We propose second-order topological insulators (SOTIs) whose lattice structure has the hexagonal symmetry $C_6$ in three and two dimensions. We start with a three-dimensional weak topological insulator constructed on the stacked triangular lattice, which has only side topological surface states. We then introduce an additional mass term which gaps out the side surface states but preserves the hinge states. The resultant system is a three-dimensional SOTI. The bulk topological quantum number is shown to be the $Z_3$ index protected by the inversion time-reversal symmetry $IT$ and the rotoinversion symmetry $C_6I$. We obtain three phases; trivial, strong and weak SOTI phases. We argue the origin of these two types of SOTIs. A hexagonal prism is a typical structure respecting these symmetries, where six topological hinge states emerge at the side. The building block is a hexagon in two dimensions, where topological corner states emerge at the six corners in the SOTI phase. Strong and weak SOTIs are obtained when the interlayer hopping interaction is strong and weak, respectively. They are characterized by the emergence of hinge states attached to or detached from the bulk bands.

Topological phase of matter remains to be a most active field of condensed matter physics. Topological insulators (TIs) are well established, where the emergence of topological boundary states is a manifestation of the bulk topological number. This is known as the bulk-boundary correspondence. Recently, the notion of topological insulators is generalized to second-order topological insulators (SOTIs). A SOTI is such an insulator that has no topological surface states though it has topological hinge states. They are one-dimensional (1D) edge states emerging at hinges of a prism respecting the symmetry based upon which the bulk topological quantum number is defined.

One powerful method to create a SOTI is to introduce a mass term to a strong TI in such a way that it gaps out surface states but preserves hinge states. A topological hinge insulator was first constructed by applying this method to the $C_4$ symmetric lattice model. However, in this model, a tetragonal prism of finite size has gapless surface states at the top and the bottom of the prism in addition to four gapless hinge states. This is because the symmetry indicator is characterized by $C_4T$ and $C_4 = C_4I$, where $T$ and $I$ are the time-reversal symmetry generator and the inversion generator, respectively. These surface states can be gapped out by introducing the Zeeman term violating $C_4T$ but preserving $C_4$. The bulk topological number, being characterized by the rotoinversion symmetry $C_4$, is given by the $Z_2$ index.

Very recently, a SOTI was experimentally materialized in Bismuth by employing topological quantum chemistry for material prediction. It has the $C_6$ symmetric lattice structure, while the bulk topological quantum number, being characterized by $C_3$, $T$, and $I$, is given by the $Z_2$ index. The tight-binding model has been proposed, but it is an eight-band model and rather too complicated.

In this paper, we propose a simple four-band model possessing the $C_6$ symmetric lattice structure realizing a SOTI. We start with a weak TI realized on the stacked triangular lattice, whose topological surface states are present only at the side surfaces. Namely, it has no gapless surface states at the top and the bottom when we consider a hexagonal prism of finite size as in Fig.1(a). Then, we gap out the side surface states by introducing an additional mass term with parameter $\Delta$. As a result, we obtain a SOTI, which has topological hinge states as in Fig.1(b). The bulk topological quantum number is shown to be the $Z_3$ index characterized by combinations of the rotoinversion symmetry $C_6 = C_6I$ and the inversion time-reversal symmetry $IT$. In accord with the $Z_3$ index, there exist two different types of SOTIs. We call them strong and weak SOTIs.

2D Hamiltonian: We start with the 2D Hamiltonian:

$$H_{2D}^0 = H_t \tau_z + H_{SO} \tau_x$$

FIG. 1: (a)–(b) A hexagonal prism is a typical structure respecting the rotoinversion symmetry $C_6$. The real-space plot of the local density of states $\rho_z$ for a hexagonal prism in the case of (a) a weak TI ($\Delta = 0$) and (b) a topological hinge insulator ($\Delta = 0.7$). The amplitude is represented by the radius of spheres. The length of one side of the hexagon is $L = 8$, and the height of the prism is $H = 11$. (c)–(d) A hexagon is a typical structure respecting the rotoinversion symmetry $C_6$. The real-space plot of $\rho_z$ for a hexagon in the case of (c) a TI and (d) a topological corner insulator. We have set $t = 1$, $t_z = 2$, $\lambda = \lambda_z = 1$ and $m = 3$. 

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on the triangular lattice, where

\[ H_t = \sum_{n=1}^{3} \left[ m - t \sum \cos(d_n \cdot k) \right] , \tag{2} \]

\[ H_{SO} = \lambda \sum_{n=1}^{3} C_{\mu}^{n} \sigma_{x} C_{3}^{-\mu} \sin(d_n \cdot k) \tag{3} \]

in the momentum space. Here, \( m, t, \lambda \) are real parameters, \( k = (k_x, k_y) \), and \( d_n = |d_n|[\cos(2\pi n/3), \sin(2\pi n/3)] \) is the pointing vector; \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) and \( \tau = (\tau_x, \tau_y, \tau_z) \) represent the Pauli matrices for the spin and the pseudospin corresponding to the orbital degrees of freedom, respectively; \( C_3 = \tau_0 \exp[-i\pi \sigma_z/3] \) is the generator of the \( \pi/3 \) rotation. It has been shown that the Hamiltonian \( H_{2D}^0 \) describes a 2D TI. According to the bulk-boundary correspondence there emerge gapless edge states for a hexagon as in Fig.2(c).

We propose to consider the Hamiltonian

\[ H_{2D} = H_{2D}^0 + H_{\Delta} \tau_0 \] \tag{4}

with

\[ H_{\Delta} = \Delta \sum_{n=1}^{3} C_{\mu}^{n} \sigma_{y} C_{3}^{-\mu} \cos(d_n \cdot k) \] \tag{5}

where \( \Delta \) is a real parameter. This term is a hexagonal generalization of the term proposed for the tetragonal symmetric system\(^{29}\). Its role is to gap out edge states except for the corners, leading to a 2D topological corner insulator as in Fig.1(d), about which we discuss at the end of this paper.

3D Hamiltonian: We may stack triangular lattices to generate a 3D lattice. The relevant Hamiltonian is given by

\[ H_{3D}^0 = H_{2D}^0 + H_z \quad \text{or} \quad H_{3D} = H_{2D} + H_z \] \tag{6}

depending whether \( \Delta = 0 \) or \( \Delta \neq 0 \), with

\[ H_z = -t_z \tau_z \cos k_z + \lambda_z \tau_x \sin k_z , \] \tag{7}

which is a well-known term describing interlayer hopping with real parameters \( t_z \) and the spin-orbit interaction \( \lambda_z \).

We consider a hexagonal prism of finite size subject to \( H_{3D}^0 \). Provided both \( t_z \) and \( \lambda_z \) are small enough, since the prism is simply obtained by stacking hexagons having the density of state as in Fig.1(c), it has naturally topological surface states at the six sides but none at the top and bottom. This remains true even if the parameters \( t_z \) and \( \lambda_z \) are not small based on explicit calculations. See Fig.2(a)–(c) with respect to the absence of gapless surface states at the top and the bottom. Such an insulator is called a weak TI. The problem is how to gap out the side surface states preserving the hinge states. This is the main issue of the present work. Our result demonstrates
that the $H_{\Delta\tau_0}$ term transforms the weak TI into a topological
hinge insulator as in Fig. 1(b).

**Topological phase diagram:** We analyze the Hamiltonian
$\mathcal{H}_{3D}$. The band structure is obtained by diagonalizing it. The
essential point is that the bulk topological quantum number is
defined by the band structure at the six high-symmetry points with respect to the six-fold rotoinversion: See (15) with (14). They are $\Gamma = (0, 0, 0)$, $K = (4\pi/3, 0, 0)$,
$K' = (-4\pi/3, 0, 0)$, $A = (0, 0, \pi)$, $H = (4\pi/3, 0, \pi)$,
$H' = (-4\pi/3, 0, \pi)$. Consequently, to determine the topological
phase boundaries, it is enough to solve the zero-energy condition ($E = 0$) at these six high-symmetry points.

The energies at these points are analytically obtained as

$$E(\Gamma) = \pm (3t + t_z - m),$$  \hspace{1cm} (8)

$$E(K) = E(K') = \pm (3t/2 - t_z + m),$$  \hspace{1cm} (9)

$$E(A) = \pm (3t - t_z - m),$$  \hspace{1cm} (10)

$$E(H) = E(H') = \pm (3t/2 + t_z + m).$$  \hspace{1cm} (11)

The topological phase boundary is given by $t_z = \pm 3t + m$
and $t_z = \pm 3t/2 - m$, which are shown in Fig 2(m). They are
independent of the values of $\lambda, \lambda_z, \Delta$.

**Symmetries:** In order to identify the bulk topological quantum
number, it is necessary to study the symmetry of the
Hamiltonian $\mathcal{H}_{3D}$. We note that the Hamiltonian
$\mathcal{H}_{3D}$ has both the time-reversal symmetry $T \mathcal{H}_{3D}(k) T^{-1} = \mathcal{H}_{3D}(-k)$
and the inversion symmetry $I \mathcal{H}_{3D}(k) I^{-1} = \mathcal{H}_{3D}(-k)$, where
$T = -i\tau_0\sigma_y K$ generates the time reversal symmetry (TRS)
with the complex conjugation $K$, while $I = \tau_z\sigma_0$ is the
inversion symmetry generator. In addition, there is the six-fold
rotational symmetry $C_6$,

$$C_6 \mathcal{H}_{3D}(k_x, k_y, k_z) \mathcal{C}_6^{-1} = \mathcal{H}_{3D}(k'_x, k'_y, k'_z),$$  \hspace{1cm} (12)

where $C_6 = \tau_0 \exp[-i\pi\sigma_z/6]$ is the generator of the $\pi/6$
rotation, and

$$k'_x = k_x/2 + \sqrt{3}k_y/2, \hspace{1cm} k'_y = \sqrt{3}k_x/2 + k_y/2.$$  \hspace{1cm} (13)

The term $H_{\Delta}$ breaks both the TRS and the inversion symmetry
but preserves the combined symmetry $IT$ and the rotoinversion
symmetry $C_6 = C_6 I$, which is similar to the case of the
tetragonal system.

**Symmetry indicator:** The symmetry indicator is already
known for the tetragonal system possessing the $C_4$ and $IT$
symmetries. By making its hexagonal generalization, we define the symmetry indicator $\kappa_6$ protected by the $C_6$ and $IT$
symmetries by the formula

$$\kappa_6 = \frac{1}{2\sqrt{3}} \sum_k \sum_\alpha e^{i\alpha \pi} n^\alpha_K,$$  \hspace{1cm} (14)

where $k$ runs over the symmetry invariant points associated with the $C_6$, $\Gamma$, $K$, $K'$, $A$, $H$ and $H'$; $n^\alpha_K$ is the number of the
occupied bands with the eigenvalue $e^{i\alpha \pi}$ of the symmetry
operator $C_6$, $C_6|\psi\rangle = e^{i\alpha \pi} |\psi\rangle$. The symmetry indicator is
shown to be quantized and real. First, $\alpha$ is quantized to be
$\alpha = 1, 3, 5, 7, 9, 11$, because of the relation $(C_6)^{\alpha} = -1$.

Second, $\kappa_6$ is real, since the band structure is always
two-fold degenerated in the presence of the $IT$ symmetry. The
symmetry eigenvalues form a conjugate pair for these bands
due to the commutation relation $[C_6, IT] = 0$ and the fact
that the $IT$ symmetry is anti-unitary. Third, $\kappa_6$ is a constant
within one topological phase since it can change its value only
when a phase boundary is crossed by changing system parameters.
Consequently it is a candidate of the topological quantum
number. We explicitly evaluate $\kappa_6$ using the formula (14),
which is shown in the phase diagram Fig 2(m).

**Surface states:** We first examine the surface states by analyzing
the band structure of a thin film. (i) When $\Delta = 0$, gapless
modes are found in the side surfaces [Fig 2(d)–(e)] in the
TI phase, but not in the up and bottom surfaces [Fig 2(a)–(b)],
which shows that the system is a weak TI. (ii) When $\Delta \neq 0$, these
surface states are gapped [Fig 2(g)–(h)]. These features are
consistent with the local density of states for the hexagonal prism
as shown in Fig 3(a)–(b). Hence, the system is naively a trivial insulator according to the bulk-boundary correspondence. However, as we now see, hinge states appears.

**Hinge states and $\mathbb{Z}_3$ index protected by $C_6$ and $IT$:** We
next investigate the hinge states by analyzing the band structure
of a hexagonal prism [Fig 2(i)–(j)] at various points in the
phase diagram [Fig 2(m)]. According to the band structure of a
hexagonal prism, hinge states emerge in the two phases indexed by $\kappa_6 = \pm 1$ as in Fig 2(i)–(k), while no hinge states are present in the phase indexed by $\kappa_6 = 0, \pm 3$ as in Fig 2(l). They are identified with SOTI and trivial phases. The two
SOTI phases indexed by $\kappa_6 = \pm 1$ are distinguished by the band structure of hinge states. Namely, hinge states are detached from (attached to) the bulk band for $\kappa_6 = -1$ ($\kappa_6 = 1$): See Fig 2(i) and (k). Consequently, the bulk topological index
is given by the $Z_3$ index defined by
\[ \nu_{3D} = \text{mod}_3 \kappa_6, \] (15)
which is a generalization of the $Z_2$ index $\nu_0$ into the hexagonal symmetric system in the absence of the TRS and the inversion symmetry.

It is intriguing that we have two different types of hinge states. We may understand their origin as follows. Recall that the hexagonal prism is described by the Hamiltonian $H_{3D} = H_{2D} + H_z$. The building block of a hexagonal prism is a hexagon described by $H_{2D}$. As we soon discuss, it has six detached corner states protected topologically, as shown in Fig.1(4). Hence, when we construct a prism by stacking hexagons, we would obtain a perfect flat band for the hinge states in the vanishing limit of interlayer hopping ($H_z \to 0$). Since the flat band is deformed solely by the interlayer hopping interaction, we expect that such hinge states are determined by the Hamiltonian $H_z$. Indeed, the band structure of the detached hinge states is obtained analytically by diagonalizing the Hamiltonian $H_z$, and given by
\[ E = \pm \frac{1}{\sqrt{2}} \sqrt{t_z^2 + \lambda_z^2 + (t_z^2 - \lambda_z^2) \cos 2k_z}. \] (16)

This solution well reproduces the detached hinge states in Fig 2(i). This is the origin of hinge states in the SOTI phase with $\kappa_6 = -1$, which we call a weak SOTI phase. On the other hand, when the interlayer hopping interaction is strong, a mixed occurs between $H_{2D}$ and $H_z$, making the corner states a part of the bulk bands. The resultant hinge states form the SOTI phase with $\kappa_6 = 1$, which we call a strong SOTI phase.

2D SOTI: We study a hexagonal SOTI model in two dimensions. The Hamiltonian is $H_{2D}$ given by [1]. The symmetry analysis is almost the same as in the 3D case just by neglecting the $z$ coordinate. The properties of the 2D hexagonal SOTI are summarized as follows.

First, the topological phase diagram is obtained by setting $t_z = 0$ in Fig.2(m). Namely, there emerge a SOTI phase for $-3/2 < m/t < 1$, and trivial phases for $m/t < -3/2$ and $m/t > 3$. Second, the $\kappa_6$ index is obtained as $\kappa_6 = 3/2$ for $m/t < -3/2$, $\kappa_6 = -1/2$ for $-3/2 < m/t < 1$ and $\kappa_6 = -3/2$ for $m/t > 3$. Hence, we define the bulk topological quantum number as
\[ \nu_{2D} = \text{mod}_3 (2\kappa_6). \] (17)

Third, we show the band structure of a nanoribbon in Fig.3. When $\Delta = 0$, there are helical edge states in Fig.3(b). We have previously shown [22] that the system is a TI. They are gapped for $\Delta \neq 0$ as in Fig.3(e), indicating that the system would be topologically trivial. Actually, it is not trivial but it is in the SOTI phase. Indeed, when we evaluate the eigenvalues of a hexagonal nanodisk, six-fold degenerate zero-energy corner states emerge for the SOTI phase as in Fig.3(h), showing the system is a topological corner insulator as in Fig.1(d).

In this work we have presented a simple model for a hexagonal topological hinge insulator. Although the hinge structure at the sides looks the same as that of Bismuth, there are some difference between them. Indeed, the topological quantum number is the $Z_3$ index in the present model but it is the $Z_2$ index in the Bismuth model. The origin of the difference is traced back to the fact that a hexagonal prism is constructed by stacking hexagons which are weak TIs. It yields two types of SOTIs depending on the interlayer hopping interaction whether it is strong or weak.

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