Dual Topological Character of Chalcogenides: Theory for Bi_2Te_3

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A topological insulator is realized via band inversions driven by the spin-orbit interaction. In the case of $\mathcal{Z}_2$ topological phases, the number of band inversions is odd and time-reversal invariance is a further unalterable ingredient. For topological crystalline insulators, the number of band inversions may be even but mirror symmetry is required. Here, we prove that the chalcogenide Bi_2Te_3 is a dual topological insulator: it is simultaneously in a $\mathcal{Z}_2$ topological phase with $\mathcal{Z}_2$ invariants $(\nu_0;\nu_1\nu_2\nu_3) = (1;000)$ and in a topological crystalline phase with mirror Chern number -1. In our theoretical investigation we show in addition that the $\mathcal{Z}_2$ phase can be broken by magnetism while keeping the topological crystalline phase. As a consequence, the Dirac state at the (111) surface is shifted off the time-reversal invariant momentum $\bar{\Gamma}$; being protected by mirror symmetry, there is no band gap opening. Our observations provide theoretical groundwork for opening the research on magnetic control of topological phases in quantum devices.

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Introduction.—$\mathcal{Z}_2$ topological insulators are band insulators featuring surface states that are spin polarized and cross the fundamental band gap [1,2]. This is a consequence of an odd number of inversions of bulk bands that are driven by the spin-orbit interaction alone or in combination with crystal lattice distortions [3–5] or chemical disorder [6,7]. The odd number of bulk-band inversions distinguishes a $\mathcal{Z}_2$ topological insulator phase from a conventional band insulator phase, as has been proven for the $\mathcal{Z}_2$ topological insulators Bi_xSb_{1-x} and the chalcogenides Bi_2Se_3, Sb_2Te_3 and Bi_2Te_3 [6,8,9]. The Dirac surface state of a $\mathcal{Z}_2$ topological insulator is located at a time-reversal invariant momentum (TRIM) of the two-dimensional Brillouin zone. Since it is protected by time-reversal symmetry, the surface state is robust against time-reversal-invariant perturbations (e.g., nonmagnetic adatoms).

Narrow band gap semiconductors, like SnTe, show an even number of band inversions [10] and, thus, do not belong to the $\mathcal{Z}_2$ topological class ($\nu_0 = 0$). However, they show a Dirac surface state that is protected by crystal symmetry, rather than by time-reversal symmetry. Hence, they belong to the class of topological crystalline insulators [11]; their mirror Chern number is -2 [10,12]. The two Dirac surface states are located within a mirror plane perpendicular to the surface but not necessarily at a TRIM of the two-dimensional Brillouin zone.

An insulator that belongs simultaneously to the $\mathcal{Z}_2$ phase and to the topological crystalline phase—a *dual* topological insulator—would allow us to manipulate its topological phase, and consequently its conducting Dirac surface state, by magnetism, either by an external magnetic field or by doping with magnetic atoms. Applying a magnetic field perpendicular to a mirror plane of the crystal lattice would on one hand break time-reversal symmetry and, as a consequence, destroy the $\mathcal{Z}_2$ topological phase. On the other hand, the mirror symmetry is maintained and the topological crystalline phase is kept. The Dirac surface state that is still protected by mirror symmetry would be shifted off the TRIM, without opening of a band gap (Fig. 1). Applying a magnetic field with a component within the mirror plane would destroy both the $\mathcal{Z}_2$ phase and the topological crystalline phase; a band gap will open up in the Dirac state, leading to a conventional insulator phase [13].

In this Letter, we prove that the exemplary chalcogenide Bi_2Te_3 is such a *dual* topological insulator: besides being in its well-established $\mathcal{Z}_2$ phase, it is simultaneously in the topological crystalline phase. Teo *et al.* have predicted that $Bi_{1-x}Sb_x$ is a dual topological insulator [6]. On top of this, we show by theoretical electronic structure calculations that the above sketched scenario of magnetic control of topological phases holds. Furthermore, Bi_2Te_3 has $\mathcal{Z}_2$ invariants of $(\nu_0;\nu_1\nu_2\nu_3) = (1;000)$; consequently, a Dirac surface state would exist on any crystal truncation plane. In other words, a sphere made of Bi_2Te_3 would show a Dirac state anywhere on its surface. In contrast, a topological crystalline insulator would show a Dirac state only in surface planes normal to the mirror plane. Hence, a Bi_2Te_3 sphere in a magnetic field perpendicular to the mirror plane would host Dirac states only on circles that lie within the mirror plane.

$\mathcal{Z}_2$ invariant and mirror Chern number.—To prove that Bi_2Te_3 is a dual topological insulator we first calculate the $\mathcal{Z}_2$ invariant and the mirror Chern number for the bulk system, using a first-principles-based tight-binding method (see the Supplemental Material [14]). The $\mathcal{Z}_2$ invariants are computed to $(\nu_0;\nu_1\nu_2\nu_3) = (1;000)$, in agreement with earlier calculations [8,15]. For the computation of the mirror Chern number [6], we consider a mirror plane

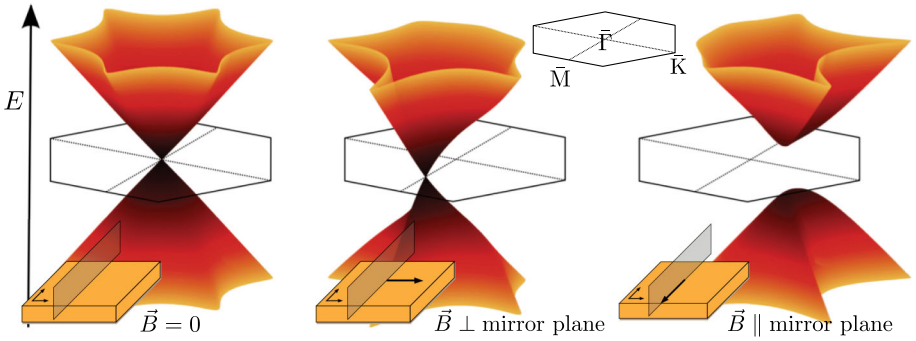

FIG. 1 (color online). Variation of a Dirac surface state's dispersion with respect to the topological phase (schematic): without magnetic field (left, $\vec{B} = 0$: dual topological insulator), with magnetic field perpendicular to a mirror plane (center, $\vec{B}\perp$ mirror plane: topological crystalline insulator), and with magnetic field within the mirror plane (right, $\vec{B}\parallel$ mirror plane: conventional insulator). The dispersions calculated from Fu's model [20] are shown in perspective view. The inset displays the surface Brillouin zone. The $\bar{M}$-$\bar{\Gamma}$-$\bar{M}$ direction lies within a mirror plane.

perpendicular to the (111) surface [like for the (001) surface of SnTe [10,16]; left in Fig. 2]. The mirror Chern number equals -1 and is interpreted as follows. On one hand, its modulus gives the number of nonequivalent Dirac surface states, as has been established in Ref. [6]; indeed, $Bi_2Te_3(111)$ hosts a single Dirac state. On the other hand, its sign gives the chirality of the spin texture of the Dirac surface state: the spin polarization of the Dirac states rotates clockwise about the surface normal at energies above the Dirac point. Already these findings prove that Bi_2Te_3 is a dual topological insulator, that is both a $\mathcal{Z}_2$ topological insulator and a topological crystalline insulator.

Now we show that the $\mathcal{Z}_2$ topological phase can be broken while keeping the topological crystalline phase. For this purpose we mimicked an external magnetic field by adding a Zeeman term to the tight-binding Hamiltonian. In this case, time-reversal symmetry is broken [17] and a $\mathcal{Z}_2$ invariant cannot be defined. If the magnetic field (i.e., an axial vector) is perpendicular to the mirror plane, the reflection symmetry is maintained and the mirror Chern number is still computed to -1, proving the topological crystalline phase. If the magnetic field lies within the mirror plane, both time-reversal and mirror symmetry are broken: neither the $\mathcal{Z}_2$ invariant nor the mirror Chern number can be defined in this case.

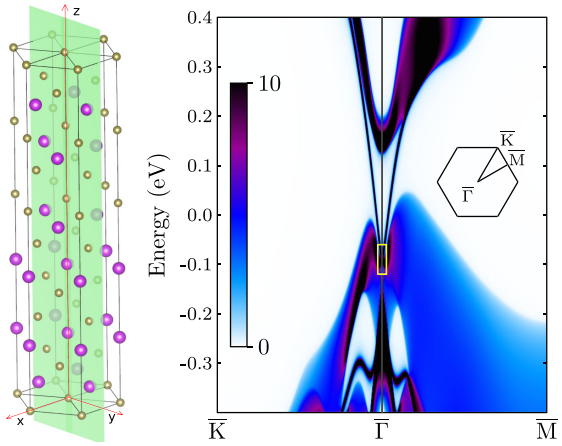

FIG. 2 (color online). Left: perspective view of Bi_2Te_3. Each of the quintuple layers shown consists of two Bi atoms (large magenta spheres) and three Te atoms (small brown spheres). The shaded green area depicts the yz mirror plane of the crystal (z along [111]). Right: Dirac surface state in $Bi_2Te_3(111)$, obtained from tight-binding calculations. The spectral density of the topmost quintuple layer is shown as color scale (in states per eV) along a $\bar{K}$-$\bar{\Gamma}$-$\bar{M}$ path of the two-dimensional Brillouin zone (inset). The yellow rectangle highlights the (E, k) area addressed in Fig. 3.

These findings suggest that the topological character of Bi_2Te_3 can be controlled by magnetism: from a dual topological insulator (no magnetic field) via a solely topological crystalline insulator (magnetic field perpendicular to mirror plane) to a conventional insulator (magnetic field within mirror plane).

Surface electronic structure.—The next step is to show how the Dirac surface state of Bi_2Te_3 is affected by the topological character. We computed the electronic structure of $Bi_2Te_3(111)$, using the tight-binding method and a renormalization scheme for semi-infinite systems [18]. Without magnetic field, the well-known Dirac surface state with its unique spin texture [15,19] has its Dirac point located very close to the valence band in the pocket at $\bar{\Gamma}$, the center of the surface Brillouin zone (right in Fig. 2). This electronic state is mostly affected by magnetism in an (E, k) region close to its Dirac point; hence, a zoom into this region is indispensable (rectangle in Fig. 2). In the following, we present exemplary results for a magnetic field with 0.03 eV Zeeman energy.

For a magnetic field $\vec{B}$ perpendicular to the mirror plane, the surface state is shifted off the TRIM by $\delta k = 0.01$ Å^{-1} (Fig. 3); this displacement lies within the mirror plane (here: k_y). There is no band gap opening [compare (e) and (f) in Fig. 3]; the Dirac point "survives," which indicates a topological nontrivial phase. In contrast, the dispersion along the magnetic field (here: k_x, i. e., normal to the

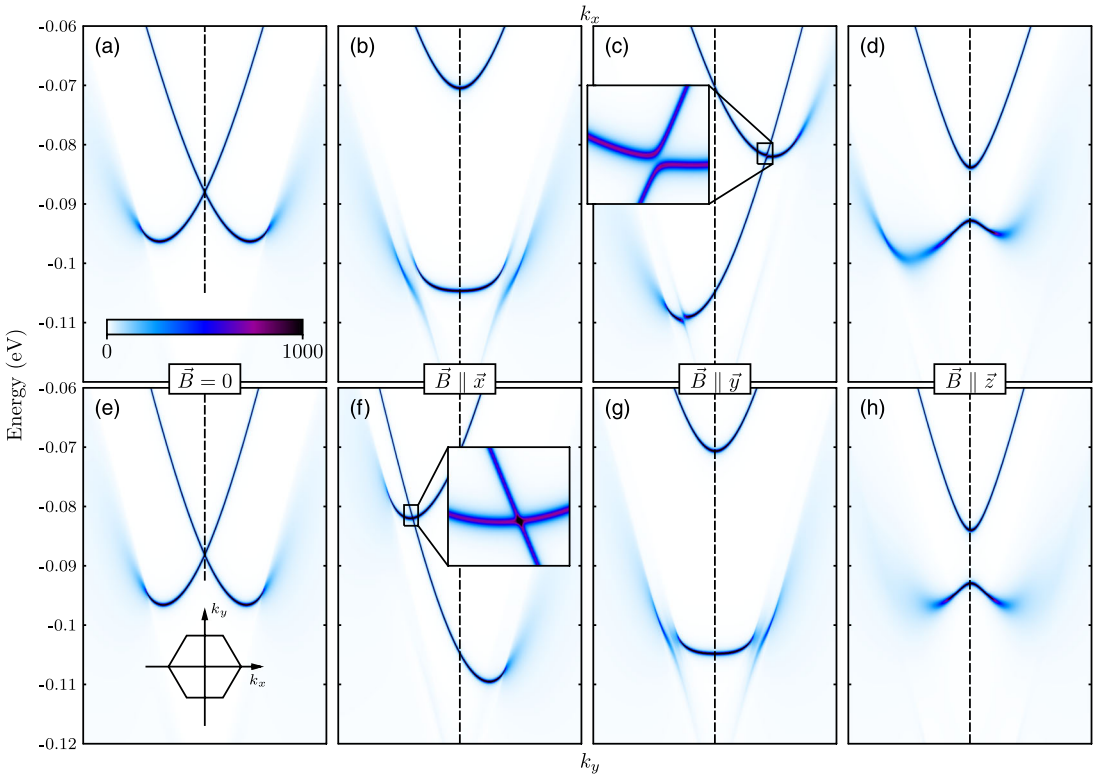

FIG. 3 (color online). Dispersion of the Dirac state at $Bi_2Te_3(111)$ for different magnetic configurations. Only a small part of the two-dimensional Brillouin zone (indicated in Fig. 2) is displayed (top row: k_x; bottom row: k_y; the respective zeroes are indicated by vertical dash-dotted lines). Without magnetic field [$\vec{B} = 0$, (a) and (e)], Bi_2Te_3 is in its dual topological phase (Dirac point at $\vec{k}_\parallel = 0$). For an in-plane magnetic field $\vec{B} \| \vec{x}$ [(b) and (f)] it stays in its topological crystalline phase; the inset in (f) zooms into the Dirac point shifted along k_y. For both $\vec{B} \| \vec{y}$ [(c) and (g)] and $\vec{B} \| \vec{z}$ [(d) and (h)] the topological phase is trivial: there is no Dirac point [cf. the zoom into the tiny band gap in (c)]. The color scale, in states per eV, displays the spectral density of the topmost quintuple layer. In regions in which the Dirac state hybridizes with bulk electronic states, the spectral density becomes blurred.

mirror plane) is gapped, with an energy splitting of about 34 meV [(b) in Fig. 3].

For $\vec{B}$ within the mirror plane (here: normal to the surface, i.e., along the z direction), Bi_2Te_3 becomes a conventional insulator: a band gap opens in the entire Brillouin zone [panels (d) and (h) in Fig. 3]. The gap width is smallest at the "avoided Dirac point" at $\bar{\Gamma}$, with a magnitude of 9 meV.

For $\vec{B}$ along the y direction (i.e., within both the surface plane and the mirror plane), a tiny gap shows up, with a width of 0.3 meV [panel (c) in Fig. 3]. Hence, also in this setup, Bi_2Te_3 is in principle a conventional insulator; however, the gap width is much smaller than the thermal energy of 25 meV at room temperature. Thus, this band gap is not relevant in device applications. A closer analysis reveals that this gap is due to spin-orbit coupling, while that for $\vec{B} \| \vec{z}$ is attributed to exchange splitting.

These electronic structure calculations for the (111) surface fully confirm the considerations based on the topological invariants. We provide further qualitative support by a model Hamilton operator for a two-dimensional electron gas [20] that has been extended to account for magnetism.

Model calculations.—To investigate the effect of the topological character on the Dirac state we derived a $\vec{k} \cdot \vec{p}$ model Hamilton operator [21]; magnetism is mimicked by a Zeeman term (see Supplemental Material [14]). This operator without the Zeeman term agrees within third order of the wave vector components with that derived by Fu [20].

The model Hamilton operator illustrates in the case of zero magnetic field the different dispersions of the Dirac state along the two different high symmetry lines $\bar{\Gamma}$-$\bar{M}$ and $\bar{\Gamma}$-$\bar{K}$ in the surface Brillouin zone, cf., the warping in Figs. 1 and 2. The spin structure of the Dirac state, especially the out-of-plane component, fits to experimental findings [9,22]. If magnetism is taken into account, the Hamilton operator is not invariant under time-reversal and one expects a gap to open up at the Dirac point (Fig. 1). However, for a magnetic field pointing perpendicular to a mirror plane, there is no gap but the Dirac point is shifted within the mirror plane. These findings are in line with the tight-binding calculations and corroborate the dual topological character of Bi_2Te_3.

Because the magnetism-induced band gaps are small, the contours of the Dirac surface state in constant energy cuts

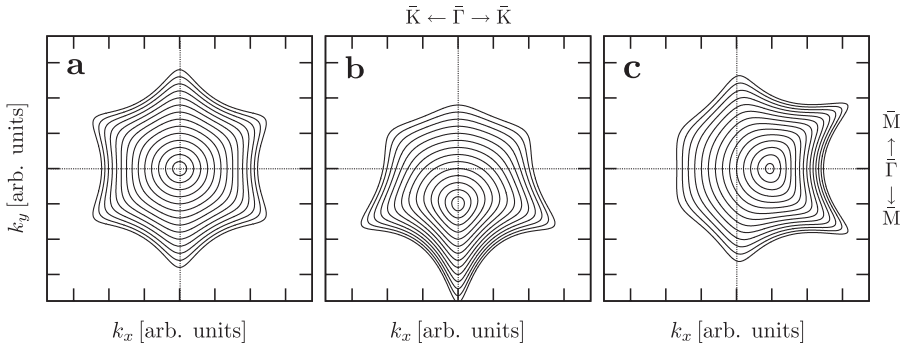

FIG. 4. Effect of a magnetic field on the dispersion of a Dirac state, obtained from a model calculation (schematic; see text). Constant energy contours are calculated (a) without magnetic field ($\vec{B} = 0$), (b) with magnetic field perpendicular to a mirror plane ($\vec{B} \| \vec{x}$), and (c) with magnetic field within the mirror plane ($\vec{B} \| \vec{y}$). The k_x (k_y) axis is along $\bar{K}$-$\bar{\Gamma}$-$\bar{K}$ ($\bar{M}$-$\bar{\Gamma}$-$\bar{M}$).

may be used as a signature for a shift of the Dirac point. These contours can be investigated in very high resolution photoelectron spectroscopy [23]. For $\vec{B} = 0$, the circular contours at energies close to the Dirac point become hexagonally warped at increased energies (Fig. 4a). These 'snowflake' shapes are distorted for in-plane magnetic fields [(b) and (c)] and show in addition centers shifted in direction perpendicular to $\vec{B}$.

Concluding remarks.—Our investigations prove theoretically that the topological character of dual topological insulators can be manipulated by magnetism: from the dual "$\mathcal{Z}_2$ plus crystalline" phase via the topological crystalline phase to the conventional insulating phase. The associated opening of a band gap in the Dirac state could be exploited in device applications. Although our study provides strong support for this scenario—by means of model calculations and semi-empirical calculations for the realistic system Bi_2Te_3—experimental verification is necessary, for example by means of photoelectron spectroscopy [24]. An alternative is Landau level spectroscopy [25] which has been applied to the Dirac surface state of Bi_2Se_3 [26] and to BiTeI [27].

Considering transport measurements, the dual topological character of $Bi_2Te_3(111)$ thin films suggests a new setup for the quantum anomalous Hall effect, as has been proposed by Liu *et al.* [28]. So far, it was believed the quantum anomalous Hall effect requires an external magnetic field perpendicular to the film to achieve an insulating state [29,30]. As shown by Liu and co-workers, an in-plane magnetic field also results in a nonzero Hall conductance, provided the field is not perpendicular to a mirror plane. If the field is in-plane and perpendicular to a mirror plane, Bi_2Te_3 is a topological crystalline insulator—shown in this Letter—and, as a consequence, the Dirac surface state is not gapped and the Hall conductance vanishes.

In this Letter, we consider magnetism brought about by an external magnetic field, resulting in small band gaps in the Dirac surface state (Fig. 3). In view of applications, larger gap widths are obtained by doping the topological insulator with magnetic constituents [31,32]. By controlling the directions of the magnetic moments by an external magnetic field, the topological character can be varied from topologically crystalline to trivial, provided the doping maintains the mirror symmetry.

This work focuses on Bi_2Te_3; calculations of the topological invariants for the other chalcogenides —Sb_2Te_3 and Bi_2Se_3—prove that these are also dual topological insulators. This is expected for they show the same crystal symmetry and the same topology of the bulk electronic structure (e.g., the band inversion at the Brillouin zone center).

A question arises whether there exist, besides the chalcogenides, other dual topological insulators. One might expect that each $\mathcal{Z}_2$ topological insulator with band inversions in a mirror plane could be a dual topological insulator. In a detailed theoretical investigation, Teo *et al.* have shown that $Bi_{1-x}Sb_x$ ($x > 0.03$) is a strong topological insulator with $\mathcal{Z}_2$ invariants (1;1 1 1) and mirror Chern number -1 [6].

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