The discovery of time reversal invariant topological insulator has attracted great attention in condensed matter physics [3, 4]. With time-reversal symmetry broken on the surface, the electromagnetic response of three dimensional (3D) insulators are described by the topological \( \theta \) term of the form 
\[
S_\theta = \frac{e^2}{4\pi} \int d^3x dt \mathbf{E} \cdot \mathbf{B}
\]
together with the ordinary Maxwell terms, where \( \mathbf{E} \) and \( \mathbf{B} \) are the conventional electromagnetic field inside the insulator, \( \alpha = e^2/\hbar c \) is the fine structure constant, and \( \theta \) is the dimensionless pseudoscalar parameter describing the insulator, which refers to “axion” field in axion electrodynamics [10]. For a system without boundary, all the physical quantities are invariant if \( \theta \) is shifted by integer multiple of \( 2\pi \). Therefor all time reversal invariant insulator fall into two distinct classes described by either \( \theta = 0 \) (trivial insulator) or \( \theta = \pi \) (topological insulator) [11]. Such a universal value of \( \theta = \pi \) in topological insulators leads to magneto-electric effect with an universal coefficient, which has several unique experimental consequences such as a topological contribution to the Faraday rotation or Kerr rotation [11, 13], and the image monopole induced by an electron [12, 14]. \( \theta \) has an explicitly microscopic expression of the momentum space Chern-Simons form which depends on the band structure of the insulator [11]

\[
\theta = \frac{1}{4\pi} \int d^3k e^{ijk} \text{Tr} \left[ A_i \partial_j A_k + i \frac{2}{3} A_i A_j A_k \right],
\]

where \( A_i^{\mu\nu}(k) = -i \langle u_\mu | \partial_\nu | u_\nu \rangle \) is the momentum space non-abelian gauge field, with \( |u_\mu\rangle, |u_\nu\rangle \) referring to the Bloch wavefunction of occupied bands.

If strong electron correlation exists in a topological insulator, a long-range antiferromagnetic (AFM) order can be established under low enough temperature. Since the AFM order breaks time-reversal symmetry spontaneously, \( \theta \) can deviate from \( \pi \), and also becomes a dynamical field which has fluctuations associated with some spin collective modes. The spin collective mode inducing fluctuations of \( \theta \) are thus coupled to the photons by \( \theta \mathbf{E} \cdot \mathbf{B} \) term, which means they become “axions” in the term used in high energy physics. Such a nonconventional antiferromagnetic insulator supporting axion excitations is proposed as topological magnetic insulator (TMI) [15].

Due to its coupling to photons, the axion field hybridizes with photons, leading to axion polariton, with a polariton gap tunable by an external magnetic field. Thus such a material can be used as a novel type of optical modulator to control the transmission of light through the material.

To realize the TMI phase, we need both the nontrivial topology of the electron bands and strong electron correlation. The materials with electrons in 4d or 5d-orbital can have both strong spin-orbit coupling (SOC) and strong interaction, which is ideal for this purpose. Recently, models for topological insulators with strong electron correlation have been proposed [10–19], also first principle calculations show topological phases exist in thallium-based III-V-IV ternary chalcogenides [20, 21] as well as ternary heusler compounds which contain the rare earth element Ln, where additional properties ranging from superconductivity to magnetism and heavy-fermion behavior can be realized [22–24]. In this Letter, we study theoretically the transition metal oxide \( ABO_3 \) of corundum structure with \( B = A \) standing for some transition metals such as Fe, Ti, Ru, Rh, Ir, Os, etc [24]. A tight binding model is obtained by using point group symmetry of this structure, from which we find a topological magnetic insulator phase with certain SOC strength and electron-electron interaction.

The corundum structure is shown in Fig. 1(a). Each transition metal atom is surrounded by oxygen octahedron, and the d orbitals are split by the octahedral crystalline field into doublet \( e_g(x^2-y^2, 3z^2-r^2) \) and triplet \( t_{2g}(xy, yz, zx) \) orbitals (See Fig. 1(c)). We will neglect small distortion of the oxygen octahedra which may lead to minor corrections to electronic structure [24]. The energy of \( t_{2g} \) stays lower with respect to \( e_g \), because
the latter point towards the negatively charged oxygens. The SOC is effective in $t_{2g}$ orbitals and negligible in $e_g$ orbitals. Including the SOC, $t_{2g}$ splits into total angular momentum $j_{\text{eff}} = 3/2$ and $j_{\text{eff}} = 1/2$. We focus on those materials where the Fermi level lies completely in the $j_{\text{eff}} = 1/2$ sub-bands. For example, the ions Ir$^{4+}$, Os$^{5+}$, Ru$^{3+}$ etc with five $d$-electrons satisfy this requirement [20].

To obtain the electron dynamics in this system, we start by a symmetry analysis to the corundum structure. The space group of this structure is $D_3d(R3c)$ with four atoms in each unit cell. It has a trigonal axis (three-fold rotation symmetry $C_3$) defined by $z$ axis, a binary axis (two-fold rotation symmetry $C_2$), defined by $y$ axis, and inversion symmetry with the inversion center at the middle of the two neighbor transition metal atoms. The primitive lattice vectors $t_{1,2,3}$ and primitive unit cells are shown in Fig. 1(a), where each unit cell consists of four transition metal atoms denoted as $1_{2,3}$. Since the O $p$-level $\varepsilon_p$ are far away from the fermi level, we can consider a model describing only $d$-electrons, with the hopping mediated by the oxygen $p$-orbitals. The model is generally written as

$$H_0 = -\sum_{\langle i,j \rangle} \left[ d_{i}^\dagger t_{ij} d_{j} + \text{h.c.} \right] + \sum_{\langle \langle i,j \rangle \rangle} \left[ d_{i}^\dagger t_{ij} d_{j} + \text{h.c.} \right], \quad (2)$$

where $\langle i,j \rangle$ and $\langle \langle i,j \rangle \rangle$ denote the nearest-neighbor (NN) and next-nearest-neighbor (NNN) sites, respectively, and the hopping terms $t_{ij}$ and $t_{ij}^\dagger$ are in general $2 \times 2$ matrices. The form of the parameters $t_{ij}, t_{ij}^\dagger$ can be simplified by symmetry considerations. Due to space limitation, we will only present the result of the symmetry analysis. The NN transfer integral $t_{ij}$ are real and spin independent, with two independent parameters, the intra-plane hopping $t_1$ and the inter-plane hopping $t_{\bot}$. $t = (p\sigma_n)^2/(p\sigma_n + 3(pp\pi))/3(\varepsilon_d - \varepsilon_p)^2$, where $(p\sigma_n), (pp\pi)$, and $(pp\pi)$ are Slater-Koster parameters between $pd$ and $pp$, respectively [27]. The contribution of the order of $(p\sigma_n)^2/(\varepsilon_d - \varepsilon_p)$ cancel out in the honeycomb lattice, in sharp contrast to Sr$_3$IrO$_4$ with the perovskite lattice [28, 29]. The NNN transfer integrals are spin dependent, and it is essential for the realization of the topological insulator phase. For intra-plane in A plane, $\gamma \rightarrow \gamma$ hopping can be written as

$$\vec{t}_{\gamma 1} = i|\vec{t}_{\gamma 1}| \vec{\sigma} \cdot \vec{r}_{\gamma 1} + t_{\gamma 1}, \quad (3)$$

$\vec{r}_{\gamma 1}$ is a unit vector $\vec{r}_{\gamma 1} \propto \vec{r}_{\gamma 1} + 1/\sqrt{2} \hat{z}$; $\vec{t}_{\gamma 1}$ is the hopping link. $\vec{t}_{\gamma 1} = \vec{t}_{\gamma 1}$ due to inversion symmetry. While in B plane, $\vec{t}_{\gamma 3} = e^{-i\pi/2} t_{\gamma 1} e^{i\pi/2}$, $\vec{t}_{\gamma 4} = e^{-i\pi/2} t_{\gamma 1} e^{i\pi/2}$ due to $C_2$ symmetry. For intra-plane ($A \rightarrow B$),

$$\vec{t}_{\gamma 1} = i|\vec{t}_{\gamma 1}| \vec{\sigma} \cdot \vec{r}_{\gamma 1} + t_{\gamma 1} + t_{\gamma 1} \quad (4)$$

$\vec{r}_{\gamma 1}$ is a unit vector $\vec{r}_{\gamma 1} \propto \vec{r}_{\gamma 1} + \alpha \hat{z}$, $\vec{r}_{\gamma 1}$ is the hopping link, $\alpha$ is some parameter which depend on materials and cannot be determined purely by symmetry, below we choose $\alpha = 1/\sqrt{2}$ which has almost the same amplitude as intra-plane. $\vec{t}_{\gamma 1} = \vec{t}_{\gamma 1} e^{i\pi/2} = \vec{t}_{\gamma 1} e^{i\pi/2}$. Explicitly, $\vec{t}_{\gamma 1}$ for the intra-plane $1 \rightarrow 1, 2 \rightarrow 2$ hopping are $x_1, y_1, z_1$, and $3 \rightarrow 3, 4 \rightarrow 4$ are $x_2, y_2, z_2$ denoting in Fig. 1(a).

In summary, the transfer integrals are real and spin independent for NN links, while complex and spin dependent for NNN links. The accurate hopping parameters vary in different materials. As an example, in the following we will use the transfer integrals of Ir oxide introduced in Ref. [17]. One can always define all the parameters in the unit of in-plane nearest neighbor hopping $t_1$, which leads to $t_1 = 1$, $t_{11} = 0.33$, $t_{11} = -0.1$, $t_{\perp} = y$, $t_{21} = 0.5y$, $t_{21} = 0.4y$. Here $\lambda$ is the SOC strength which determines the ratio of spin-dependent hopping and spin-independent hopping. For Ir oxide we have $\lambda = 0.8$. All the inter-plane hopping matrix elements are rescaled by a factor $y$ which incorporates the anisotropy between intra-plane and inter-plane directions. The energy dispersion for $y = 0.3$ (dashed line) and $y = 0.55$ (solid line) are shown in Fig. 2(a), which shows that the system at half filling is an insulator in both case. Due to inversion symmetry, all the energy bands are doubly degenerate.

In three-dimensional topological band insulators, four independent $Z_2$ topological invariants can be defined [30–32]. For inversion symmetric systems, all the topological invariants can be simply determined by the parity of the wave-functions at the 8 time-reversal invariant momenta (TRIM) in the Brillouin zone [3]. Denote $G_1, G_2, G_3$ are the three basis vectors of the
reciprocal lattice, then the 8 TRIM’s are defined by $k_i = (k_1 G_1 + k_2 G_2 + k_3 G_3)/2\pi$ with $k_1, k_2, k_3 = 0$ or $\pi$. For each TRIM $k_i$, one can define a $Z_2$ quantity $\delta_i$ as the multiplication of the parity of all occupied bands $\delta_i = \prod_{s \in occ} \xi_s$, with $\xi_s$ the parity of $s$-th band. It should be noticed that a Kramers pair of bands are only counted in (c) and $y = 0.55$ in (d). The red curves in (d) stands for surface states. The inset shows the surface Brillouin zone. The system changes from trivial insulator to topological insulator (TI) with the topological invariant $\nu = \prod_{s \in occ} \xi_s$ for all val- ues of anisotropy parameter $\lambda$. The topological invariants can be calculated for all values of anisotropy parameter $\lambda$ and spin-orbit coupling $\lambda$. From this result we see that a band inversion occurs at $F$ points upon the change of $y$. In Fig. 2(b) we show the energy at $F$ point versus $y$, from which one can see clearly a level crossing at $y \approx 0.42$. The topological invariants can be calculated for all values of anisotropy parameter $\lambda$ and spin-orbit coupling parameter $\lambda$, which leads to the phase diagram shown in Fig. 3. One can see that the topological nontrivial band structure can be realized at large $y$ (i.e., small anisotropy) even for infinitesimal spin-orbit coupling. However, one should notice that for some parameters the band structure is actually a semi-metal (similar to Sb), which has a direct gap but does not have in-direct gap. We also solve the Hamiltonian in a slab geometry with two 001 surfaces to study explicitly the topological surface states. Fig. 2(c)&(d) shows the 2D energy dispersion of the two systems shown in Fig. 2(a). In addition to the bulk states, for $y = 0.55$ there are surface states with three Dirac cones at $M$ points of the surface BZ, while no surface state is found for $y = 0.3$, in consistency with the bulk topological invariants.

To get better understanding of the physical properties of this system, a low energy effective model can be obtained by expanding the Hamiltonian around the $F$ points. Around each $F$ point, the effective model is $4 \times 4$ which describes two Kramers pairs of low lying bands and has Dirac-like form. In the following, we will denote the momentum by its coordinate in the basis of reciprocal lattice, i.e., $\mathbf{k} = (k_1 G_1 + k_2 G_2 + k_3 G_3)/2\pi$. The $F$ points are given by $(\pi, 0, 0)$ and $(0, \pi, 0)$ and $(\pi, \pi, 0)$. Around the point $(\pi, 0, 0)$ the Hamiltonian has the following form:

$$H_{\text{eff}}(\pi 0 0) = \epsilon_0(\mathbf{q}) \mathbb{I}_{4 \times 4} + \sum_{a=1}^{5} d_a(\mathbf{q}) \Gamma_a, \quad (5)$$

Here the Dirac $\Gamma$-matrices are defined as $\Gamma_a = (\tau_x \otimes \sigma_x, \tau_x \otimes \sigma_y, \tau_y \otimes 1, \tau_z \otimes 1, \tau_z \otimes \sigma_z)$ where $\tau_i$ and $\sigma_i$ ($i = x, y, z$) denote the Pauli matrices in the space of orbital and spin, respectively. $\mathbf{q} = \mathbf{k} - (\pi 0 0)$, $d_a(\mathbf{q}) = \sum_{i=1,2,3} A_i^a q_i$ for $a = 1, 2, 3, 5$, $d_4(\mathbf{q}) = M + \sum_{i=1,2,3} B_i q_i^2$, and $\epsilon_0(\mathbf{q}) = C + \sum_{i=1,2,3} D_i q_i^2$. For $\lambda = 0.8$, around the topological phase transition point we have

$$A_i^a = \begin{pmatrix} 0.14 & -0.12 & 0.37 & -0.34 \\ -0.47 & 0.06 & -0.13 & 0.09 \\ 0.014 & 0.038 & 0.015 & 0.055 \end{pmatrix},$$

$$B_i = \begin{pmatrix} 0.625, 0.32, 0.24 \end{pmatrix},$$

$$D_i = \begin{pmatrix} 0.375, 0.04, 0.04 \end{pmatrix}$$
\[ C = 0.064. \text{ The mass parameter } M \text{ depends on } y \text{ as } M \approx -23y + 9.76 \text{ which changes sign at } y \approx 0.42 \text{ and leads to the topological phase transition. The effective Hamiltonian around the other two } F \text{ points at } (0\pi 0) \text{ and } (\pi \pi 0) \text{ can be obtained by } C_3 \text{ rotation.} \]

Now we study the effect of electron correlation. The leading term in the interaction Hamiltonian is the onsite Hubbard repulsion for the \( j_{\text{eff}} = 1/2 \) orbitals

\[ H_{\text{int}} = U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (6) \]

Magnetic ordering in this system can be studied in mean-field approximation. For simplicity, we will only consider the order parameters that do not break translation symmetry. The mean-field calculation predicts a SDW phase above a critical \( U \), as shown in the phase diagram in Fig. 4. The spin moments of this SDW phase lie in the honeycomb plane, which are ordered antiferromagnetically within each honeycomb layer and non-collinear between the two neighboring honeycomb layers, as shown in Fig. 4.

Such a SDW order breaks both time-reversal symmetry \( \mathcal{T} \) and inversion symmetry \( \mathcal{P} \) spontaneously, but preserves the combination \( \mathcal{PT} \). Thus the magneto-electric coefficient \( \theta \) in the \( \Phi \mathcal{E} \cdot \mathbf{B} \) term may deviate from the time-reversal invariant values 0 and \( \pi \) in the SDW phase, and certain spin wave fluctuations are coupled to photon as axions \[ 13. \]

To estimate the value of \( \theta \) in the SDW phase, we can study the effect of the SDW order in the effective model \( (5) \). To the leading order, the \( \mathcal{T}, \mathcal{P} \) breaking but \( \mathcal{PT} \) preserving perturbation to the effective model must have the form \( \delta H_{\text{eff}}(\mathbf{q}) = \sum_{a=1,2,3,5} m_a \Gamma_a \), where \( m_a \) depends linearly on the spin moment \( \langle S \rangle \) obtained from mean-field theory. Thus the perturbed Hamiltonian can still be written as \( \hat{H}(\mathbf{q}) = \sum_{a=1,2,3,5} d_a(\mathbf{q}) \Gamma_a \) with \( d_a(q)(a = 1, 2, 3, 5) = \sum_{x=x,y,z} A_{xy,k_i + m_a}^a d_{i}(\mathbf{q}) \) unchanged. For this effective model, \( \theta \) has an explicit expression \[ 13 \]

\[ \theta = \frac{1}{4\pi} \int d^3 k \frac{2(|d| + d_4)}{(|d| + d_4)^2} \epsilon^{ijkl} d_i \partial_x d_j \partial_y d_k \partial_z d_l \quad (7) \]

where \( i, j, k, l = 1, 2, 3, 5 \), and \(|d| = \sqrt{\sum_{a=1}^{5} d_a^2}\). Since the main contribution to \( \theta \) comes from the region close to Dirac points, \( \theta \) can be approximated by the sum of \( \theta_s \)s calculated separately for each Dirac point using the effective model. The numerical results of \( \theta \) is shown in Fig. 4(b).

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FIG. 4: (Color Online) (a) The phase diagram with the out of plane hopping \( y \) and onsite repulsion \( U \) as parameters. The phase on the right is the topological magnetic insulator (TMI) which carries the dynamic axion. (b) The value of \( \theta \) (see text) along the blue line in the phase diagram. (c) The SDW order pattern. The purple arrows represent the spin in the honeycomb layer A and the green arrows represent the spin in the adjacent honeycomb layer B. Other possible spin configurations can be obtained by six-fold rotations of this one.

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