GPa, and $\delta_{TI} = -0.85$ GPa all represent the transition pressure of phase change. (b) The curves of SOC of Bi ions (take the quotient of the system containing pressure and the absence of pressure) and the magnetic moment of Fe ion along the z-direction as a function of pressure. Different color regions visually show different topological phases.

Fig. 5 The existence of the type-II Weyl semimetal phase. (a) Band structure of FM-z order under -0.5 GPa pressure, where the zoom-in diagram demonstrates the Weyl point W. (b) Topological surface states in (110) termination and (c) the motion of the sum of WCCs on a small sphere centered at W (C=1) and W' (C=-1) in momentum space. (d) Fermi arc (on the isoenergy plane of the Weyl points) of FM-z order under -0.5 GPa pressure.

Fig. 6 Comparison of topological properties of FM-z FeBi$_2$Te$_4$ with or without pressure. (a)/(c) Topological surface states in (001) termination and (b)/(d) spin textures (on the isoenergy plane of the Weyl points) of FM-z order at the absence of pressure or under -0.5 GPa pressure. The zoom-in diagram in Fig. 6(c) is shows a gapped topological surface state.

Fig. 7 Low-energy effective model confirms topological quantum phase transition. (a) Schematic of FM Weyl semimetal from NM insulator. As $M_{1,2}$ increases, a pair of Weyl points is generated. (b) Schematic diagram of the band inversion at $\Gamma$. (c) Schematic diagram of the phase transition for SOC reduction.
Crystal structures and energies of FeBi2Te4 in different orders. Crystal structures of bulk FeBi2Te4 (a) FM ordering and (b) A-type AFM ordering. (c) The First Brillouin zone with (001) and (110) planes. (d) Comparison of the global band gap of the bulk FeBi2Te4 for different magnetic orders (FM, AFM and NM) with and without SOC, where the magnetic moment orientations [001] and [100] are calculated when SOC effects are considered. The direct band gap and indirect band gap are marked with D and I respectively in parentheses. (e) The relative energies of FM and AFM magnetic orders $\Delta E_{\text{FM-AFM}}$, where positive values indicate lower energy in the AFM order. To visualize the energy difference values close to 0 (like EuBi2Te4), we break the axes at certain positions. We considered AFM orders in both [100] and [001] directions, while the AFM states of the cited references a[5] and b[46] are along the [001] direction.
Band structures of FeBi2Te4 in AFM order. (a) Bulk band structure and (b) projected band structure of AFM order FeBi2Te4 without SOC. Projected band structures of (c) AFM-z and (d) AFM-x orders. The black and green lines in the projected band structure indicate the global band gap and the local band gap at $\Gamma$, respectively, and in addition, the global band gap size is visualized by the yellow shading.
Figure 3

Topological properties of AFM-z and AFM-x orders FeBi2Te4. WCC calculation results for two configurations considering SOC for (a) AFM-z and (b) AFM-x. Topological surface states in (110) termination of (c) AFM-z and (d) AFM-x orders.
Pressure induced a series of topological phase transitions in FM-z order FeBi2Te4. (a) FeBi2Te4 of the FM order undergoes multiple phase transitions under pressure: topological insulators, Dirac semimetal, type-I Weyl semimetals, type-II Weyl semimetals, and ordinary insulators. The upper panel shows the band structure of each phase at different pressures, and the lower panel shows the corresponding phase transition results. Where $\delta_{\text{DSM}} = -0.34 \text{ GPa}$, $\delta_{\text{Weyl}} = -0.6 \text{ GPa}$, and $\delta_{\text{TI}} = -0.85 \text{ GPa}$ all represent the transition pressure of phase change. (b) The curves of SOC of Bi ions (take the quotient of the system containing pressure and the absence of pressure) and the magnetic moment of Fe ion along the z-direction as a function of pressure. Different color regions visually show different topological phases.
Figure 5

The existence of the type-II Weyl semimetal phase. (a) Band structure of FM-z order under -0.5 GPa pressure, where the zoom-in diagram demonstrates the Weyl point W. (b) Topological surface states in (110) termination and (c) the motion of the sum of WCCs on a small sphere centered at W (C=1) and W' (C=-1) in momentum space. (d) Fermi arc (on the isoenergy plane of the Weyl points) of FM-z order under -0.5 GPa pressure.
Figure 6

Comparison of topological properties of FM-z FeBi2Te4 with or without pressure. (a)/(c) Topological surface states in (001) termination and (b)/(d) spin textures (on the isoenergy plane of the Weyl points) of FM-z order at the absence of pressure or under -0.5 GPa pressure. The zoom-in diagram in (c) is shows a gapped topological surface state.
Figure 7

Low-energy effective model confirms topological quantum phase transition. (a) Schematic of FM Weyl semimetal from NM insulator. As M1,2 increases, a pair of Weyl points is generated. (b) Schematic diagram of the band inversion at $\Gamma$. (c) Schematic diagram of the phase transition for SOC reduction.

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