The recent discovery of antiferromagnetic (AFM) topological insulator (TI) in MnBi$_2$Te$_4$ has triggered great research efforts on exploring novel magnetic topological physics. Based on first-principle calculations, we find that the manipulation of magnetic orientation and ordering not only significantly affects material symmetries and orbital hybridizations, but also results in new magnetic topological phases in MnBi$_2$Te$_4$. We thus predict various types of unusual topological quantum phase transitions that are magnetically controllable in the material, including phase transitions from AFM TI to AFM mirror topological crystalline insulator, from type-II to type-I topological Weyl semimetal, and from axion insulator to Chern insulator. The findings open new opportunities for future research and applications of magnetic topological materials.

The subject of antiferromagnetic (AFM) topological insulators (TIs) has attracted enormous research interests in condensed matter physics and material science, since the first theoretical model proposed in 2010 [1]. AFM TIs are new states of quantum matter characterized by a Z$_2$ topological invariant, in analogy to time-reversal invariant (TRI) TIs [2, 3]. However, their topological surface states can be inherently gapped and the gap size can be significantly tuned by changing surface termination. Remarkably, the surface gap is originated from the interplay of massless Dirac-like fermions with intrinsic magnetization and featured by a quantized Berry phase of $\pi$, which is able to create the novel half-quantum Hall effect on the surface and the long-sought topological axion states [3–6]. Therefore, AFM TIs provide an ideal platform to explore exotic topological quantum phenomena, including axion electrodynamics, topological magneto-electric effects, the quantum anomalous Hall (QAH) effect and topological superconductivity, etc. The same kind of phenomena, in principle, could be realized in TRI TIs, which, however, relies critically on extrinsic magnetic structure on topological properties is thus expected to be crucial, which, however, has not been well studied for AFM TIs.

In the work, we systematically study the influence of magnetic structure on electronic and topological properties of AFM TI material MnBi$_2$Te$_4$ by first-principles calculations. Our results find that the interlayer coupling of MnBi$_2$Te$_4$ is strongly restricted by $PT$ symmetry and can be significantly tuned by breaking $PT$ symmetry. Hence, the change of magnetic order and orientation, which is controllable by applying magnetic field, has profound effects on orbital hybridization and band structure of MnBi$_2$Te$_4$. Remarkably, variant novel topological states, including AFM mirror topological crystalline insulator and type-I topological WSM in 3D as well as Chern insulator in 2D, can be realized in MnBi$_2$Te$_4$ by tuning magnetic structure. Unusual quantum phase transitions between these intriguing topological states are thus accessible, which could not only greatly enrich our understanding of magnetic topological physics but also inspire the design of new functional devices.

MnBi$_2$Te$_4$ is a van der Waals layered material crystal-
lized in a rhombohedral structure with the space group $R3m$ [22], formed by ABC-stacked Te-Bi-Te-Mn-Te-Bi-Te septuple layers (SLs). The ground state of the material has an A-type AFM order with an out-of-plane easy axis, displaying FM order within SL and AFM order between neighboring SLs as schematically presented in Fig. 1. In nonmagnetic state, there exist some key material symmetries, including $C_{3z}$ rotational symmetry, $M_x$ mirror symmetry, space inversion $P$, time reversal $T$ and $PT$. Here the $x$ and $z$ axes are defined along the in-plane and out-of-plane directions, respectively. When the AFM order is formed in MnBi$_2$Te$_4$ below the Néel temperature ($\sim 25$ K) [10, 11, 13–15], $M_x$ and $T$ get broken, while other symmetries are preserved. Different magnetic orders and orientations, however, could be realized by applying magnetic field. For instance, magnetic orientation could be tuned from out-of-plane to in-plane under a moderate magnetic field, and even further magnetic order can be driven from AFM to FM under a relatively stronger magnetic field of $\sim 6$ Tesla, as demonstrated experimentally [11]. Different magnetic structures (Fig. 1), labeled as AFM-$z$, AFM-$x$, FM-$z$ and FM-$x$ ($x$ and $z$ represent magnetic orientation), are thus accessible, which give different material symmetries as summarized in Table I. Hereafter, we will study electronic and topological properties of MnBi$_2$Te$_4$ for different magnetic structures.

**TABLE I: Material symmetries of MnBi$_2$Te$_4$ bulk in different magnetic configurations.**

|               | $P$ | $PT$ | $M_x$  | $C_{3z}$ | $S = T_{1/2}T$ |
|---------------|-----|------|--------|---------|---------------|
| AFM-$z$       | ✓   | ✓    | ✓      | ✓       | ✓             |
| AFM-$x$       | ✓   | ✓    | ✓      | ✓       | ✓             |
| FM-$z$        | ✓   | ×    | ×      | ✓       | ×             |
| FM-$x$        | ✓   | ×    | ✓      | ×       | ×             |

Let us first discuss the influence of magnetic order on interlayer coupling by comparing 2-SL MnBi$_2$Te$_4$ with different magnetic structures of AFM-$z$ and FM-$z$. The influence is visualized by looking at the differences in their band structures (Figs. 2a and 2b), since both systems would approach the same monolayer limit if the interlayer coupling is turned off. One major difference is that FM order generally induces spin-split bands, while AFM order always shows spin-degenerate bands as ensured by $PT$ symmetry. This is a well-known result from symmetry argument. However, the coupling between two FM SLs, each of which is spin-split by itself, would usually give rise to four bonding and antibonding states. A nontrivial question naturally arises: why the AFM system only displays two copies of bonding and antibonding states, irrespective of the strength of interlayer coupling. Detailed analysis finds that the top-layer spin-up state and the bottom-layer spin-down state are degenerate in energy, which would typically couple strongly with each other. These two states, however, are forbidden to couple by $PT$ symmetry (Fig. 2d). Only interlayer coupling between two states with the same spin but different energies are allowed. The analysis implies that the interlayer coupling is strongly restricted by $PT$ symmetry.

Conversely, interlayer coupling would be significantly enhanced by breaking $PT$ symmetry. This is really true when changing magnetic order from AFM to FM. For the FM state, the stronger interlayer coupling leads to a topological band inversion between Bi $p^+_z$ and Te $p^-_z$ (Fig. 2e), thus driving the system to Chern insulator phase. Our edge-state calculations indeed find gapless chiral edge mode within the bulk gap (Fig. 2h), which supports the above statement. In contrast, there is no such kind of band inversion for the 2-SL AFM system, explained by the restricted interlayer coupling. Therefore, when applying an out-of-plane magnetic field, a magnetic transition from AFM to FM state would be accompanied by a quantum phase transition from trivial insulator to Chern insulator.

The change of magnetic orientation also has important effects on electronic and topological properties. This is exemplified by studying 2-SL MnBi$_2$Te$_4$ with different magnetic structures of FM-$z$ and FM-$x$. Their band structures are noticeably different, especially for some valence bands (cf. Figs. 2b and 2c), implying strong influence of magnetic orientation on orbital hybridizations. Importantly, $M_x$ symmetry is broken for FM-$z$, while it is preserved for FM-$x$. The existence of $M_x$ requires a vanishing Hall conductance $\sigma_{xy}$, which thus suggests the FM-$x$ system has a zero Chern number. The symmetry argument is supported by orbital analysis that finds no topological band inversion (Fig. 2f) as well as by edge-state calculations that find no chiral edge state (Fig. 2i). Remarkably, our calculations suggest that by gradually tuning magnetic orientation from out-of-plane to in-plane, a topological quantum phase transition from $C = -1$ to $C = 0$ and further to $C = 1$ would occur, which is accompanied by closing and reopening of band
The tunable band gap and controllable topological quantum phase transition could be useful for designing new functional devices, like quantum topological transistors.

We then move forward to MnBi$_2$Te$_4$ bulk, which also shows rich topological phase transition phenomena when tuning its magnetic structure. By changing magnetic orientation from AFM-z to AFM-x, the band structure varies considerably, as shown in Fig. 3b. This is possibly due to the breaking of $C_{3z}$ and the emergence of $M_x$, which imposes different symmetry selection rules and thus results in distinct orbital hybridizations. Nevertheless, the topological band inversion between Bi $p_z^+$ and Te $p_z$ exists, independent of magnetic orientation. Therefore, AFM-x and AFM-z systems belong to the same $Z_2$ topological class, both of which are AFM TIs characterized by $Z_2 = 1$ and protected by $S = T_{1/2} T$ symmetry ($T_{1/2}$ represents a half magnetic-unit-cell translation). Therefore, they both have gapless surface states on the side surfaces that have preserved $S$ symmetry (Fig. 3a). Significant differences occur on the (111) surface. The surface state is gapped for AFM-z order, which gives a half-integer quantum Hall conductance $\sigma_{xy} = e^2/2h$. In contrast, the surface gap of AFM-x, if existing, would also give $\sigma_{xy} = e^2/2h$, which contradicts with $M_x$ symmetry. Therefore, its surface gap is enforced to be zero by $M_x$ symmetry. This symmetry argument is verified by surface-state calculations, which find gapless Dirac-like surface states within the bulk gap for the (111) termination. These surface states are nearly isotropic in 2D momentum space, in contrast to the anisotropic Dirac-like states on the side (110) surface (Figs. 3c and 3d).

Next we argue that the existence of both $M_x$ and $PT$ symmetries enables a new topological classification characterized by mirror Chern number $C_M = (C_{+,i} - C_{-,i})/2$ [23]. Since $M_x$ mirror reflection operation is commutative with $PT$, mirror eigenvalues $\pm i$ can be used to label the two-fold degeneracy protected by $PT$. Then, if one of the doubly degenerate states is labeled by $+i$, the other (i.e., $PT$ partner of the former) would be labeled by $-i$, and vice versa. Thus one can define Chern number for either $+i$ or $-i$ on the $M_x$ invariant plane in momentum space. The total Chern number $C = C_{+,i} + C_{-,i}$ is required to be zero by $PT$ symmetry, but $C_M$ can be nonzero. Specifically for MnBi$_2$Te$_4$ with AFM-x order, there exists a topological band inversion at $\Gamma$, which leads to nonzero $C_{+,i}$ and thus $|C_M| = 1$. This refers to a new topological phase, called AFM mirror topological crystalline insulator (TCI), which has gapless (111) surface protected by $M_x$ symmetry and gapless side surfaces protected by $S$ symmetry. Note that on the (111) surface, the Dirac-point of topological surface states is located at the $\Gamma$ point. This is in contrast to topological surface states of TRI TIs in proximity to magnetism oriented along the $x$ direction, which would have Dirac point shifted away from $\Gamma$.
The gapless (111) surface of AFM mirror TCI is of particular interest from the point view of symmetry and topology. The surface magnetism typically introduces a mass term into the Dirac-like surface states by breaking $T$. However, this mass term is enforced to zero by mirror symmetry. Based on this unique feature, one can control the $T$-breaking mass term by simply tuning mirror symmetry breaking. Or one could introduce another type of mass term, for instance, by superconducting proximity effect that could induce topological superconductivity [24]. Therefore, rich topological quantum physics would emerge by controlling symmetry breaking. Note that there are some intrinsic magnetic insulators in the MnBi$_2$Te$_4$ family, like XBi$_2$Te$_4$ (X=V, Ni, Eu), whose magnetic ground state is AFM-$x$ [7]. Therefore, the novel AFM mirror TCI phase would be realized intrinsically in these materials.

Let us discuss how things change when tuning magnetic order from AFM to FM. The FM-$z$ order of bulk MnBi$_2$Te$_4$ corresponds to a type-II topological Weyl semi-metal (WSM) phase [7, 8], in which Lorentz invari-
ance is violated and some part of electron pockets are located below hole pockets in the Weyl cone [25]. Importantly, only simple pair of Weyl points (WPs) exist in the material, due to the breaking of $T$. WPs are located along the $\Gamma$-$Z$ direction as ensured by $C_{3z}$ rotational symmetry and related to each other by $P$. When rotating magnetic orientation away from the $z$ axis by applying magnetic field (Fig. 4a), $C_{3z}$ gets broken but $P$ is preserved. Therefore, WPs would shift away from $\Gamma$-$Z$ to general $k$ points. More importantly, due to the layered structure of the material, Zeeman field induced band splitting is much larger for FM-$z$ than for FM-$x$, as verified by our calculations. Based on these insights, it is expected that varying magnetic orientation considerably change band dispersion near WPs, which has important influence on the physics of Weyl fermions.

We define a polar angle $\theta$ to quantify magnetic orientation and set $\theta = 0^\circ$ ($\theta = 90^\circ$) for FM-$x$ (FM-$z$). Figure 4b displays the motion of WPs in momentum space when varying $\theta$. A topological phase transition from type-II to type-I WSM phase happens at $70^\circ < \theta < 80^\circ$ (Fig. 4c). When $\theta = 0^\circ$, two WPs eventually merge, leading to annihilation of Weyl fermions and a topological transition to trivial phase. Remarkably, the type-I topological WSM phase in MnBi$_2$Te$_4$ is the simplest WSM, which has only one single pair of WPs located exactly at the charge neutral point. For comparison, we show band structures (Fig. 4d) for $\theta = 80^\circ$ and $\theta = 40^\circ$ as representative examples of type-II and type-I topological WSMs, and present their calculated surface states on the (1T1) termination (Fig. 4e). While both Fermi arcs and trivial electron pocket around $\Gamma$ simultaneously appear near the Fermi level in the type-II case, only Fermi arcs with no interfering signal from other bulk states can be obtained in the type-I case. In contrast to other WSM materials with multiple pairs of WPs and complex Fermi surfaces [25-28], this material hosts the simplest topological WSM phase, which is more advantageous for exploring Weyl physics and transport experiments. Moreover, its Weyl fermions are greatly tunable, which could lead to emergent quantum phenomena. For instance, artificial black-hole horizon emerges at the critical point of topological phase transition between type-I and type-II WSM phases [29, 30].

Finally, we would like to discuss topological properties of few-layer MnBi$_2$Te$_4$. For AFM-$x$ order, the few-layer film is either an insulator with zero Chern number or is gapless as required by $M_z$ symmetry. For the later case, the breaking of $M_z$, for instance, by changing magnetic orientation or by applying strain, could open the band gap, which may generate topological nontrivial phases.

For the magnetic ground state AFM-$x$, previous work found that Chern number of MnBi$_2$Te$_4$ changes in an unique oscillating behavior between even and odd layers, giving rise to axion insulators and QAH insulators [7], respectively. When changing magnetic order into FM-$z$ by applying an out-of-plane magnetic field, topological properties can be largely tuned. Figures 5a and 5b display band structures of 3-SL and 4-SL films with FM-$z$ order, respectively. Both of them show gapped Dirac cone-like band structures near the Fermi level. Our calculations of anomalous Hall conductance (Fig. 5c), edge states, and bandgap as function of spin-orbit coupling consistently suggest that they are Chern insulators. Chern numbers and bandgaps for varying thickness with FM-$z$ order are summarized in Table II. Thicker films can have higher Chern numbers, which is an inherent feature of topological WSM phase. Therefore, when changing magnetic order from AFM to FM, thin films can display topological quantum phase transition from axion insulators to Chern insulators that possibly have high Chern numbers.

In summary, based on first-principles calculations, we find that the change of magnetic order and orientation has profound influence on material symmetries and orbital hybridizations in AFM TI material MnBi$_2$Te$_4$, which results in a few new topological quantum states, including the AFM mirror TCI and the type-I topological WSMs. We thus predict a variety of quantum phase transitions between novel topological states, which is experimentally feasible and controllable. These novel topo-

![Fig. 5: Band structures and anomalous Hall conductance of few-layer FM MnBi$_2$Te$_4$. (a) and (b) Band structures for 3-SL and 4-SL FM films, respectively. (c) Anomalous Hall conductance of FM films of different thicknesses.](image-url)
logical states and quantum phase transitions, if confirmed by experiments, could greatly stimulate future research of magnetic topological physics and materials.

*Note added:* Recently, quantum phase transition from axion insulator to Chern insulator was realized experimentally in few-layer MnBi$_2$Te$_4$ [31].

| Gap (meV) | C  |
|-----------|----|
| 3-SL      | 78 | 1  |
| 4-SL      | 76 | 1  |
| 5-SL      | 63 | 1  |
| 6-SL      | 57 | 1  |
| 7-SL      | 49 | 1  |
| 8-SL      | 46 | 1  |

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[1] R. S. Mong, A. M. Essin, and J. E. Moore, Phys. Rev. B **81**, 245209 (2010).
[2] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
[3] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).
[4] X.-L. Qi, T. L. Hughes, and S.-C. Zhang, Phys. Rev. B **78**, 195424 (2008).
[5] F. Wilczek, Phys. Rev. Lett. **58**, 1799 (1987).
[6] A. M. Essin, J. E. Moore, and D. Vanderbilt, Phys. Rev. Lett. **102**, 146805 (2009).
[7] J. Li, Y. Li, S. Du, Z. Wang, B.-L. Gu, S.-C. Zhang, K. He, W. Duan, and Y. Xu, arXiv:1808.08608 (2018).
[8] D. Zhang, M. Shi, T. Zhu, D. Xing, H. Zhang, and J. Wang, arXiv:1808.08014 (2018).
[9] Y. Gong, J. Guo, J. Li, K. Zhu, M. Liao, X. Liu, Q. Zhang, L. Gu, L. Tang, X. Feng, et al., arXiv:1809.07926 (2018).
[10] M. M. Otvorkov, I. I. Klimovskikh, H. Bentmann, A. Zeugner, Z. S. Aliev, S. Gass, A. U. B. Wolter, A. V. Koroleva, D. Estyunin, A. M. Shikin, et al., arXiv:1809.07389 (2018).
[11] J. Cui, M. Shi, H. Wang, F. Yu, T. Wu, X. Luo, J. Ying, and X. Chen, Phys. Rev. B **99**, 155125 (2019).
[12] M. M. Otvorkov, I. Rusinov, M. Blanco-Rey, M. Hoffmann, A. Vyazovskaya, S. Eremeev, A. Ernst, P. Echenique, A. Arnau, and E. V. Chulkov, Phys. Rev. Lett. **122**, 107202 (2019).
[13] A. Zeugner, F. Nietschke, A. U. B. Wolter, S. Gaβ, R. C. Vidal, T. R. F. Peixoto, D. Pohl, C. Damm, A. Lubk, R. Hentrich, et al., Chem. Mater. **31**, 2795 (2019).
[14] S. H. Lee, Y. Zhu, Y. Wang, L. Miao, T. Pilisbury, S. Kempinger, D. Graf, N. Alem, C. Cui-Zu, N. Samarth, et al., arXiv:1812.00339 (2018).
[15] J.-Q. Yan, Q. Zhang, T. Heitmann, Z. L. Huang, W. D. Wu, D. Vaknin, B. C. Sales, and R. J. McQueeney, arXiv:1902.10110 (2019).
[16] R. C. Vidal, H. Bentmann, T. R. F. Peixoto, A. Zeugner, S. Moser, C. H. Min, S. Schatz, K. Kissner, M. Unzelmann, C. I. Fornari, et al., arXiv:1903.11826 (2019).
[17] B. Chen, F. Fei, D. Zhang, B. Zhang, W. Liu, S. Zhang, P. Wang, B. Wei, Y. Zhang, J. Guo, et al., arXiv:1903.09934 (2019).
[18] Y. Deng, Y. Yu, M. Shi, J. Wang, X. Chen, and Z. Yuanbo, arXiv:1904.11468 (2019).
[19] J. Zhang, C.-Z. Chang, Z. Zhang, J. Wen, X. Feng, K. Li, M. Liu, K. He, L. Wang, X. Chen, et al., Nat. Commun. **2**, 574 (2011).
[20] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Science **314**, 1757 (2006).
[21] B. Huang, G. Clark, D. R. Klein, D. MacNeill, E. Navarro-Moratalla, K. L. Seyler, N. Wilson, M. A. McGuire, D. H. Cobden, D. Xiao, et al., Nature Nanotechnol. **13**, 544 (2018).
[22] D. S. Lee, T.-H. Kim, C.-H. Park, C.-Y. Chung, Y. S. Lim, W.-S. Seo, and H.-H. Park, Cryst. Eng. Comm. **15**, 5532 (2013).
[23] J. C. Y. Teo, L. Fu, and C. L. Kane, Phys. Rev. B **78**, 045426 (2008).
[24] Y. Peng and Y. Xu, arXiv:1809.09112 (2018).
[25] A. A. Soluyanov, D. Gresch, Z. Wang, Q. Wu, M. Troyer, X. Dai, and B. A. Bernevig, Nature **527**, 495 (2015).
[26] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B **83**, 205101 (2011).
[27] H. Weng, C. Fang, Z. Fang, B. A. Bernevig, and X. Dai, Phys. Rev. X **5**, 011029 (2015).
[28] N. Armitage, E. Mele, and A. Vishwanath, Rev. Mod. Phys. **90**, 015001 (2018).
[29] K. Volovik, G. E. and Zhang, J. LOW Temp. Phys. **189**, 276 (2017).
[30] H. Huang, K.-H. Jin, and F. Liu, Phys. Rev. B **98**, 121110 (2018).
[31] Chang Liu, et al. Unpublished.