Topological phases in Iridium oxide superlattices: quantized anomalous charge or valley Hall insulators

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We study topological phases in Iridium (Ir) oxide superlattices of orthorhombic perovskite-type grown along the [001] crystallographic axis. Due to strong spin-orbit coupling of Ir 5d-orbitals and electronic correlation effects, Ir oxide bilayer superlattices display topological magnetic insulators exhibiting quantized anomalous Hall effects. Depending on stacking of two layers, we also found a valley Hall insulator with counter-propagating edge currents from two different valleys and a topological crystalline insulator with edge states protected by the crystal lattice symmetry. In a single layer Ir oxide superlattice, a topological insulator can be achieved, when a strain field is applied to break the symmetry of a glide plane protecting the Dirac points. In the presence of a magnetic ordering or in-plane magnetic field, it turns into a topological magnetic insulator. We discuss essential ingredients for these topological phases and experimental signatures to test our theoretical proposals.

I. INTRODUCTION

Considerable attention has been recently devoted to investigations of non-trivial physics arising from strong spin-orbit coupling (SOC). Such studies were initiated by theoretical proposals of topological insulators with conducting surface states protected by time reversal (TR) symmetry\textsuperscript{11,12} which was then experimentally confirmed in two-dimensional (2D) HgTe/Hg$_{1-x}$Cd$_x$Te quantum wells\textsuperscript{13,14} and indirectly by angle resolved photoemission spectroscopy (ARPES) in three dimensional (3D) systems such as Bi$_{1−x}$Sb\textsubscript{$x$} \textsuperscript{15,16} Bi$_2$Se\textsubscript{$x$} \textsubscript{$y$} \textsubscript{$z$} Bi$_2$Te\textsubscript{$x$} \textsubscript{$y$} \textsubscript{$z$} Since then, different types of topological phases have been theoretically suggested. These include topological crystalline insulators with surface states protected by crystal lattice symmetry\textsuperscript{17,18} Weyl semimetals with chiral fermions\textsuperscript{19,20} and topological magnetic insulators with quantized anomalous Hall (QAH) effects\textsuperscript{21,22}. Furthermore, strongly interacting systems could provide a new avenue to explore more exotic phases such as topological Mott insulators and fractional Chern insulators\textsuperscript{23,24}.

While the number of topological phases in this theoretical list is still growing, experimental confirmations of topological phases are limited to the above systems of groups IV-VI elements. Why such topological insulators have not been detected in other materials such as oxides, despite that oxides are most abundant in nature because oxygen form stable chemical bonds with almost all elements to give the corresponding oxides? In particular, transition metal oxides exhibit various collective phenomena stemming from strong electronic correlations, and tremendous interests and efforts in growing oxide films have been made to find new functionalities. However, the focus on transition metal oxides so far has been mainly 3d- and 4d-orbital systems with weak or moderate SOC, and little attention has been paid to 5d-orbital systems with strong SOC until recently. Among 5d-orbital systems, Ir oxides named Iridates have provided an excellent playground to study the combined effects of SOC and electron correlations. Depending on the underlying lattice structure, Iridates have offered a rich phase diagram\textsuperscript{25}. Despite various different phases, one common ingredient is that $J_{\text{eff}} = \frac{1}{2}$ description due to a strong atomic SOC is a good starting point in building microscopic Hamiltonians. Using $J_{\text{eff}} = \frac{1}{2}$ wavefunction, a topological insulator was proposed in 3D perovskite Iridates\textsuperscript{26}. It was found that a bulk SrIrO$_3$ with P$_{bnm}$ structure exhibits a topological nodal line protected by the lattice symmetry which becomes a 3D nodal point when the mirror symmetry along the c-axis is broken. It becomes a topological insulator, when the mirror breaking term further increases\textsuperscript{27}. A successful growing of Ir oxide superlattice, [(SrIrO$_3$)$_n$SrTiO$_3$] where the integer $n$ controls the number of Ir oxide layers using pulsed laser deposition (PLD) technique has been also reported\textsuperscript{28}. It has demonstrated how a spin-orbit magnetic insulator arises by tuning the number of layers between SrIrO$_3$ and SrTiO$_3$.

Given that SrIrO$_3$ with P$_{bnm}$ structure possesses a topological nodal line, it is possible to design other topological phases by employing the current experimental techniques. While a topological insulator was proposed in an effective honeycomb bilayer by fabricating [111] superlattice structure from perovskite oxides\textsuperscript{29} atomically controlled [111] superlattice of perovskite oxides is known extremely difficult to be fabricated. On the other hand, Ir oxide superlattice grown along the [001] axis has been successfully made by J. Matsuno et al.\textsuperscript{30} as stated above. In this paper, we show how to realize topological phases in Ir oxide superlattices grown along the [001] axis; [(SrIrO$_3$)$_n$ (AMO)$_m$] for integer $n'$ and $n = 1$ or 2 where AMO$_3$ is a band insulator with closed shell of transition metal $M^{4+}$ and an alkaline earth metal $A^{2+}$. To achieve topological phases, one has to retain oxygen octahedra rotation and tilting which is necessary to generate a Rashba-like SOC in $J_{\text{eff}} = \frac{1}{2}$ basis. Thus AMO$_3$ should have the orthorhombic P$_{bnm}$ structure such as CaTiO$_3$, CaMoO$_3$, CaRuO$_3$.
II. SINGLE-LAYER IRIDATES

A. Model Hamiltonian and Dirac fermion

In bulk samples AMO$_3$ with P$_{bnm}$ structure, each M atom surrounded with six O atoms forms an octahedron. This octahedron has the rotation $\theta$ around c-axis and tilting $\phi$ along the local (110) direction as shown in Fig. 1. The rotation and tilting angles alternate between two neighboring IrO$_6$ octahedra in the plane and between adjacent layers making four M atoms in a unit cell. To engineer a single-layer Ir oxide, IrO$_2$ layer is grown from AMO$_3$ as shown in Fig. 1. $x$- and $y$-directions are rotated by 45° degree from the crystal $a$- and $b$-axis for convenience. As we stated above, the alternating rotation and tilting of neighboring IrO$_6$ is crucial to realize topological phases for the following reason. The relatively strong SOC of Ir atoms splits $t_{2g}$ states into $J_{\text{eff}} = \frac{1}{2}$ and $J_{\text{eff}} = \frac{3}{2}$, and Ir$^{4+}$ ionic configuration leading to the valence of 5$d^5$ makes these iridates to be a half-filled $J_{\text{eff}} = \frac{1}{2}$ band. Note that $J_{\text{eff}} = \frac{1}{2}$ consists of $|J_z = \pm \frac{1}{2}\rangle = \frac{1}{\sqrt{3}}(|d_{xy,s} \pm (d_{yz,-s} + i|d_{xz,-s}|)\rangle$ where $s$ represents spin-$1/2$ up and down states, respectively. In the presence of the alternating tilting and rotation between neighboring sites, a hopping integral between $d_{xy,s}$ and $d_{xz/yz,s}$ orbitals becomes finite. Since $d_{xy,s}$ and $d_{xz/yz,s}$ belong to different spin states of $|J_z\rangle$, this hopping involves $|J_z = \frac{1}{2}\rangle$ and $|J_z = -\frac{1}{2}\rangle$ states which then generates a spin-flip Rashba-like term.

For a single layer of IrO$_2$, there are two sites due to different rotation ($\theta$) and tilting angle ($\phi$) between nearest-neighbor sites. We denote these Ir sites A and B indicating different oxygen environments as shown in Fig. 1. It has a rectangle structure associated with a glide symmetry plane which corresponds to the invariance under a 1/2 translation along a certain direction, and reflection afterwards. In this lattice, it is along b-axis and thus named the b-glide. The effect of this glide plane on $t_{2g}$ orbitals is to interchange $d_{xy}$ orbital with $d_{xz}$ orbital and exchange A site with B site. Introducing the Pauli matrices $\gamma$ and $\sigma$ for the sublattice A and B, and $J_{\text{eff}} = 1/2$ pseudospin, respectively, this b-glide symmetry plane is expressed as

$$\hat{\Pi}_b = \frac{i}{\sqrt{2}}(\sigma_x - \sigma_y)\tau_b \hat{k}_{bg},$$  \hspace{1cm} (1)

where $\hat{k}_{bg}$ are the operators acting on crystal momentum space as $\hat{k}_{bg} : (k_x, k_y) \rightarrow (k_y, k_x)$.

A tight-binding model can be constructed from $J_{\text{eff}} = 1/2$ bands with the basis $(A \uparrow, B \uparrow, A \downarrow, B \downarrow)$ where A and B denotes two different Ir sites in the unit cell as discussed above, and $(\uparrow, \downarrow)$ represents $J_z = \pm \frac{1}{2}$. Taking into account the nearest and next-nearest hoppings, the Hamiltonian is given by

$$H_0(k) = \epsilon_0(k)\tau_x + \epsilon'(k)\mathbf{I} + \epsilon_1d(k)\sigma_z\tau_y + \epsilon_y(k)\sigma_y\tau_y + \epsilon_x(k)\sigma_x\tau_y,$$  \hspace{1cm} (2)
FIG. 2. (color online) Band dispersion of single layer Ir oxide (a) without tilting $\phi$. It shows four fold degeneracy along $S = (\pi, 0) \rightarrow X = (\frac{\pi}{2}, -\frac{\pi}{2})$ direction. (b) Finite rotation and tilting leaves two Dirac points at $X$ and $Y = (\frac{\pi}{2}, \frac{\pi}{2})$. (c) When the b-glide symmetry is broken, Dirac point acquires a finite gap at $X$ and $Y$ points.

where

$$
\epsilon_{0/d}(k) = 2t_{0/d}(\cos(k_x) + \cos(k_y)),
$$

$$
\epsilon_{y/x}(k) = t_1 \cos(k_{x/y}) + t_2 \cos(k_{x/y}),
$$

$$
\epsilon'(k) = \lambda + t' \cos(k_x) \cos(k_y). \tag{3}
$$

Here $t_0$ is the nearest neighbor (NN) intra-orbital hopping and $t_{1d}$ is the NN hopping between $d_{yz}$ and $d_{xz}$ orbitals. $\lambda$ is the strength of the SOC and $t'$ is the next-nearest neighbor (NNN) intra-orbital hopping. $t_1$ and $t_2$ are the NN hopping from $d_{yz}$ and $d_{xz}$ orbitals to $d_{xy}$ orbital, respectively. $t_{1d}$ and $t_2$ vanish without the rotation and tilting of octahedra. The hopping parameters are obtained based on Slater-Koster method and the parameters are functions of $\theta$ and $\phi$. For example, they are given by $(t', t_0, t_{1d}, t_1, t_2)/t = (-0.3, -0.6, -0.15, 0.15, 0.45)$ when $(\theta, \phi) \approx (7^\circ, 19^\circ)$, where $t$ is the $\pi$-bonding between $d$-orbitals $t_{dd\pi}$, and we set $t_{dd\pi}$ : $t_{dd\sigma}$ : $t_{dd\delta} = 1 : 3 \frac{1}{2} : 1$.

The band structure is shown in Fig. 2. Without the tilting angle $\phi$, two bands are degenerate along $X = (\frac{\pi}{2}, -\frac{\pi}{2})$ to $S = (\pi, 0)$ as shown in Fig. 2(a). However, when both the rotation and tilting of octahedra are present, this degeneracy is broken, and there are two Dirac points at $X$ and $Y$ protected by the b-glide symmetry as shown in Fig. 2(b). The Dirac point may appear below the Fermi energy $E_F$ when the tilting angle $\phi$ is not significant. Indirect hopping via oxygen can change the strength of hopping parameters as well, but the topological nature of phases described here is not altered by such qualitative changes. When the b-glide symmetry is broken, for example by a strain field along $x$-direction, these Dirac points are gapped as shown in Fig. 2(c). In the following subsection, we discuss the topological nature of this insulator by providing the corresponding Chern numbers and edge state analysis.

B. Topological Insulator and quantized anomalous Hall effects

Since the Dirac points are protected by the b-glide symmetry, any small perturbation that breaks the b-glide symmetry opens a gap at these two Dirac points. The b-glide operator is given by Eq. (1), and thus a small strain along $x$ (or $y$)-direction is sufficient. Such a broken b-glide symmetry term allows additional NNN and third NN hoppings as follows.

$$
\epsilon_{2n}(k) = (t_{2n} \cos(k_x + k_y) + t'_{2n} \cos(k_x - k_y))\tau_z,
$$

$$
\epsilon_{3n}(k) = 2t_{3n} \cos(2k_x) - \beta \cos(2k_y))\tau_z, \tag{4}
$$

where $t_{2n}$ and $t_{3n}$ are the NNN intra-orbital hopping. $t_{3n}$ is the third NN intra-orbital hopping, and $\beta$ is the parameter to measure the strength of a broken b-glide term. The tight-binding parameters $(t_{2n}, t'_{2n}, t_{3n}) = (0.098, -0.1, 0.06)$ obtained by Slater-Koster using the same angles of $\phi$ and $\theta$ as above, and $\beta = 0.6$ lead to the band dispersion shown in Fig. 2(c).

The non-trivial topology behind the gapped Dirac point can be revealed through the following edge state calculation. The slab computation has been performed in a zigzag slab geometry which is periodic along $b = \frac{\pi + y}{2}$ and has an open boundary along $a = \frac{\pi - y}{2}$. Along $a$ direction, it has one boundary edge ($L = 0$) terminates at atom A but the other boundary ($L = N$) ends with atom B. When there is no TR broken term exists, the system shows gapless edge modes propagating from valence band to conduction band as shown in Fig. 3(a). These two gapless edge states cross at a time reversal invariant momentum (TRIM) point indicating its protection by the TR symmetry. As long as TR symmetry is present, the degeneracy can not be lifted by disorders or weak interactions. Indeed, we have checked that the edge states are robust, even in the presence of a random sublattice potential. $Z_2$ index is another way to confirm the topological insulator. It is straightforward to compute the eigenvalues of inversion operator. The result shows that $Z_2$ index $= 1$ consistent with the edge state calculation.

Another effect of strong SOC in Iridates is an amplification of electronic correlation leading to a spin-orbit Mott insulator. The relevant bandwidth $W$ is $J_{e\text{ff}} = \frac{1}{2}$ band rather than the full $t_{2g}$ band due to the SOC, and thus the ratio of Hubbard interaction $U$ and the bandwidth $W$ is signified in Iridates. Taking into account the electronic correlations and the broken inversion symmetry on the bond between neighboring Ir and Ir atoms, Ir oxides exhibit non-collinear magnetic orderings at low temperatures, where the ordering temperature is set by the Dzyaloshinskii-Moriya (DM) interaction in $J_{e\text{ff}} = 1/2$.
spin, as it breaks the SU(2) spin rotational symmetry. Thus we consider the following form of magnetic ordering:

\[ m_{(010)} \sigma_y \tau_z + m_{(100)} \sigma_x, \]

(5)

where \( m_{(010)} \) represents the sublattice antiferromagnetic ordering, while \( m_{(100)} \) a ferromagnetic component of ordering.

In the absence of TR, the topological invariance characterizing the QAH effects is identified by charge Chern number defined as,

\[ C_p = \frac{1}{2\pi} \int d^2k \Omega_z^p(k), \]

(6)

where \( p \) is the band index and \( \Omega_z^p(k) \) is z-component of \( p \)-th band Berry curvature \( \Omega^p(k) \) given in the Appendix.

The quantized transverse Hall conductance \( \sigma_{xy} \) is then given by

\[ \sigma_{xy} = \frac{e^2}{h} \sum_{p \in \text{occupied}} C_p, \]

(7)

where the sum goes over all occupied bands below Fermi energy \( \epsilon_F \). For the single layer 2D Ir oxide, the quantized Hall conductivity is obtained as

\[ \sigma_{xy} = \frac{e^2}{h}, \]

(8)

indicating the topological invariance \( C \equiv \sum_{p \in \text{occupied}} C_p = 1 \) related to edge currents propagating one direction along the sample boundary, as shown in Fig. 3(b). Since the above result is also valid for any in-plane Zeeman magnetic field, it can be tested under an external magnetic field for temperatures above the magnetic ordering temperature.

III. BILAYER IRIDATES

To achieve the topological phases in the single layer IrO\(_2\) layer, the b-glide symmetry should be externally broken. This requires a strain field in a certain direction, which is not trivial in an experimental setting. In this section, we propose two types of bilayer IrO\(_2\) systems, which naturally hold topological phases without a lattice symmetry breaking perturbation. Since the single IrO\(_2\) layer has two different sets of rotation and tilting angles, one way to engineer bilayer systems is to stack two layers of \( A \) and \( B \) on top of each other. Note that \( A \) and \( B \) per unit cell have the rotation and tilting degree \( (\theta, \phi) \) and \( (-\theta, -\phi) \), respectively. However, the other way to stack two single layers is to make the second layer has different rotation and tilting set such as \( (\theta, -\phi) \) and \( (-\theta, \phi) \) denoted by \( C \) and \( D \) sites, respectively. We call the first case ABAB stacking and the other ABCD stacking: see Fig. 4. The distance between top and bottom layers in both cases can be manipulated by the number of AMO\(_3\) layers in between, and the nature of topological phases are not altered by such quantitative changes. Let us consider the ABAB stacking case first.

A. ABAB stacking

As presented in Fig. 4, the ABAB bilayer structure with significant rotation and tilting can be achieved by inserting one layer band insulator material MO\(_2\) (\( M=\text{Zr, Hf} \)) between two IrO\(_2\) layers. The tight-binding Hamiltonian is given by

\[ H_{ABAB}(k) = \sum_{i=1,2} H_i^0(k) + H_{12}(k), \]

(9)
\[ H_{12}(k) = \epsilon_{di}(k)\nu_x + \text{Re}(\epsilon_{dz}(k))\sigma_y\tau_y\nu_x + \text{Im}(\epsilon_{dz}(k))\sigma_z\tau_y\nu_y + \text{Re}(\epsilon_z(k))\sigma_y\nu_y + \text{Im}(\epsilon_z(k))\sigma_z\nu_y, \]

where

\[ \epsilon_{di}(k) = t_z + t_{(110)}\cos(k_x + k_y) + t_{(110)}\cos(k_x - k_y), \]

\[ \epsilon_{dz}(k) = t_{dz}(\cos(k_x + \cos(k_y)) + it_{dz}'(\sin(k_x) + \sin(k_y))), \]

\[ \epsilon_z(k) = (t_{2z} + \cos(k_y)) + t_{1z} + \cos(k_x) + i(k_x \leftrightarrow k_y), \]

\[ \epsilon_z'(k) = (t_{2z}'\sin(k_y) + t_{1z}'\sin(k_x)) + i(k_x \leftrightarrow k_y), \]

where \( t_z \) is the NN hopping between two layers. \( t_{(110)} \) and \( t_{dz} \) are the third NN intra-orbital hopping along \( (110) \) and \( (110) \), respectively. \( t_{dz} \) and \( t_{dz}' \) arises from \( d_{yz} \) orbital to \( d_{xy} \) orbital NNN hopping due to the rotation and tilting angles. \( t_{2z} \) and \( t_{1z} \) are obtained based on Slater-Koster Method and

\[ (t_z, t_{(110)}, t_{dz}, t_{dz}', t_{2z}, t_{1z}, t_{2z}', t_{1z}')/t = (-0.13, -0.01, -0.09, -0.03, -0.01, 0.014, 0.01, 0.062, 0.01) \]

for the same \( \theta \) and \( \phi \) used in the single layer. The band structure in Fig. 5(a) shows that there are two line nodes around \( X \) and \( Y \) when \( \phi = 0 \). However, a finite tilting \( \phi \) lifts the band degeneracy, but keeps one pair of Dirac points along the high symmetry line \( X \rightarrow S \) which is protected by the b-glide symmetry in Fig. 5(b).

Due to the electronic correlation, a magnetic ordering occurs which breaks the TR symmetry. A non-collinear magnetic ordering is expected due to the DM interaction on the Ir-Ir bond. One example of non-collinear ordering has the form

\[ m_{(110)}(\sigma_x + \sigma_y) + m_{(110)}(\sigma_z - \sigma_y)\tau_z, \]

where antiferromagnetic ordering is assumed to be along \( (110) \) and ferromagnetic component along \( (110) \). Since the exact direction of magnetic ordering is not important for the topological nature, we computed the Hall conductivity for (a) \( m_{(110)} \neq 0 \) and (b) \( m_{(110)} \neq 0 \) cases.
The crystal structure with ABCD stacking is displayed in Fig. 6(a). The tight-binding Hamiltonian for this stacking is given by

\[ H_{ABCD}(\mathbf{k}) = \sum_{i=\pm} H^i_0(\mathbf{k}) + H^i_{12}(\mathbf{k}), \]

where

\[ H^i_0(\mathbf{k}) = \epsilon^i(\mathbf{k}) \mathbf{I} + \epsilon_0(\mathbf{k}) \tau_z + \epsilon_{1d}(\mathbf{k}) \sigma_z \tau_y \]

\[ \pm(\epsilon_y(\mathbf{k}) \sigma_y \tau_y + \epsilon_x(\mathbf{k}) \sigma_x \tau_y), \]

\[ H^i_{12}(\mathbf{k}) = \epsilon_{d}(\mathbf{k}) \nu_x + \epsilon_{12}(\mathbf{k}) \tau_x \nu_x + t'_z(\sigma_y + \sigma_x) \tau_z \nu_y. \]

The various dispersions \( \epsilon(\mathbf{k}) \)s in \( H^\pm_0 \) have the same expression as Eq. (5), which represent intra-layer hopping integrals for top (\( i = + \)) and bottom (\( i = - \)) layer. \( H^i_{12} \) contains hopping paths between the two layers, and the dispersion \( \epsilon_d(\mathbf{k}) \) is the same as Eq. (11). \( t'_z \) represents the 1D orbital to \( d_{xy} \)-orbital hopping between the layers, and

\[ \epsilon_{12}(\mathbf{k}) = t_{12}(\cos(k_x) + \cos(k_y)), \]

where \( t_{12} \) denotes the NNN inter-layer intra-orbital hopping.

In addition to the b-glide symmetry \( \hat{\Pi}_{b} \) in Eq. (1), there exists another glide plane which transfers between top and bottom layers in this bilayer system.

\[ \hat{\Pi}_{layer} = \frac{i}{\sqrt{2}}(\sigma_x + \sigma_y) \tau_z \nu_z \hat{k}_{layer}, \]

where \( \hat{k}_{layer} \) is the operator that interchanges \( k_x \) and \( k_y \) as \( \hat{k}_{layer} : (k_x, k_y) \rightarrow (-k_y, -k_x) \). By computing the commutator of \( \hat{\Pi}_{layer} \) with \( H_{ABCD}(\mathbf{k}) \), it is straightforward to confirm that \( [\hat{\Pi}_{layer}, H_{ABCD}] = 0 \).

The band dispersion is shown in Fig. 5(c). The set of tight-binding parameters are given by \( (t_z, t_{110}, t_{110}, t_{12}, t'_z)/t = (-0.23, -0.01, -0.09, -0.11, -0.04) \) for the same \( \theta \) and \( \phi \) in the single layer. The hopping amplitude changes as a function of distance and has been estimated by introducing a scaling function \( 1/r^3 \). There are two
FIG. 7. (color online) Phase diagram when rotation degree is $\theta = 13^\circ$ in the middle panel (c) plotted as $z$-direction exchange field $h_z$ in the unite of Tesla (T) versus tilting degree $\phi$. Different phases has been characterized by different topological invariants $(C_{mv}, C_m, C_v, C)$. The edge state for each phase has been displayed in (a) QAH, (b) quantized valley Hall (QVH), (d) mirror valley Hall (MVH) and (e) topological crystalline insulator (TCI). Two gapless edge modes in (a), (b), (d) and (e) at $L = 0$ and $L = N$ boundary are represented by red and blue, respectively. Edge states are purple (mixed color of red and blue) in (d) and (e) because of the degeneracy between edge modes at $L = 0$ and $L = N$. See the main text for finite $C_{mv}$ and $C_m$ related to these edge modes.

Phases diagram contains various phase including mirror valley Hall phase, topological crystalline insulator phase, QAH phase and quantized valley Hall phase with distinguished topological feature, as displayed in Fig. 7(c). The vertical axis is the degree of tilting angle $\phi$. The horizontal axis corresponds to the strength of $z$-component of the magnetic exchange field, since the energy band gaps around $X$ and/or $Y$ exhibits different behaviors depending the strength of $h_z$ when a Zeeman field $h_x \sigma_x + h_y \sigma_y + h_z \sigma_z$ is applied and/or an antiferromagnetic ordering of $(m_x \sigma_x + m_y \sigma_y + m_z \sigma_z) \tau_z$ occurs. The phase boundaries can be modified depending on the magnetic ordering or exchange field pattern, but the qualitative picture of the phase diagram is not sensitive to the choice of magnetic ordering direction, as long as there is a finite $z$-component, $h_z$ (or $m_z$). Thus we only tune the strength of $h_z$ for simplicity. In Fig. 7(c) $h_z$ is estimated in Telsa using the tight binding parameters discussed above, and set $t \sim 100m_eV$.

Each phase separated by thick black line in Fig. 7 is characterized by the unique set of topological invariance $(C_{mv}, C_m, C_v, C)$ defined in Eq. (19). The edge states shown in Fig. 7(a), 7(b), 7(d) and 7(e) were obtained with the slab geometry under the boundary the same condition with ABAB stacking case described in the last section.

The bilayer with small tilting angle is characterized by mirror valley Hall phase with $C_{mv} = 2$. The valley physics in mirror valley Hall phase manifests explicitly in the edge state dispersion in Fig. 7(d). When the degree of tilting angle $\phi$ increases, it becomes a topological crystalline insulator with $C_m = 2$. The large tilting degree is able to inverse the sign of one of the mass term $C_v$.

The details of computations of $(C_{mv}, C_m, C_v, C)$ and the explicit expression is presented in the Appendix.

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near X or Y, and thus modifies the topology of the system. The edge state dispersion for topological crystalline insulator phase has two pairs of gapless currents moving along opposite directions. Each pair of edge modes carries opposite mirror eigenvalues. As the name suggested, these two pairs of gapless edge states are indeed protected by $\Pi_{\text{mirror}}$. The TR breaking term will not lift the degeneracy between edge states as long as the perturbation preserves $\Pi_{\text{mirror}}$.

By tuning the strength of $h_z$, the QAH phase arises. In the QAH phase, two gapless edge states localized at $L = 0$ propagating along the same direction. Each one contributes $e^2/h$ to Hall conductance and the total Hall conductivity when Fermi energy has been tuned inside the bulk gap is given by

$$ \sigma_{xy} = 2\frac{e^2}{h}. \quad (20) $$

However, in quantized valley Hall phase, within valley X (Y), the two edge states localized at $L = 0$ propagating along the same direction leads to quantized valley Hall conductivity $\sigma_{xy}^v$.

$$ \sigma_{xy}^v = C_v \frac{e^2}{h} = \frac{4e^2}{h}. \quad (21) $$

The mirror and mirror valley Chern numbers ($C_m, C_{mv}$) can be understood through the behavior of edge modes localized at $L = 0$ for instance. When the system is in mirror valley Hall phase, there are four edge modes at $L = 0$ or $L = N$ as shown in Fig. 7(d). Two edge modes are propagating from left to right with ($-, X$) and ($+, Y$) label, respectively. The other two are flowing along opposite direction carries ($+, X$) and ($-, Y$) label, respectively. Here ($\pm, X/Y$) means edge state carries ± quantum number which is the eigenvalue of $\sigma_{xy}$ localized around $X/Y$. Thus $C_{mv}$ is finite. When the gap is reversed at X, the propagating directions of the edge modes ($\pm, X$) will reverse and result in non-vanishing $C_m$. Therefore, the system is a topological crystalline insulator as shown in Fig. 7(e).

As we emphasized above, a finite bilayer hopping integral is crucial to achieve the QAH phase when TR symmetry is broken, because the z-axis ferromagnetic exchange field $h_z\sigma_z$ (or sublattice antiferromagnetic ordering $m_z\tau_z\sigma_z$) has to overcome $t_z$ to reverse the sign of Berry curvature around $X$ or $Y$ to enter the QAH insulator (see the Appendix for the proof). Using the current tight binding parameters, the strength of $h_z$ needs to be about a few Tesla as shown in Fig. 7(e). Since the critical strength of $h_z$ is tuned by the strength of $t_z$, it is desirable to make the bilayer hopping $t_z$ smaller, which is controlled by the spacing between the layers as shown in of Fig. 4.

IV. CONCLUSIONS

A recent experiment has reported a successful growth of Ir oxide superlattice ([SrIrO$_3$]$n$, SrTiO$_3$) with controllable number of layers $n$, which tailors a spin-orbit magnetic insulator for $n = 1$ and 2. Due to the smaller lattice constant in TiO$_2$ compared with IrO$_2$, it was expected that there are alternating rotations of Ir octahedra, but lacking a tiltting $(\phi)$ of octahedra to keep a tetragonal crystal structure of SrTiO$_3$. This was confirmed by the magnetic ordering patterns in $n = 1$ and 2 superlattices, consistent with the first principle calculations. However, topological phases have not been observed in these superlattices, even though bulk SrIrO$_3$ orthorhombic perovskites possess topological nodal lines protected by the lattice and TR symmetries.

One essential ingredient to realize any topological insulator is a Rashba-like SOC. In the $J_{\text{eff}}$=1/2 wavefunction formed by a strong atomic SOC, this Rashba-like SOC is generated by finite hopping integrals between different $J_z = \pm 1/2$ states. For example, finite hopping paths between $d_{xz}$ and $d_{yz}$ generate Rashba-like SOC terms in $J_{\text{eff}} = 1/2$ basis since $d_{xy}$ up-spin and one-dimensional orbitals of $d_{xz/yz}$ up-spin belong to different $J_z$ states. In perovskite layered systems, this is possible when the hopping path does not respect the mirror symmetry under $z \rightarrow -z$, as $d_{xy}$ is even while $d_{x\pm y\pm z}$ is odd under this operation. Thus the alternating octahedra rotations and tiltings are necessary for topological phases in layered perovskites.

We propose topological phases in Ir oxide superlattices or films grown from band insulator perovskites AMO$_3$ with Pbnm structure such as CaTiO$_3$, SrZrO$_3$ and SrHfO$_3$. Different topological phases were found depending how the TR and crystal symmetries are broken. For a single-layer Ir oxide, the Dirac dispersion at X and Y TRIM points is protected by the b-glide symmetry. When this b-glide symmetry is broken, it reveals a 2D topological insulator by gapping the Dirac nodes. In the presence of a magnetic ordering or in-plane Zeeman field, the system develops a topological magnetic insulator with QAH effects. In the bilayer Ir oxides, we consider two different stacking of layers. Due to finite hopping paths between the two layers, the nodal dispersion at X and Y TRIM points acquire different mass terms, even though the b-glide symmetry is present. In one case of stacking called ABAB stacking, the nodal point shifts to a non-symmetric point. Any magnetic field or magnetic ordering that breaks the b-glide symmetry turn this system into a topological magnetic insulator with QAH effects. In the ABCD stacking, it is an insulator with non-trivial valley Chern number or topological crystalline insulators depending on the degree of octahedra tilting angle $(\phi)$ in the absence of a magnetic ordering. Since there is an additional symmetry combined by the b-glide and layer symmetry, z-component of magnetic field or ordering is required to achieve a topological magnetic insulator with the quantized charge Chern number. These superlattices...
or films are grown along the [001] axis, which can be achieved by a most standard PLD growing technique. To test the proposal, ARPES measurement can be employed to investigate the Dirac point in these superlattices when TR symmetry is preserved, and Hall conductivity measurement should exhibit the QAH effect when a magnetic ordering occurs or an external magnetic field is applied.

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Appendix: Analytical Results of ABCD Bilayer

Applying the following canonical transformation in σ and ν space,

\[ \sigma_\pm \rightarrow \sigma_\pm \nu_z, \]
\[ \nu_\pm \rightarrow \nu_\pm \sigma_z, \]  

(A.1)

the Hamiltonian in Eq. (14) can be brought into a block diagonalized form.

\[ H' = \begin{pmatrix} H'_+ & 0 \\ 0 & H'_- \end{pmatrix}, \]

(A.2)

with

\[ H'_\pm = \pm \epsilon_{\pm}(k) \sigma_z + \epsilon_0(k) \tau_x + \epsilon_\nu(k) \sigma_y \tau_y + \epsilon_x(k) \sigma_x \tau_y \pm \epsilon'_z(\sigma_x - \sigma_y) \tau_z, \]

(A.3)

where ± subscripts are assigned to reflect the eigenvalues of \( \sigma_z \nu_z \) and the basis we choose for \( H' \) is a set of the eigenvectors of \( \sigma_z \nu_z \).

Consider the upper block Hamiltonian \( H'_+ \) near X point. By computing the eigenvalues of \( H'_+ \) in Eq. (A.3) along \( X \rightarrow \Gamma \), the location where the band gap vanishes near X is given by

\[ \cos(k_0^\pm) = \pm \frac{t'_z}{t_1 - t_2}. \]

(A.4)

The two solutions \((k_0^\pm, -k_0^\pm)\) in Eq. (A.4) in fact has the same topological properties. For convenience, only one point \((k_0^+, -k_0^+)\) \((= k_0, -k_0)\) will be taken into account.

Effective two band Hamiltonian for each block can be obtained by projecting the \( H'_+ \) to the relevant two bands \( |\phi\rangle \) and \( |\varphi\rangle \) at \((k_0, -k_0)\).

\[ |\phi\rangle = \frac{1}{\sqrt{2}} (|1\rangle - |2\rangle), \]
\[ |\varphi\rangle = \frac{1}{\sqrt{2}} (|1\rangle + |2\rangle). \]

(A.5)

where \( 1(2) \) refers to top (bottom) layer and \(|\uparrow\rangle \) for \( J_z = \frac{1}{2} \), \(|\downarrow\rangle \) for \( J_z = \frac{1}{2} \). Follow the perturbation theory, the effective two band Hamiltonian around X is written as

\[ H'^{\text{eff}}_{X} = \hat{P}_0 \hat{H}_0' \hat{P}_0 = \hat{A}_{+,X}(k) \cdot \hat{\sigma}, \]

(A.6)

where projecting operator is \( \hat{P}_0 = |\phi\rangle \langle \phi| + |\varphi\rangle \langle \varphi| \) and each component of \( \hat{A}_{+,X} \) is given by

\[ A_{+,X}^z = t_z + t'(110) + t'_0 + \delta_X, \]
\[ A_{+,X}^{y/z}(k) = t'_0 \delta_ky/z - t'_2 \delta_ky. \]

Here \( t'_1 = t_1 \sin(k_0), t'_2 = t_2 \sin(k_0) \), \( t'(110) = t(110) \sin(k_0) \), \( t'_0 = 4\nu_0 \cos(k_0) \) and \( \delta_kx \equiv k_x - k_0, \delta_ky \equiv k_y + k_0 \). The Berry curvature for p-th band is given as \( \Omega_p(k) = \nabla_k \times (i\langle p, k| \nabla_k |p, k \rangle) \). Thus the Berry curvature for the lowest band of \( H'^{\text{eff}}_X \) in Eq. (A.6) is

\[ \Omega_{+,X}^z(k) = \frac{(t'_2)^2 - (t'_1)^2}{|A_{+,X}^z|^3} \delta_X. \]

(A.8)

The Chern number can be computed using the formula Eq. (8) given in the main text and the expression is quite straightforward.

\[ C_{+,X} = \text{sign}(\delta_X). \]

(A.9)

Following the same procedure for lower block \( H'_- \) around X and \pm block around Y, the Chern number is given by

\[ C_{\pm,X} = \pm \text{sign}(\delta_X), \]
\[ C_{\pm,Y} = \mp \text{sign}(\delta_Y). \]

(A.10)

where \( \delta_Y = t_z + t'_0 + t(110) + t'_0 \) with \( t'(110) = t(110) \sin(k_0) \).

Various topological charges in bilayer system has been identified in Eq. (19). Plug in the expression of Eq. (A.10), we have

\[ C_{mv} = \text{sign}(\delta_X) + \text{sign}(\delta_Y), \]
\[ C_m = \text{sign}(\delta_X) - \text{sign}(\delta_Y), \]
\[ C_v = C = 0. \]

(A.11)

Here by considering the magnetic field along z-direction \( h_z \sigma_z \) with \( h_z > 0 \), TR can be explicitly broken. The only modification in two band effective Hamiltonian is the mass term appears in Eq. (A.8) changes to

\[ \delta_{X/Y} \rightarrow h_z \pm \delta_{X/Y} \].

(A.12)

And the Chern number in Eq. (A.10) has the following expression.

\[ C_{\pm,X} = \text{sign}(h_z \pm \delta_X), \]
\[ C_{\pm,Y} = -\text{sign}(h_z \pm \delta_Y). \]

(A.13)

The explicit expression of \( C_{mv}, C_m \) and \( C_v \) in Eq. (19) can be modified accordingly based on Eq. (A.13). The above analysis indicates the phase transition is driven by the z-direction magnetic field \( h_z \).
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