Exchange bias and quantum anomalous Hall effect in the MnBi$_2$Te$_4$/CrI$_3$ heterostructure

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The layered antiferromagnetic MnBi$_2$Te$_4$ films have been proposed to be an intrinsic quantum anomalous Hall (QAH) insulator with a large gap. It is crucial to open a magnetic gap of surface states. However, recent experiments have observed gapless surface states, indicating the absence of out-of-plane surface magnetism, and thus, the quantized Hall resistance can only be achieved at the magnetic field above 6 T. We propose to induce out-of-plane surface magnetism of MnBi$_2$Te$_4$ films via the magnetic proximity with magnetic insulator CrI$_3$. A strong exchange bias of $\sim 40$ meV originates from the long Cr-$e_g$ orbital tails that hybridize strongly with Te $p$ orbitals. By stabilizing surface magnetism, the QAH effect can be realized in the MnBi$_2$Te$_4$/CrI$_3$ heterostructure. Moreover, the high-Chern number QAH state can be achieved by controlling external electric gates. Thus, the MnBi$_2$Te$_4$/CrI$_3$ heterostructure provides a promising platform to realize the electrically tunable zero-field QAH effect.

INTRODUCTION

The quantum anomalous Hall (QAH) effect is a topological phenomenon characterized by quantized Hall resistance and zero longitudinal resistance (1–4). Different from the conventional quantum Hall effect, the QAH effect is induced by the interplay between spin-orbit coupling (SOC) and magnetic exchange coupling and thus can occur in certain ferromagnetic (FM) materials at zero external magnetic field. Owing to its topological and dissipation-free properties, the QAH insulator is an outstanding quantum-coherent material platform for the next-generation quantum-based technologies, including spintronics and topological quantum computations. Following the early theoretical predictions (5–7), the QAH effect was first demonstrated in magnetically (Cr or V) doped (Bi,Sb)$_2$Te$_3$ (8–11), in which magnetic doping provides the required exchange coupling between magnetic moments and electron spins and thus is essential for the occurrence of the QAH state. However, magnetic doping inevitably degrades sample quality with the presence of massive disorders and thus limits the critical temperature of the QAH state below 2 K (11). Therefore, it is desirable to realize the QAH effect in intrinsic magnetic materials with stoichiometric crystals.

Recently, a tetradymite-type layered compound, MnBi$_2$Te$_4$, was proposed to be a promising topological material platform (12–15), with intrinsic A-type anti-FM (AFM) order, in which the magnetic moments of Mn atoms are ferromagnetically coupled within one septuple layer (SL) and anti-ferromagnetically coupled between the adjacent SLs, for the realization of the QAH effect, as well as other magnetic topological phases (16–18). Early first-principles calculations show that the QAH state can be realized in the MnBi$_2$Te$_4$ films with odd numbers of SLs at zero magnetic field for the ideal AFM order (13–19). The A-type AFM order was demonstrated via magnetization measurements for bulk MnBi$_2$Te$_4$ as the typical spin-flip transition was observed when the external magnetic field perpendicular to the SL plane was increased above 3.5 T (15, 20–24). However, the magnetotransport experiments in the MnBi$_2$Te$_4$ films only revealed a quantized Hall resistance for the magnetic field above 6 T (21, 25, 26), larger than the critical field of spin-flop transition. Therefore, the thin film has already become FM under this magnetic field. The predicted zero-field QAH state induced by the ideal AFM order has yet been demonstrated experimentally. The early angular-resolved photon emission spectroscopy (ARPES) measurements observed a band gap, ranging from 50 meV to hundreds of meVs (15, 20, 27, 28), of topological surface states (TSSs) in MnBi$_2$Te$_4$. However, this gap is shown to persist well above the Néel temperature and could be observed even at room temperature (20, 27, 15), making it unlikely originated from the AFM order. More recent high-resolution ARPES studies based on synchrotron and laser light sources show that the TSS remains gapless below the Néel temperature (29–32). The negligible magnetic gap of TSS is consistent with the absence of the zero-field QAH effect in magnetotransport measurements (20, 21, 23, 25, 26). The absence of magnetic gap of TSSs suggests that the surface magnetism may not be well developed and different from the bulk AFM order. Physically, this is not unexpected since more complex magnetic interactions, including dipole-dipole interaction and Dzyaloshinskii-Moriya interaction, may play an important role for the surface magnetic mechanism. Consequently, the surface Mn magnetic moments may be canted, or lie in the SL plane, or become disordered, all of which may lead to a gapless TSS. Furthermore, magnetic domains ubiquitously exist in AFM materials and cannot be easily eliminated even by field cooling. All these problems hamper the realization of zero-field QAH state in the MnBi$_2$Te$_4$ films.

In this work, we propose to overcome the challenge of surface magnetism by coupling the MnBi$_2$Te$_4$ films to a two-dimensional (2D) FM insulator with the example of CrI$_3$ via exchange bias. Our density functional theory (DFT) calculations on the MnBi$_2$Te$_4$/CrI$_3$ heterostructure show a FM exchange bias around 40 meV, much larger than the Néel temperature of MnBi$_2$Te$_4$ [24 K (15)] and the Curie temperature of CrI$_3$ [61 K for bulk (33) and 45 K for monolayer (34)]. Moreover, CrI$_3$ has little influence on electronic band structure of MnBi$_2$Te$_4$ films, and thus, the QAH state with the Chern number (CN) = 1 can exist in 3- and 5-SL-thick MnBi$_2$Te$_4$, consistent with the early studies on pure MnBi$_2$Te$_4$ films. We also studied the electric gating effect and the CrI$_3$/MnBi$_2$Te$_4$/CrI$_3$ heterostructures. Our results show that (i) the high-CN QAH state with CN = 3 can be achieved by tuning gate voltages and (ii) the strong exchange bias...
can always align the magnetization of both surfaces of MnBi$_2$Te$_4$ films, thus driving even SL MnBi$_2$Te$_4$ into the QAH state in the CrI$_3$/MnBi$_2$Te$_4$/CrI$_3$ heterostructure.

RESULTS

FM exchange bias at the MnBi$_2$Te$_4$/CrI$_3$ interface

The required exchange bias material should provide strong magnetic coupling at the interface but not change the electronic states near the Fermi energy. Therefore, we choose a magnetic insulator, CrI$_3$ (34). Its monolayer is FM and can couple with MnBi$_2$Te$_4$ through the van der Waals interface, which may weakly disturb the band structure of MnBi$_2$Te$_4$. Because the interaction is determined by the interface layer, we only choose a monolayer of CrI$_3$ for the interface model.

We construct interface models with one layer of CrI$_3$ and different layers of MnBi$_2$Te$_4$ on its top, as shown in Fig. 1. Both materials share the same triangular lattice but different in-plane lattice parameters, 7.04 Å for CrI$_3$ and 4.36 Å for MnBi$_2$Te$_4$ from our DFT calculations, which is consistent with recent works (13, 14, 35). A 2 × 2 supercell of CrI$_3$ can match well with a 3 × 3 supercell of MnBi$_2$Te$_4$. Alternatively, the primitive unit cell of CrI$_3$ can also match a $\sqrt{3} \times \sqrt{3}$ supercell of MnBi$_2$Te$_4$ with a mismatch of 7%. Because we are mostly interested in the band structure of MnBi$_2$Te$_4$, we stretch the CrI$_3$ lattice to match the $\sqrt{3} \times \sqrt{3}$ MnBi$_2$Te$_4$ supercell. We fully optimized the atomic structures by including the van der Waals interactions in DFT calculations within the generalized gradient approximation (GGA) and the Hubbard U. We have tested both models and found that they give similar results in the exchange coupling and band structure (see figs. S1 and S3). Thus, we choose the smaller model, $\sqrt{3} \times \sqrt{3}$ MnBi$_2$Te$_4$/1 × 1 CrI$_3$, for further investigations in the following.

At the interface, MnBi$_2$Te$_4$ exhibits strong FM coupling with CrI$_3$. For 1-SL MnBi$_2$Te$_4$ on top of CrI$_3$, the energy difference between the FM and AFM coupling is about 40 meV. We note that different ways of stacking between two materials give very similar strength of exchange coupling, which is also true for the 3 × 3 MnBi$_2$Te$_4$/2 × 2 CrI$_3$ case (fig. S3). When increasing the MnBi$_2$Te$_4$ layer to 2 SLs and more, the interface FM coupling remains with the same exchange energy and the two SLs still couple in the AFM way (fig. S2). Therefore, the CrI$_3$ layer couples only with the neighboring MnBi$_2$Te$_4$ layer and does not affect the AFM order between different MnBi$_2$Te$_4$ layers.

We point out that such an exchange coupling is much stronger than the magnitude of the exchange interactions between two MnBi$_2$Te$_4$ layers (~3 meV for $\sqrt{3} \times \sqrt{3}$ supercell) or two CrI$_3$ layers (~10 meV for 1 × 1 unit cell (36)). Therefore, CrI$_3$ can stably pin the FM order of the proximity MnBi$_2$Te$_4$ layer and act as an effective exchange bias. In addition, we find that the SOC weakly affects the magnetic coupling strength (see figs. S1 to S4) and the magnetic moments prefer the out-of-plane direction (see fig. S8).

The strong exchange coupling originates in the orbital feature at the interface. The Mn site has $d^9$ configuration as $t^2_2g_2e^5_0$ and the Cr site has $d^5$ as $t^2_2g_2e^2_0$. There is a long exchange pathway from Cr-$e_g$ to Mn-$t_{2g}$ states through the intermediate I, Te, Bi, and Te atoms, which is beyond the simple superexchange interaction. In the localized Wannier orbitals, we observe a crucial feature in the Cr-$e_g$ states. Tails of the Cr-$e_g$ Wannier functions extend beyond the van der Waals gap and strongly overlap with the neighboring Te $\rho$ orbitals (see Fig. 1C). This strong orbital overlap rationalizes the strong coupling between two materials. We also notice that the exchange channels from Cr-$e_g$ to Mn-$t_{2g}$ and Cr-$e_g$ to Mn-$e_g$ are both of FM type, further enhancing the overall exchange coupling strength. This is in sharp contrast to the exchange coupling between two CrI$_3$ layers, which is of FM type for the channel from Cr-$e_g$ to Cr-$t_{2g}$ and of AFM type from Cr-$t_{2g}$ to Cr-$t_{2g}$ (36). In addition, AFM-type coupling at the interface can also play a role of the exchange bias, although the present specific interface structure exhibits the FM coupling.

QAH effect

We next investigate the electronic band structure and discuss its topological properties. Figure 2 shows band structures for 1 to 6 MnBi$_2$Te$_4$ SLs on top of CrI$_3$. As discussed above, there is FM coupling between CrI$_3$ and neighboring the MnBi$_2$Te$_4$ SL and AFM coupling between MnBi$_2$Te$_4$ SLs. The interface band structure can be approximately regarded as an overlap of two different materials. An essential feature is the existence of an energy gap in these band structures, which is crucial for the realization of QAH effect. The occupied Cr-$t_{2g}$ bands are far below the valence bands of MnBi$_2$Te$_4$. The Cr-$e_g$ states overlap with the conduction band bottom of MnBi$_2$Te$_4$ and remain unoccupied. This means that there is no charge transfer through the van der Waals junction. The calculated Cr-$t_{2g}$ and Cr-$e_g$ gap is about 1 eV, which is consistent with previous GGA calculations and can be corrected to about 1.5 eV by hybrid functionals (37). Although some Cr-$e_g$ bands appear as the lowest conduction bands at the interface for thinner MnBi$_2$Te$_4$ films (1 to 4 SLs), they will be pushed to even higher energy by the self-energy correction and do not affect our understanding of the band structure topology. When the MnBi$_2$Te$_4$ layer is thicker (e.g., 5 to 6 SLs), the MnBi$_2$Te$_4$ states become the lowest conduction bands in the GGA band structure. Thus, CrI$_3$ serves an ideal proximity exchange bias without destroying the MnBi$_2$Te$_4$ band structure.

We find that isolate MnBi$_2$Te$_4$ layers are trivial magnetic insulators for 1, 2, 4, and 6 SLs thick and QAH effect insulators for 3 and...
5 SLs, which is consistent with recent theoretical studies (13, 19). Here, the QAH insulator has the CN = 1, as showed by our Berry phase calculations using the Wilson loop method (38, 39) and the Berry curvature distribution in the 2D Brillouin zone. In proximity to the CrI3 layer, MnBi2Te4 band structures are modified weakly without changing their topological nature. For example, the isolated MnBi2Te4 layer of 2, 4, or 6 SLs thick exhibits the double degeneracy in the band structure caused by the symmetry combining spatial inversion and time reversal. The existence of the CrI3 layer weakly breaks this symmetry and splits the degenerate bands. We verify the topological character of the interface structures by observing the band gap evolution with respect to the SOC strength. For 3- and 5-SL thick MnBi2Te4/CrI3, the bandgap closes at about 90% of the normal SOC strength but reopens an energy gap with increasing SOC, showing a topological phase transition (TPT) (see figs. S5 and S6). The QAH insulator gaps are 49 and 14 meV for the 3- and 5-SL interface, respectively. For 1-, 2-, 4-, and 6-SL-thick MnBi2Te4/CrI3, however, the bandgap remains open as varying SOC from 0 to 100%.

**Electrically tunable high-CN QAH effect**

The 2D layered structure offers an opportunity to tune the band structure topology by applying a vertical electric field. The electric field induces different potential variation at different layers and subsequently modifies the overall band structure and its topological nature. For the interface structure, an electric field (ε) along the −z direction can push the Cr-e_g states up in the conduction band, as illustrated in Fig. 1B, leaving only MnBi2Te4 states right above and below the energy gap. Further increasing the electric field can induce an inversion between the occupied and unoccupied bands, giving rise to the TPT. Since the CrI3 brings little modifications to the low-energy band structure of MnBi2Te4, we only consider isolated MnBi2Te4 models when applying an electric field in following discussions.

The electric field can induce the high-CN QAH state. In a simple two-band model (5), a band inversion at the Γ point usually leads to a change of the CN by ±1. If the band inversion occurs at generic k-points, then it can induce a jump of the CN by the number of the transition points. The MnBi2Te4 film under an electric field exhibits two important symmetries, the threefold rotation (denoted as C3) and a combined symmetry between the time reversal and mirror reflection (denoted as TM). Since the mirror plane crosses the Γ–M line in the Brillouin zone and perpendicular to the layer plane, the Γ–K line is invariant under the TM symmetry. Therefore, if a transition happens at a generic k-point away from the Γ–K line, then the gapless points must exist at six different k-points related by C3 and TM symmetries. If a transition happens along the Γ–K line that is invariant under TM, then the gapless points must simultaneously appear at three different k-points related by C3 (see the inset of Fig. 3A). If a transition appears at Γ that is invariant under both C3 and TM symmetries, then a single Dirac point transition can occur.

To verify this scenario, we carried out band structure calculations on 3-SL-thick MnBi2Te4 and demonstrate that the CN can...
jump by both 1 and 3 via applying a small electric field, as shown in Fig. 3. At zero electric field, the 3-SL-thick MnBi₂Te₄ is a QAH state with CN = 1 and changes to a trivial insulator for $\epsilon = 0.005 \text{V/Å}$. This transition is through a gap-closing point at $\Gamma$ for $\epsilon = 0.002 \text{V/Å}$. For a larger electric field ($\epsilon = 0.015 \text{V/Å}$), another transition occurs with three gap-closing points along the $\Gamma$–$K$ lines, leading to a QAH state with CN = 3. The gap-closing and reopening points can be recognized as hot spots of the Berry curvature in Fig. 3C. Furthermore, the electric field can also drive the MnBi₂Te₄ film with even numbers of SLs from a trivial magnetic insulator with zero CN to the QAH state. For instance, red $\epsilon = 0.025 \text{V/Å}$ induces a TPT with three gapless points along the $\Gamma$–$K$ lines in the 2-SL-thick MnBi₂Te₄ film at $\epsilon = 0.0223 \text{V/Å}$, resulting in the QAH state with CN = −3 (see fig. S7).

**Sandwiched MnBi₂Te₄ structures**

Given the short range nature of exchange bias, the CrI₃ is expected to align the magnetization of the bottom MnBi₂Te₄ layer in the MnBi₂Te₄/CrI₃ heterostructure but may have little influence on the top MnBi₂Te₄ layer when the film thickness is large. This issue can be resolved by considering a sandwiched structure CrI₃/MnBi₂Te₄/CrI₃. For the MnBi₂Te₄ films with an odd number of SLs, the AFM order in MnBi₂Te₄ is compatible with the FM orders in the top and bottom CrI₃ monolayers. In contrast, for the MnBi₂Te₄ films with an even number of SLs, the compensated AFM ordering between MnBi₂Te₄ layers can be changed by CrI₃. As an example of the 4-SL case in Fig. 4, the magnetization of the top MnBi₂Te₄ SL feels frustration from the upper CrI₃ layer and the lower MnBi₂Te₄ layer. Because the MnBi₂Te₄/CrI₃ coupling is much stronger than the MnBi₂Te₄/MnBi₂Te₄ coupling, magnetic moments of the top MnBi₂Te₄ SL aligns parallel to those of the CrI₃ layer. Such a rearrangement of magnetic moments in the MnBi₂Te₄ SL leads to a net magnetization for the MnBi₂Te₄ film. As verified by our band structure calculations, reversing magnetic moments of the top MnBi₂Te₄ SL layer is indeed energetically favored by 30 to 40 meV (fig. S4). Subsequently, the system becomes a QAH state with an energy gap of 34 meV. As shown by the Wilson loop calculations, it exhibits a nontrivial CN = −1. Therefore, the sandwich configuration may always provide a QAH insulator for either odd or even numbers of MnBi₂Te₄ SLs.

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**Fig. 3. Electrically tunable band structure topology and the QAH effect.** (A) Band structure evolution of 3-SL-thick MnBi₂Te₄ as the electric field ($\epsilon$) increases. Two topological transitions occur at $\epsilon = 0.002$ at the $\Gamma$ point and 0.0141 V/Å along $\Gamma$–$K$ lines. (B) The Berry phase $\theta$, i.e., the Wannier charge center, accumulated along a Wilson loop ($k_1 \in [−\pi, \pi]$) as varying $k_2$. It is topologically equivalent to the edge state spectra. Corresponding CNs are one, zero, and three for $\epsilon = 0.000,0.004$ and 0.015 V/Å, respectively. (C) Corresponding Berry curvature ($\Omega$) distribution in the first Brillouin zone. The integration of $\Omega$ gives the CN (multiply by 2$\pi$).

**Fig. 4. Interface exchange field induced magnetic order and the QAH effect.** (A) Band structure of a 4-SL-thick MnBi₂Te₄ with a special magnetic order. When it was sandwiched between two CrI₃ layers, the AFM-type coupling between MnBi₂Te₄ layers are changed by the top CrI₃ layer, as illustrated in the inset. This band structure is calculated without CrI₃ layers, in the tight-binding scheme. The CrI₃-sandwiched DFT band structure can be found in fig. S4. (B) Corresponding Berry phase of the Wilson loop, with a CN = −1. (C) The Berry curvature distribution in the first Brillouin zone.
DISCUSSION
In summary, the magnetic order of MnBi$_2$Te$_4$ thin film can be pinned and also manipulated by a strong exchange bias in proximity to CrI$_3$. Thus, the heterostructures with MnBi$_2$Te$_4$ and CrI$_3$ provide an experimentally feasible platform to realize the QAHE effect. An external electric field can further modify the thin-film band structure and induce QAHE effect with large CNs. Since the magnetic insulator CrI$_3$ weakly disturbs the electronic states of MnBi$_2$Te$_4$, it can also be used to pin the surface magnetic order of the bulk MnBi$_2$Te$_4$ and assist the observation of the axion insulator phase ($16, 17$) in ARPES. In addition, it is worth noting that other magnetic insulators with out-of-plane magnetization, such as Tm$_2$Fe$_2$O$_{12}$ (TmIG) and Cr$_2$Ge$_2$Te$_6$, may also play the same role of exchange bias as CrI$_3$.

In the proof stage of our manuscript, we were aware of the recent experimental report on the zero-field QAHE effect in MnBi$_2$Te$_4$ thin layers ($41$).

METHODS

DFT calculations were performed using the Vienna ab initio simulation package ($40$), with core electrons represented by the projector augmented wave potential. The Perdew-Burke-Ernzerhof exchange-correlation functional with GGA + $U$ method was used in the DFT calculations. The parameter $U = 2.9$ and $3.0$ eV was chosen to describe the localized $d$ orbitals of Cr and Mn, respectively. Plane waves with a kinetic energy cutoff of $270$ eV were used as the basis set. Geometry optimization was carried out until the residual force on each atom was less than $0.01$ eV/$\AA$. The DFT-D3 correction ($d = 2.9$ and $3.0$ eV) was chosen to de-

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