Topological Crystalline Insulators

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The recent discovery of topological insulators has revived interest in the band topology of insulators. In this work, we extend the topological classification of band structures to include certain crystal point group symmetry. We find a class of three-dimensional “topological crystalline insulators” which have metallic surface states with quadratic band degeneracy on high symmetry crystal surfaces. These topological crystalline insulators are the counterpart of topological insulators in materials without spin-orbit coupling. Their band structures are characterized by new topological invariants. We hope this work will enlarge the family of topological phases in band insulators and stimulate the search for them in real materials.

PACS numbers: 73.20.-r, 73.43.-f

The topology of band structures is important in the study of topological phases of matter. Historically the quantization of Hall conductance in the integer quantum Hall effect was explained by the Thouless-Kohmoto-Nightingale-den Nijs integer (also known as Chern number or the Wannier functions with the same symmetry as the electronic states). We assume that these bands do not overlap with the electronic states. In particular, we are interested in the energy bands derived from the $p$, $d$, and $f$ orbitals. We study a class of three-dimensional topological crystalline insulators which have four-fold ($C_4$) or six-fold ($C_6$) rotational symmetry. As we will show, its (001) surface, which preserves the rotational symmetry, supports gapless surface states. These topological crystalline insulators are the counterpart of topological insulators in materials without spin-orbit coupling. Instead electron’s orbital degrees of freedom play a role similar to spin. Unlike the linearly dispersing Dirac surface states of topological insulators, the (001) surface states of topological crystalline insulators have quadratic band degeneracy protected by time reversal and discrete rotational symmetry.

The outline of this paper is as follows. First we introduce a simple tight-binding model in a tetragonal crystal with $C_4$ symmetry. We explicitly show that gapless surface states exist on the (001) crystal face. The topological stability of surface states suggests a nontrivial phase in this model. Next we define a new $Z_2$ topological invariant for generic time reversal invariant band structures with $C_4$ or $C_6$ symmetry in three dimensions. This establishes the topological crystalline insulator phase. Finally we discuss the electronic properties of quadratic surface bands.

**Tight-Binding Model:** Consider a tetragonal lattice with a unit cell of two inequivalent atoms $A$ and $B$ along the $c$-axis, as shown in Fig.1a. The 3D crystal can be viewed as a stack of bilayer square lattices in the $ab$ plane. We now introduce a tight-binding model to describe the band structure of electron’s $p$ orbitals (or $d$ orbitals, see the next paragraph). In particular, we are interested in the energy bands derived from $p_x$ and $p_y$ orbitals. We assume that these bands do not overlap with the $p_z$ bands, and construct a tight-binding model from Wannier functions with the same symmetry as $p_x$ and $p_y$.
orbitals. The Hamiltonian \( H \) consists of intra-layer hopping \( H^A \) and \( H^B \), as well as inter-layer hopping \( H^{AB} \):  
\[
H = \sum_n H_n^A + H_n^B + H_n^{AB},
\]
\[
H_n^A = \sum_{i,j} t^a(r_i - r_j) \sum_{\alpha,\beta} c_{\alpha \alpha}^i (r_i, n) c_{\beta \beta}^j (r_j, n),
\]
\[
H_n^{AB} = \sum_{i,j} t'(r_i - r_j) \left[ \sum_\alpha c_{A \alpha}^i (r_i, n) c_{B \alpha}^j (r_j, n) + h.c. \right]
\]  
\[+ t_z' \sum_{i} \left[ \sum_\alpha \left| c_{A \alpha}^i (r_i, n) c_{B \alpha}^i (r_i, n+1) + h.c. \right] (1)
\]

Here each site is specified by \((n, r, a)\): \( n \) labels the bilayer unit cell along \( c \)-axis; \( r = (x, y) \) labels the \( ab \)-plane coordinate; \( a = A, B \) labels the sublattice. \( \alpha, \beta \) label the \( p_x, p_y \) orbital. Two types of \( p \)-orbital hopping terms appear in \( H \). The intra-layer hopping in \( H^A \) is of \( \sigma \)-bonding type; it depends on the relative orientation of \( p \)-orbital and the hopping direction \( e^{ij} = (r_i - r_j)/|r_i - r_j| \). The inter-layer hopping in \( H^{AB} \) is orbital-independent. Written in this form, the tight-binding Hamiltonian manifestly preserves crystal symmetries. The hopping amplitudes \( t^a, t' \) and \( t_z' \) between two sites depend on their \( ab \)-plane distance \( r_i - r_j \). Throughout this work, we assume spin-orbit coupling is negligible, so that electron’s spin index is omitted.

We emphasize that the form of the Hamiltonian \( H \) is entirely determined by crystal symmetry. Because \( d_{xz, yz} \) orbitals transform in the same way as \( p_{x, y} \) orbitals under \( C_4 \), it also applies to materials with these \( d \)-orbital. Therefore (1) is potentially relevant to a large class of materials including transition metal compounds with \( t_{2g} \) orbitals near Fermi energy.

To obtain a minimal model for topological crystalline insulators, we include the nearest and next-nearest neighbor intra-layer hoppings in \( H^A \) with the amplitude \( t_1^A \) and \( t_2^A \), as well as nearest and next-nearest neighbor inter-layer hoppings in \( H^{AB} \) with the amplitude \( t_1^{AB} \) and \( t_2^{AB} \). The corresponding Bloch Hamiltonian \( H(k) \) is obtained by Fourier transform:

\[
H(k) = \begin{pmatrix}
H^A(k) & H^{AB}(k) \\
H^{AB}(k) & H^B(k)
\end{pmatrix}
\]

\[
H^a(k) = 2t_1^A \begin{pmatrix}
\cos k_x & 0 \\
0 & \cos k_y
\end{pmatrix}
\]
\[
+ 2t_2^A \begin{pmatrix}
\cos k_x \cos k_y & \sin k_x \sin k_y \\
\sin k_x \sin k_y & \cos k_x \cos k_y
\end{pmatrix}
\]

\[
H^{AB}(k) = [t_1^{AB} + 2t_2^{AB} (\cos k_x + \cos k_y) + t_z^{AB} e^{ik_z}] I. \tag{2}
\]

The band structure is shown in Fig.2a for the following set of parameters: \( t_1^A = -t_2^B = 1, t_1^A = -t_2^B = 0.5, t_1^{AB} = 2.5, t_2^{AB} = 0.5, t_z^{AB} = 2 \). We have checked that the energy gap is finite everywhere in the Brillouin zone. As long as the energy gap does not close, the system remains in the same topological class within a finite parameter range.

To study surface states, we solve \( H \) in a slab geometry. We find that the existence of gapless surface states crucially depend on the surface termination. Consider the high symmetry (001) surface, which preserves the \( C_4 \) symmetry. Here surface states exist and transverse the whole energy gap as shown in Fig.2, leading to a 2D surface metal. Note that surface states are doubly degenerate at \( \bar{M} = (\pi, \pi) \): one in \( p_x \) orbital and the other in \( p_y \) orbital. Because \( M \) is a fixed point under four-fold rotation, the doublet form a two-dimensional irreducible real representation of \( C_4 \) symmetry, as a result of time reversal symmetry for electrons without spin-orbit coupling (i.e., spinless fermions). Surface band dispersion near \( M \) can be obtained from \( k \cdot p \) theory. We introduce a pseudospin \( \sigma_z = \pm 1 \) to label the \( p_x \) and \( p_y \) orbital of the doublet. In this basis, \( C_4 \) rotation is represented by \( e^{i\sigma_z \pi/4} \) and time reversal operator \( T \) is represented by complex conjugation. Up to a gauge transformation, the form of the \( k \cdot p \) Hamiltonian \( H \) is dictated by symmetry:

\[
\mathcal{H}(k_x, k_y) = \frac{k^2}{2m_0} + \frac{k_x^2 - k_y^2}{2m_1} \sigma_z + \frac{k_x k_y}{2m_2} \sigma_x. \tag{3}
\]

Perturbations which break either \( C_4 \) or \( T \) symmetry can open up an energy gap and destroy the protected surface states. This can be seen explicitly by adding a \( C_4 \)-breaking term \( M_1 k_x \sigma_y + M_2 \sigma_z \) or a \( T \)-breaking term \( M \sigma_y \).
to $\mathcal{H}$. Similar quadratic bands have been recently studied in 2D photonic crystals \(^{12}\) and fermion models \(^{13}\).

Our tight-binding model does not have gapless surface states for other surface terminations which break the $C_4$ symmetry.

When $T$ and $C_4$ symmetry are preserved, the surface states shown above are topologically protected. This can be understood by considering the surface band dispersion along $\Gamma M$. Within our model, surface states (if present) must be doubly degenerate at $\Gamma$ and $M$. As a consequence, there exists two distinct types of surface band connectivity along $\Gamma M$, having an even or odd number of band crossings at Fermi energy respectively. Surface states with even crossings are fragile: they can be pushed out of the energy gap by changing the surface potential. Surface states with odd crossings have a Fermi surface connectivity along $\bar{\Gamma} \bar{\Gamma}$ which encloses $\Gamma$ an odd number of times. They cannot be removed. These two types of surface states imply the existence of two topologically distinct phases of time-reversal-invariant band insulators with four-fold symmetry. The reasoning here closely follows the previous study of topological insulators \(^{14}\).

**$Z_2$ Topological Invariant:** We now show that a $Z_2$ topological invariant $\nu_0 = 0,1$ characterizes the band structure of 3D time-reversal-invariant insulators with four-fold rotation symmetry (without spin-orbit coupling). $\nu_0 = 0$ corresponds to a trivial phase adiabatically connected to an atomic insulator. $\nu_0 = 1$ corresponds to a topological crystalline insulator which has gapless surface states on the (001) surface.

We start by examining the symmetry property of Bloch wavefunctions of occupied bands: $|\psi_n(k)\rangle = e^{ik \cdot r}|u_n(k)\rangle$, where $|u_n(k)\rangle$ is the cell-periodic eigenstates of the Bloch Hamiltonian $H(k) = e^{-ik \cdot r}H e^{ik \cdot r}$. Here the unit cell is chosen to be invariant under $C_4$ rotation around the $z$ axis. $H(k)$ satisfies

$$H(k_x, k_y, k_z) = U H(k_y, -k_x, k_z) U^{-1}$$

$$H(k_x, k_y, k_z) = T H(-k_x, -k_y, -k_z) T^{-1}. \quad (4)$$

Here the unitary operator $U = e^{iL_z \pi/2}$ implements $C_4$ rotation within the unit cell ($L_z = xP_y - yP_x$ is an angular momentum operator). The anti-unitary operator $T = K$ (complex conjugation) implements time reversal transformation for spinless fermions, with the property $T^2 = 1$. As a result, time reversal symmetry by itself does not guarantee a two-fold degeneracy. However, the combination of time reversal and four-fold rotational symmetry can lead to protected degeneracies at four special momenta $\Gamma = (0,0,0), M = (\pi, \pi, 0), A = (\pi, \pi, \pi), Z = (0,0,\pi)$ in the 3D Brillouin zone (Fig.1b).

At such a high symmetry point $k_0$, $H(k_0)$ commutes with $U$, so that the energy bands $|u_n(k_0)\rangle$ are eigenstates of four-fold rotation with possible eigenvalues $1,-1,i$ and $-i$. Moreover, because $H(k_0)$ is real, energy bands at $k_i$ with $\pm i$ eigenvalues are guaranteed to be degenerate, forming a two-dimensional irreducible real representation of $C_4$. For example, such doublet bands can derive from $(p_x, p_y)$ or $(d_{xz}, d_{yz})$ orbitals.

From now on, we consider a set of energy bands $|u_n(k)\rangle$, $n = 1, ...2N$ which are doubly degenerate $E_{2n-1}(k) = E_{2n}(k)$ at $\Gamma, M, A$ and $Z$. As we will see below, only these doublet bands admit a $Z_2$ classification.

The $Z_2$ topological invariant $\nu$ is defined in terms of the electron wavefunctions:

$$(-1)^{\nu_0} = (-1)^{\nu_M} (-1)^{\nu_{A_2}}, \quad (5)$$

$$(-1)^{\nu_{k_1,k_2}} = \exp(i \int_{k_1}^{k_2} d\mathbf{k} \cdot \mathbf{A}_k) \frac{\text{Pf}[w(k_2)]}{\text{Pf}[w(k_1)]}. \quad (6)$$

$$A_k = \sum_j \langle u_j(k)|\partial_k|u_j(k)\rangle,$$

$$w_{mn}(k_1) \equiv \langle u_m(k_1)|U|u_n(k_1)\rangle.$$  

$A_k$ is the $U(1)$ Berry connection. $w(k_1)$ is an anti-symmetric $U(2N)$ matrix because $\{H(k_1), UT\} = 0$ and $(UT)^2 = -1$. Pf stands for the Pfaffian. We now specify the integration path in \((6)\). For $\nu_M$, the integral is along an arbitrary line connecting $\Gamma$ and $M$ which lies within the 2D plane $k_z = 0$ in the Brillouin zone as shown in Fig.1b. Likewise, the integration path for $\nu_{A_2}$ lies in the plane $k_z = \pi$.

Both $A$ and $w$ depend on the choice of basis $|u_j(k)\rangle$, but we now prove that $\nu_{k_1,k_2}$ is gauge invariant. Two different basis $|u_n(k)\rangle$ and $|u_m(k)\rangle$ are related by a $U(2N)$ gauge transformation:

$$|\tilde{u}_n(k)\rangle = G_{nm}(k)|u_m(k)\rangle, \quad G \in U(2N) \quad (7)$$

This leads to the corresponding gauge transformation of $A$ and $w$:

$$\tilde{A} = A - i Tr[G^{-1} \partial_k G] = A - i \partial_k \log(\det[G]),$$

$$\tilde{w} = G^* w G^\dagger. \quad (8)$$

Using the identity $\text{Pf}[X^T M X] = \det[X]\text{Pf}[M]$, it is straightforward to verify that $\nu_{k_1,k_2} = \nu_{k_1,k_2}$ is gauge invariant.

We now further show that $(-1)^{\nu_{k_1,k_2}} = \pm 1$ is a $Z_2$ quantity. It follows from \((7)\) that at the two 2D planes $k_z = 0$ and $k_z = \pi$, $H(k)$ has the symmetry property: $H(k) = \Xi H(k) \Xi$, $\Xi \equiv U^T T$. This allows us to choose a real gauge along the integration path to evaluate \((6)\):

$$\Xi|u_n(k)\rangle = -|u_n(k)\rangle, \quad (9)$$

Because $\Xi$ is anti-unitary, $\mathcal{A} = 0$ everywhere along the integration path. So in this gauge $(-1)^{\nu_{k_1,k_2}}$ reduces to

$$(-1)^{\nu_{k_1,k_2}} = \text{Pf}[w(k_2)]/\text{Pf}[w(k_1)]. \quad (10)$$

Because $|u_n(k)\rangle$ belong to the two-dimensional representation of $C_4$ group, we have $U^2|u_n(k)\rangle = -|u_n(k)\rangle$, so that the gauge condition \((9)\) at $k_i$ is equivalent to
Surface States with Quadratic Degeneracy:

Quadratic degeneracies in 2D band structure have attracted considerable interest recently. The $k \cdot p$ Hamiltonian (3) is widely used as a low energy approximation for the band structure of bilayer graphene near $\pm K$ points. However, unlike topological crystalline insulators, the quadratic degeneracy there is not protected by symmetry. Instead, the band dispersion very close to $\pm K$ becomes linear due to trigonal warping effects.

Electron interactions can drive 2D bands with quadratic degeneracy into a variety of interesting broken symmetry phases including quantum anomalous Hall state, nematic phase and etc [13]. The competition between different ordered phases is of great interest in bilayer graphene. It remains to see what happens in the single-valley quadratic surface states of topological crystalline insulators.

It would be interesting to generalize the concept of topological crystalline insulators to interacting systems. For example, crystal symmetry is known to play an important role in the topological classification of spin liquids [13], spin chains [19], and Mott insulators [20]. A unifying theory of symmetry protected topological phases remains to be developed. We also note that analogs of topological crystalline insulators can be potentially realized in photonic crystals.

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SUPPLEMENTARY MATERIAL

We study the stability of surface states with quadratic degeneracy when the doublet bands coexist with singlet band in the bulk. The latter may come from, e.g., $p_z$ orbitals so far neglected in our tight-binding model on tetragonal lattice. Provided there is no band crossing between doublet and singlet bands, the $Z_2$ invariant $\nu$ for the former remains well-defined. However, as we now demonstrate, the quadratic surface states of a nontrivial $\nu = 1$ phase can in principle be damaged by hybridizing with additional singlet surface band.

We assume that the singlet band in the bulk gives rise to a branch of unprotected nondegenerate surface state with the usual dispersion $E_3(k) = \epsilon_3 + k^2/(2m_3)$. $\epsilon_3$ is the energy difference between the doublet and singlet surface state at $k = 0$. This extra surface state can hybridize with the original surface states with quadratic degeneracy. A hybridization term is symmetry allowed in the $k \cdot p$ Hamiltonian:

$$\mathcal{H}' = \begin{pmatrix}
\mathcal{H} & 0 \\
0 & \epsilon_3 + \frac{k^2}{2m_3}
\end{pmatrix} + \lambda \begin{pmatrix}
0 & 0 & ik_x \\
0 & 0 & ik_y \\
-ik_x & -ik_y & 0
\end{pmatrix}.$$

Here $\mathcal{H}$ is the $2 \times 2$ Hamiltonian defined in Eq. (\[\text{Eq. 3}\]), $\lambda$ is the coupling strength between them responsible for hybridization. For $\epsilon_3m_3 < 0$ and $\lambda = 0$, singlet and doublet surface bands cross at $k \neq 0$. A finite coupling $\lambda \neq 0$ turns the band crossing into an avoided crossing and opens up an energy gap. The resulting surface states cease to be protected: they can be smoothly pushed into the bulk continuum. This shows that the intervention from singlet bands can in principle destroy the gapless surface state with quadratic degeneracy. However, the above scenario requires the coexistence of singlet surface state under particular conditions, which seems very non-generic in real materials. Therefore we are optimistic that surface states with quadratic degeneracy on topological crystalline insulators are robust for practical purposes.