Axion Insulator State with ferromagnetic ordering in CrI$_3$/Bi$_2$Se$_3$/MnBi$_2$Se$_4$ Heterostructure

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Abstract
Realizing axion insulator state with a uniform magnetization considerably facilitates experimental explorations of the intriguing topological magnetoelectric effect, a hallmark of three-dimensional (3D) topological insulators (TIs). Through density functional theory calculations and four-band model studies, we find that magnetic ions Cr$^{3+}$ in monolayer CrI$_3$ and Mn$^{2+}$ in septuple-layer MnBi$_2$Se$_4$ have opposite exchange couplings to the topological surface states of 3D TI Bi$_2$Se$_3$. As an exciting result of such opposite exchange couplings, axion insulator state is realized by a uniform magnetization in CrI$_3$/Bi$_2$Se$_3$/MnBi$_2$Se$_4$ heterostructure. Our work opens up opportunities for exploring topological magnetoelectric effect realized by the uniform magnetization induced axion insulator state in heterostructures of 3D TIs and two-dimensional van der Waals ferromagnetic insulators.

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The topological magnetoelectric (TME) effect is the hallmark response of three-dimensional (3D) topological insulators (TIs) to an electromagnetic field [1-7]. This effect is evoked by the topological term $\theta$ and shows up in the so-called axion insulators [5, 8-11]. Most strikingly, it is one of the topological quantization phenomena in units of the fundamental fine structure constant and manifests itself as mutual controls between magnetic and electric polarizations [5]. Hence, the TME effect has a significant impact on the fundamental physics and is promising for applications in spintronics and quantum information operations [4-7, 12, 13]. Current experimental observations of the TME effect are nevertheless rather elusive owing to the difficulty for finding suitable axion insulators. To date, experimental realization of the axion insulator state has been reported by only a handful cases, by doping 3D TI films with different magnetic elements on their two surfaces [9-11]. There are two challenges that seriously impede experimental progresses in realizing the TME effect in this way. The first is the need of extremely low critical temperature to reach the axion insulator state, primarily due to the ultra-small gap of the magnetized topological surface states (TSSs) of randomly doped 3D TIs [9-11, 14]. The second is the requirement of an antiparallel alignment between magnetizations at the top and bottom surfaces of the TI films, which can only be maintained in a sizable magnetic field [9-11].

In principle, the TME effect should be more easily observable in axion insulators that are produced by putting two-dimensional (2D) van der Waals (vdW) ferromagnetic (FM) insulators (Fig. 1a) on 3D TIs. The magnetization for TSS is more uniform via the proximity effect and hence the band gap is typically very large, as found in both theory and experiments [15, 16]. As 2D vdW FM insulators such as CrI$_3$ monolayer (ML) can have high Curie temperatures [17], it is conceivable that the TME effect can be observed in more practical conditions. Furthermore, by carefully selecting 3D TIs and 2D vdW FM insulators, it is possible to achieve uniform magnetization induced axion insulators. In such axion insulator, the TME effect can be observed in either very low or very high magnetic field (Fig. 1b). So a large TME signal can be obtained in experiments because it is proportional to the external magnetic field [5]. Therefore, it is appealing to explore
uniform magnetization induced axion insulator state in potential heterostructures of 3D TIs and 2D vdW FM insulators that gives robust TME effects.

In this letter, we report results of systematic studies based on the density functional theory (DFT) calculations and furthermore on the effective four-band model analyses. We demonstrate the possibility of realizing the uniform magnetized induced axion insulator state in CrI$_3$/Bi$_2$Se$_3$/MnBi$_2$Se$_4$ heterostructure. Interestingly, Cr$^{3+}$ ions in CrI$_3$ ML and Mn$^{2+}$ ions in septuple-layer (SL) MnBi$_2$Se$_4$ (MBS) have opposite exchange couplings to the TSSs of the prototypical 3D TI Bi$_2$Se$_3$ (BS), even when their magnetizations are parallel to each other. This allows the establishment of the axion insulator state in a broad range of magnetic field. Our work indicates that CrI$_3$/BS/MBS heterostructure is very promising for being used in nanodevices for operations based on the TME effect.

Our DFT calculations are carried out using the Vienna Ab initio Simulation Package (VASP) at the level of the generalized gradient approximation [18-21]. We utilize the projector-augmented wave pseudopotentials [21-23]. An energy cutoff of 500 eV is adopted for the plane-wave basis expansion. The LSDA+U method [24] is used to take into consideration the strong correlation effect of Cr and Mn 3$d$ electrons. For Cr, the on-site Coulomb interaction $U$ is $U_{\text{Cr}}=3.0$ eV and the Hund exchange interaction is $J^H_{\text{Cr}}=0.9$ eV [25]; for Mn, $U_{\text{Mn}}=6.0$ eV and $J^H_{\text{Mn}}=1.0$ eV [26]. For heterostructures of CrI$_3$/BS/CrI$_3$ and MBS/BS/MBS and CrI$_3$/BS/MBS, the BS film has ten quintuple layers (QLs). At the CrI$_3$/BS interface, Cr atoms sit on the top of Se anions [25]. At the MBS/BS interface, we use the atom alignment as in Ref. [15, 27]. A 12 Å vacuum space is inserted between adjacent slabs in all heterostructures. The nonlocal vdW functional (optB86b-vdW) [28, 29] is included in calculations. The z-axis is perpendicular to the BS slab and x- and y-axis are in its surface plane.

To explore the uniform magnetization induced axion insulator state, we study the low-energy electronic properties of the heterostructure of a 3D TI film and two 2D vdW FM insulators (Fig. 1a, denoted as FM-t/TI/FM-b) by means of a four-band model. This four-
band model includes the TSSs ($H_{\text{surf}}$) of the 3D TI film, exchange field ($H_{\text{Zeeman}}$) and interfacial potential ($H_{\text{interface}}$) [5, 6, 9-11]. The latter two result from the presence of the two 2D vdW FM insulators. With the basis of $\{|t, \uparrow\}, |t, \downarrow\}, |b, \uparrow\}, |b, \downarrow\}$, this four-band model [30-33] is written as follows:

$$H\left(k_x, k_y\right) = H_{\text{surf}}\left(k_x, k_y\right) + H_{\text{Zeeman}}\left(k_x, k_y\right) + H_{\text{interface}}\left(k_x, k_y\right)$$

$$= A k^2 + \begin{bmatrix} v_F \left(-k_x \sigma_x + k_y \sigma_y\right) & 0 \\ 0 & v_F \left(-k_y \sigma_y + k_x \sigma_x\right) \end{bmatrix} \begin{bmatrix} \Delta_t \sigma_z & 0 \\ 0 & \Delta_b \sigma_z \end{bmatrix} + \begin{bmatrix} V \sigma_0 & 0 \\ 0 & -V \sigma_0 \end{bmatrix}$$

In Eq. (1), spin up (down) state is represented by $\uparrow$ ($\downarrow$); top (bottom) surface is denoted by $t$ ($b$); $v_F$ is the Fermi velocity; $k_x, k_y$ and $k^2 = k_x^2 + k_y^2$ are wave vectors in the surface plane; $\Delta_t$ and $\Delta_b$ are exchange fields sensed by the top and bottom TSSs; $\sigma_{x,y,z}$ and $\sigma_0$ are Pauli and 2-by-2 unit matrices, respectively. Inversion asymmetry potential $2V$, due to the structure inversion asymmetry, is the potential difference between the top and bottom surfaces of the 3D TI film [30, 34-36]. Here the 3D TI film is assumed to be thick enough so that the hybridization between the top and bottom TSSs is excluded to obtain the quantized TME effect [5, 6]. By studying this mode at length, we gain two key guidances to the appearance of the uniform magnetization induced axion insulator.

Figure 1 (color online) (a) Illustration of FM-t/TI/FM-b heterostructure with opposite exchange couplings $J_t$ and $J_b$. $H_{tc}$ and $H_{bc}$ are the coercive fields of the top and bottom 2D vdW FM insulators, respectively. (b) External field dependence of the presence of the uniform magnetization induced axion insulator state (zero Hall conductivity $\sigma_{xy}$) in FM-t/TI/FM-b heterostructure. The blue and red arrows indicate the magnetization directions of the top and bottom 2D vdW FM insulators, respectively. (c) Phase diagram of the four-band model Eq. (1). IAP is short for inversion asymmetry potential.
Opposite exchange fields $\Delta_t$ and $\Delta_b$, i.e., $\Delta_t\Delta_b < 0$, is necessary to the formation of axion insulator state in the FM-$t$/TI/FM-$b$ heterostructure [5, 6, 30]. Phenomenologically, exchange field $\Delta$ is determined as $\Delta = J m_z$ [7, 37-39], where $J$ is the intrinsic exchange coupling between TSSs and magnetic ions of the 2D vdW FM insulator and $m_z$ is the extrinsic magnetization of the 2D vdW FM insulator that points perpendicular to the top/bottom surface of the 3D TI film. When $J_t$ and $J_b$ have opposite signs (Fig. 1a), a uniform magnetization of the top and bottom 2D vdW FM insulators, i.e., $m'_t = m'_b$, leads to $\Delta_t\Delta_b < 0$. Therefore, the first guidance is to find two different 2D vdW FM insulators whose magnetic ions have opposite exchange couplings to the TSSs. Obviously, two identical 2D vdW FM insulators cannot give birth to the uniform magnetization induced axion insulator state in FM-$t$/TI/FM-$b$ heterostructure, because $J_t$ and $J_b$ are inherently same in this case.

Since the two 2D vdW FM insulators are required to be different, there exists an inherent structure inversion asymmetry producing a nonvanishing inversion asymmetry potential $2V$. Now we elucidate its effect on the bands. According to the four-band model Eq. (1), we obtain the band dispersions as follows:

$$\varepsilon_t^+ (k_x, k_y) = A k^2 \pm \sqrt{\Delta_t^2 + \nu_1^2 k^2} + V$$

$$\varepsilon_b^+ (k_x, k_y) = A k^2 \pm \sqrt{\Delta_b^2 + \nu_1^2 k^2} - V$$

Eq. (2) and (3) indicate that $V$ shifts the bands of the top and bottom surfaces in opposite ways; for example, when $V$ is positive, the top-surface bands are shifted upward while the bottom-surface bands are shifted downward. Through such shift, the inversion asymmetry potential $2V$ has a decisive effect on the occurrence of axion insulator state. When $2|V|$ is smaller and larger than the critical point $|\Delta_t| + |\Delta_b|$, FM-$t$/TI/FM-$b$ heterostructure is in the phases of axion insulator and metal, respectively (Fig. 1c). Besides, the gap of the axion insulator is linearly reduced when $2|V| > |\Delta_t| - |\Delta_b|$. So the second guidance is to select 2D vdW FM insulators that open a large gap (namely large exchange field $\Delta$) at the TSSs so as to prevent FM-$t$/TI/FM-$b$ heterostructure from becoming metallic.
Armed with these two guidances, we choose 2D vdW FM insulators ML CrI$_3$ and SL MBS and 3D TI BS. It has been demonstrated that ML CrI$_3$ induces a sizable nontrivial gap into the TSSs of BS film without any detrimental effect to their transport properties [25]. A recent experiment has already observed those: (I) the TSSs of BS film is opened a large gap by the FM SL MBS; (II) the ferromagnetism at MBS/BS interface persists up to room temperature [15]. As already pointed out, the large gap at the TSSs is exactly desired. Besides, the room-temperature ferromagnetism at the MBS/BS interface is really beneficial to observe axion insulator state in more practical conditions. Lastly and importantly, there is a high possibility that magnetic ions Cr$^{3+}$ and Mn$^{2+}$ have opposite exchange couplings to the TSSs of BS film, because they have different electronic configurations, i.e., $t_{2g}^{3e} e_{g}^{0d}$ in the former and $t_{2g}^{3e} e_{g}^{0d}$ in the latter.

![Figure 2 (color online) Band structures of (a) CrI$_3$/BS/CrI$_3$ and (b) MBS/BS/MBS. In (a) and (b), right insets sketch the magnetization configurations and left insets show the spin-projected bands near the Fermi level. Spin weights are indicated by the color bar.](image)

We first acquire the exchange coupling parameter $J_{Cr}$ between the TSSs of BS and magnetic ions Cr$^{3+}$ of ML CrI$_3$. To this end, we calculate the band structure of CrI$_3$/BS/CrI$_3$ in the case of $m_{Cr}>0$, namely, the magnetizations of ML CrI$_3$ pointing at the positive direction of $z$ axis (left inset in Fig. 2a). From the band structure as shown in Fig. 2a, one observes that the TSSs of BS is magnetized by ML CrI$_3$ and thus a gap of 5.6
meV opens at the $\Gamma$ point. Projecting the bands to the spin-up and spin-down channels (right inset in Fig. 2a) indicates that valence band tops have spin-down components while conduction band bottoms have spin-up components. This reveals exchange field $\Delta_{\text{Cr}} > 0$. Combining $\Delta_{\text{Cr}} = J_{\text{Cr}} m_{\text{Cr}}$ and $m_{\text{Cr}} > 0$, we obtain a positive $J_{\text{Cr}}$.

Fig. 2b shows the band structure of MBS/BS/MBS in the case of $m_{\text{Mn}} > 0$, i.e., the magnetizations of SL MBS pointing at the positive direction of $z$ axis (left inset of Fig. 2b). In consistent with previous studies [15], SL MBS magnetizes the TSSs of BS and opens a large gap of 52.2 meV at the $\Gamma$ point. From the spin projections (right inset in Fig. 2b), we see that valence band tops have spin-up components whereas conduction band bottoms have spin-down components, suggesting exchange field $\Delta_{\text{Mn}} < 0$. According to $\Delta_{\text{Mn}} = J_{\text{Mn}} m_{\text{Mn}}$ and $m_{\text{Mn}} > 0$, we obtain a negative $J_{\text{Mn}}$. Hence, as expected, magnetic ions Cr$^{2+}$ of ML CrI$_3$ and Mn$^{2+}$ of SL MBS have opposite negative exchange couplings to the TSSs of BS.

Now that the desired opposite exchange couplings $J_{\text{Cr}}$ and $J_{\text{Mn}}$ have been confirmed, we assemble ML CrI$_3$, BS film and SL MBS into a sandwich heterostructure and investigate the possibility of realizing the uniform magnetization induced axion insulator state. The magnetizations of ML CrI$_3$ and SL MBS are set to be along the same direction, i.e., along the positive direction of $z$ axis (left inset in Fig. 3a). The band structure shown in Fig. 3a indicates that CrI$_3$/BS/MBS is an insulating with a sizable gap of 6.4 meV. Through resolving the bands to the top and bottom QLs of BS, we observe that the magnetized top-surface TSSs well separate from the magnetized bottom-surface TSSs (Fig. 3b). The left inset of Fig. 3a and Fig. 3b suggest the spin components of the top- and bottom-surface TSSs around the $\Gamma$ point. As desired, the top- and bottom-surface TSSs sense opposite exchange fields, i.e., $\Delta_t \Delta_b < 0$.

To examine if the above-mentioned insulator state in CrI$_3$/BS/MBS is axion insulator state, we fit its band structure using the four-band model Eq. (1) (see Fig. S1 in Supplementary Material (SM)) [40]. The fitted top and bottom exchange fields are
Δₜ = 3.2 meV and Δₓ = -27.6 meV, respectively. Besides, the inversion asymmetry potential 2|V| induced by the two different 2D vdW FM insulators ML CrI₃ and SL MBS is fitted to be 2|V| = 19.4 meV. Based on these fitted parameters, we have \( |Δₓ| - |Δₜ| > 2|V| \).

So the asymmetric interface potential 2V has no any effect on the topological properties of CrI₃/BS/MBS. By integrating the Berry curvatures of the occupied bands in the Brillouin zone, we obtain that the top- and bottom-surface Chern numbers are \( C_N^t = 1/2 \) and \( C_N^b = -1/2 \), respectively. That is to say, the top and bottom surfaces have opposite half-quantum Hall conductances \( σ_{xy}^t = e^2/2h \) and \( σ_{xy}^b = -e^2/2h \), respectively. This is the direct signature of axion insulator state in CrI₃/BS/MBS. Taking this opposite half-quantum Hall conductances and the uniform magnetizations as shown in inset of Fig. 3a together, we come to a conclusion that the uniform magnetization induced axion insulator state can indeed be realized in CrI₃/BS/MBS.

The uniform magnetization induced axion insulator state in CrI₃/BS/MBS is very robust against the choice of the on-site Coulomb interaction \( U_{Cr} \) of Cr³⁺ and \( U_{Mn} \) of Mn²⁺. As

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**Figure 3 (color online)** (a) Band structure of the uniform magnetization induced axion insulator state in CrI₃/BS/MBS. Left inset sketches the uniform magnetization. The spin-projected four bands near the Fermi level are shown in the right inset. Color bar indicates the spin-projected weights. (b) Top-QL-BS (blue) and bottom-QL-BS (red) projected bands. (c) Berry curvatures \( Ω \) of the occupied magnetized TSSs of top (up panel) and bottom (bottom panel) surfaces.
shown in Fig. 4a, as $U_{Cr}$ changes, exchange field $\Delta_{Cr}$ in CrI$_3$/BS/CrI$_3$ remains positive even though its magnitude varies slightly. This indicates that exchange coupling $J_{Cr}$ is positive and its sign is not changed by $U_{Cr}$. Besides, the $U_{Mn}$ dependence of exchange field $\Delta_{Mn}$ in MBS/BS/MBS (Fig. 4b) clearly shows that exchange coupling $J_{Mn}$ keeps negative in a large range of $U_{Mn}$. Most importantly, the uniform magnetization induced axion insulator state appears in CrI$_3$/BS/MBS independently on the choice of $U_{Cr}$ and $U_{Mn}$ and it has a sizable gap in order of several meV (Fig. 4c and Fig. S2, S3, S4 in SM). This demonstrates that the uniform magnetization induced axion insulator state in CrI$_3$/BS/MBS is robust and should be easily observed in experiments.

**Figure 4 (color online)** (a) $U_{Cr}$ dependence of exchange field $\Delta_{Cr}$ in CrI$_3$/BS/CrI$_3$. (b) $U_{Mn}$ dependence of exchange field $\Delta_{Mn}$ in MBS/BS/MBS. (c) Dependence of the band gap of the uniform magnetization induced axion insulator state on $U_{Cr}$ and $U_{Mn}$ in CrI$_3$/BS/MBS.

To summarize, we demonstrate based on a four-band model study and systematic DFT calculations that CrI$_3$/Bi$_2$Se$_3$/MBS heterostructure displays the uniform magnetization induced axion insulator state. This attractive axion insulator state arises from the fact that the TSSs of BS interact with magnetic ions Cr$^{3+}$ of ML CrI$_3$ and Mn$^{2+}$ of SL MBS via opposite exchange couplings. From an experiments perspective, it is feasible to fabricate CrI$_3$/BS/MBS. Cl$_3$/BS can be mechanically assembled thanks to the vdW-type structure of CrI$_3$ and BS [41, 42]. BS/MBS has been successfully synthesized [15] and can be also grown by molecular beam epitaxy [43]. Moreover, it is encouraging that the critical temperature of axion insulator state in CrI$_3$/BS/MBS could be high up to a few tens Kelvins, because its gap is in order of 6 meV which corresponds to 70 K and is higher.
than the Curie temperature 45 K of ML CrI$_3$ [17]. We believe that our findings could stimulate experimental and theoretical investigations of the easily observable TME effect that is produced by the uniform magnetization induced axion insulator state in heterostructures of 3D TIs and 2D vdW FM insulators.

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