Spin-polarization control driven by a Rashba-type effect breaking the mirror symmetry in two-dimensional dual topological insulators

Carlos Mera Acosta\textsuperscript{1,2,}\* and Adalberto Fazzio\textsuperscript{1,2}

\textsuperscript{1}Institute of Physics, University of Sao Paulo, CP 66318, 05315-970, Sao Paulo, SP, Brazil
\textsuperscript{2}Brazilian Nanotechnology National Laboratory, CP 6192, 13083-970, Campinas, SP, Brazil

Three-dimensional topological insulators protected by both the time reversal (TR) and mirror symmetries were recently predicted and observed. Two-dimensional materials featuring this property and their potential for device applications have been less explored. We find that in these systems, the spin-polarization of edge states can be controlled with an external electric field breaking the mirror symmetry. This symmetry requires that the spin-polarization is perpendicular to the mirror plane, while in QSHIs, the electric field induces spin-polarization components parallel to the mirror plane. Since this field preserves the TR topological protection, we propose a transistor model using the spin-direction of protected edge states as a switch. In order to illustrate the generality of the proposed phenomena, we consider compounds protected by mirror planes parallel and perpendicular to the structure, e.g., Na\textsubscript{3}Bi and half-functionalized (HF) hexagonal compounds, respectively. For this purpose, we first construct a tight-binding effective model for the Na\textsubscript{3}Bi compound and predict that HF-honeycomb lattice materials are also dual topological insulators.

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The quantum geometrical description of the insulator state gave rise to a breakthrough in the understanding of the topological phases in solids [1–4]. Topological invariants, e.g., the Z\textsubscript{2} invariant and the Chern number \( C \), classify insulators according to the preserved symmetries and the "symmetry-charge" pumped to the boundary [5]. Systems featuring a non-zero topological invariant, i.e., topological insulators (TIs), support dissipationless metallic boundary (edge/surface) states protected by a specific crystal symmetry on a bulk insulator [6]. For instance, quantum spin Hall insulators (QSHIs) and topological crystalline insulators (TCIs) are two-dimensional (2D) materials characterized by Z\textsubscript{2} = 1 [7–9] and a non-zero mirror Chern number [10–12], \( C_M \), respectively. In QSHIs, the edge states are protected by the time-reversal (TR) symmetry, while in TCIs by either point or mirror symmetries. Topological transitions are typically related to band inversions [13]: the transition from normal insulators to either QSHIs or TCIs with \( C_M = \pm 1 \) requires an odd number of band inversions, while TCIs with \( C_M = \pm 2 \) exhibit even band inversions. Naturally, \( C_M \neq 0 \) or \( \pm 2 \) intrinsically avoid the QSH state (Z\textsubscript{2} = 1).

Materials with a dual topological character (DTC), i.e., systems that are simultaneously QSHIs (TIs in three-dimensions) and TCIs [14], requires both Z\textsubscript{2} = 1 and \( C_M = \pm 1 \), which imposes a condition: it must occur only an odd number of band inversion at k-points preserving both the mirror and the TR symmetries. In view of the TR invariant momentum points always come in pairs, this condition is only satisfied by the \( \Gamma \) point. Since 2D-TCIs are typically systems with \( C_M = \pm 2 \), e.g., SnTe multilayers [11, 15], monolayers of SnSe, PbTe, PbSe [16–18], TlSe [19], and SnTe/NaCl quantum wells [20], DTC in 2D compounds have been predicted only for Na\textsubscript{3}Bi layers [21]. Three dimensional materials exhibiting DTC not only have been predicted in Bi\textsubscript{2}Te\textsubscript{3} [14], Bi\textsubscript{4}Se\textsubscript{3} [22], and Bi\textsubscript{1−x}Sb\textsubscript{x} [23], but also experimentally observed in the stoichiometric superlattice [Bi\textsubscript{2}]\textsubscript{1}[Bi\textsubscript{2}Te\textsubscript{3}]\textsubscript{2} [24].

The search for novel systems featuring DTC and the study of their potential for device applications is desired for the development of spintronics. For instance, in systems featuring DTC external, electric and magnetic fields allow the control of topological states. This intrinsic property arises from the possible separate manipulation of QSHI [25–27] and TCIs [28–30] states due to the symmetry breaking induced by the external fields, i.e., the magnetic (electric) field breaks the TR (mirror) symmetry, but the edge states could still be protected by the mirror (TR) symmetry.

In this letter, we propose the control of the edge states spin-polarization orientation through an external electric field breaking the mirror symmetry in systems exhibiting DTC, i.e., this field induced a Rashba-type effect resulting in spin-polarization components parallel to the mirror plane. Based on this effect, we suggest a transistor model using the spin-direction as a switch. In order to illustrate the generality of the proposed phenomena, we consider compounds protected by mirror planes parallel and perpendicular to the structure, e.g., Na\textsubscript{3}Bi and half-functionalized (HF) hexagonal compounds, respectively. For this purpose, we first i) construct a tight-binding effective model for the Na\textsubscript{3}Bi compound [21], and ii) predict that the TR-symmetry protected edges states in HF-honeycomb lattice materials Ref. 31 are also protected by mirror planes perpendicular to the layer, which is different from the conventional TCIs. Using the proposed models, we then study the in- and out-plane electric field breaking the mirror symmetry in Na\textsubscript{3}Bi and HF-hexagonal compounds, verifying the change of the
spin-polarization in TR-symmetry protected edge states.

**Effective Hamiltonian describing the DTC of Na\(_3\)Bi:** The Na\(_3\)Bi compound satisfies the symmetry operations: i) three-fold rotation symmetry \(R_3\) along the \(z\)-axis, ii) TR symmetry \(T\), iii) mirror symmetry \(M_x\) (\(x \rightarrow -x\)), and iv) mirror symmetry \(M_z\) (\(z \rightarrow -z\)). The TC phase is protected by the reflection symmetry respect to the plane containing the 2D layer, i.e., \(M_z\), which is schematically represented in Fig 1. In the inverted order, the valence band maximum (VBM) has a \(p\)-orbital character, mainly dominated by \(p_x\) and \(s\)-orbitals of the Bi atoms, whereas the conduction band minimum (CBM) mainly consists of \(p_y\) and \(p_z\)-Bi orbitals. At the \(\Gamma\) point, the valence (conduction) band is described by the effective states \(\{|\text{Bi} j, j_z\rangle\}\) with the total angular momentum \(J = 3/2\) (\(J = 1/2\)), i.e., \(|\text{Bi}_{1/2}, \pm 1/2\rangle\) and \(|\text{Bi}_{3/2}, \pm 1/2\rangle\), respectively. Using the symmetry operations for these states, we find an effective tight-binding Hamiltonian model describing the Na\(_3\)Bi band structure near the Fermi energy (See supplemental material). In the limit \(\vec{k} \rightarrow \Gamma\), the effective Hamiltonian reads

\[
\mathcal{H}_{Na_3Bi} = \begin{pmatrix}
-\varepsilon + \xi k^2 & 0 & 0 & \ell_- (\vec{k}) \\
0 & -\varepsilon + \xi k^2 & \ell_+ (\vec{k}) & 0 \\
0 & \ell_- (\vec{k}) & \varepsilon - \xi k^2 & 0 \\
\ell_+ (\vec{k}) & 0 & 0 & \varepsilon - \xi k^2
\end{pmatrix},
\]

where \(k_{\pm} = k_x \pm ik_y\) and \(k_2 = k_x^2 + k_y^2\). Here, \(\ell_\pm = \gamma k_{\pm} + \tilde{\gamma} k_{\pm}^2\) is the interaction term between the \(J = 1/2\) and \(J = 3/2\) states. The on-site energy (mass term) and the kinetic term for states with \(J = 1/2\) (\(J = 3/2\)) are represented by \(\varepsilon\) and \(\xi\) (\(\varepsilon\) and \(\tilde{\xi}\)), respectively. This model reproduces our density functional theory (DFT) calculation, performed using the SIESTA code[32] with the on-site approximation for the SOC[33, 34] and the Perdew-Burke-Ernzenhof generalized gradient approximation[35] for the exchange-correlation functional.

The mirror symmetry protection becomes evident when the Hamiltonian is written in the basis formed by the mirror operator eigenvectors. For any generic \(\vec{k}\)-point in the BZ, the wave-function \(|\psi_{\vec{k}} (k_x, k_y)\rangle\) (with \(\sigma = \uparrow, \downarrow\)) can be indexed with the eigenvalues of the mirror operator \(M_z\), \(m_{z,j}\). This is a consequence of commutation relation \([\mathcal{H}(k_x, k_y), M_z]\), which can be easily verified using the matrix representation \(M_z = -i\tau_z \otimes \sigma_z\), i.e., the mirror operator \(M_z\) transforms the orbitals as \(M_z |\text{Bi}_{1/2}, \pm 1/2\rangle = \mp i |\text{Bi}_{1/2}, \pm 1/2\rangle\) and \(M_z |\text{Bi}_{3/2}, \pm 1/2\rangle = \pm i |\text{Bi}_{3/2}, \pm 1/2\rangle\). Using this representation, we find the eigenvalues \(m_{z,1/2} = \pm i\) and \(m_{z,3/2} = \pm i\), and the eigenvectors \(|\phi_{z,1/2}^\pm \rangle = (Z_{\pm 1} \ 0 )\) and \(|\phi_{z,3/2}^\pm \rangle = (0 \ Z_{\mp 1} )\). Here, \(Z_i = (0 1 )\), \(Z_{-i} = (1 0 )\) and \(\vec{0} = (0 0 )\). The Hamiltonian in the basis \(|\phi_{z,1/2}^\pm \rangle, |\phi_{z,3/2}^\pm \rangle, |\phi_{\bar{z},1/2}^\pm \rangle, |\phi_{\bar{z},3/2}^\pm \rangle\) is a block diagonal matrix,

\[
\mathcal{H}_{Na_3Bi} = \begin{pmatrix}
\ell_+ (\vec{k}) & 0 \\
0 & \ell_- (\vec{k})
\end{pmatrix},
\]

where the blocks describing the mirror projected states reads

\[
h_{z,\pm i}(k_x, k_y) = \begin{pmatrix}
-\varepsilon + \xi k^2 & \ell_\pm (\vec{k}) \\
\ell_{\mp}(\vec{k}) & \varepsilon - \xi k^2
\end{pmatrix}.
\]

Thus, a perturbation breaking the mirror symmetry introduces off-diagonal matrix elements in Eq. 2. For instance, according to our *ab initio* calculations, a perpendicular electric field can be effectively included as a Rashba-type term that couples the Hamiltonians \(h_{z,\pm i}\) and \(h_{z,-i}\), i.e., \(h_R = i\lambda k x\). (See supplemental material).

The mirror Chern number, \(C_M\), is defined in terms of the states at the mirror symmetry invariant \(k\)-points. For instance, in the 3D-TCI SnTe, \(C_M\) is computed using only the \(k\)-points at the intersection between the mirror plane and the 3D-BZ. Here, since the intersection between the BZ and the mirror plane is the BZ itself, all \(k\)-points are mirror symmetry invariant. Thus, \(C_M\) is calculated through the Berry phase, \(\Omega_{n_+}^{\pm i}(k_x, k_y)\), defined in the whole BZ [10, 19], i.e., \(C_M = (C_i - C_{-i}) / 2\), where \(C_{\pm i}\) Chern number for mirror eigenvalues \(\pm i\),

\[
C_{\pm i} = \frac{1}{2\pi} \sum_{n < \ell_j} \int_{BZ} \Omega_{n_+}^{\pm i}(k_x, k_y) dx dy.
\]

Using the proposed model, we verified that \(C_{\pm i} = \mp 1\), indicating that the Na\(_3\)Bi monolayer is a TCI with \(C_M = -1\), as predicted in Ref. 21.
**Prediction of DTC in HF-honeycomb materials:** Graphene-like materials functionalized with group-VII atoms are predicted to behave as QSHIs [36]. When a VII-atom is removed from the unit cell, one sublattice exhibits dangling bonds and hence, magnetic moments due to unpaired electrons possibly spontaneously evolve into a magnetic order, spoiling the QSH states and given rise to the quantum anomalous Hall effect [37]. The electrons can be paired by substituting the non-passivated IV-atoms by atoms with an odd number of valence electrons. Thus, HF IV-V hexagonal-lattices materials, formed by two triangular sub-lattices, one consisting of an IV-VII dimer and the other of atoms V (See Fig 1), have no magnetic moment. Therefore, this systems are predicted to be mechanically stable QSHIs [31]. Since the functional moment, the systems are predicted to dimer and the other of atoms V (See Fig 1), have no magnetic moment. Thus, HF IV-V hexagonal-lattices materials, formed by two triangular sub-lattices, one consisting of an IV-VII dimer and the other of atoms V (See Fig 1), have no magnetic moment.

In these systems, the TCI phase is protected by the reflection symmetry respect to the three planes that are perpendicular to the lattice and contain the lines connecting the nearest neighbors in the honeycomb lattice.

HF-honeycomb lattice materials can display an inverted band character dominated by Bi-atoms with an odd number of valence electrons. The Fermi level lines the nearest neighbors in the honeycomb lattice. In the Na3Bi compound, a perpendicular electric field (parallel to the mirror plane) and mirror symmetries with a perpendicular magnetic field (parallel to the mirror plane) also allows to manipulate the edge states with in-plane magnetic fields. In the general case, the magnetic field $\mathbf{H}_{bi,By} = \mathbf{1} \otimes (\sigma_y B_y + \sigma_z B_z)$, gives rise to a coupling term between $h_i$ and $h_{-i}$, inducing a spin-polarization in the direction in which is applied, even for $k$-point at the mirror plane.

**Electric field effect in 2D-materials with DTC:** Metallic edge states, the most interesting feature in both TCIs and QSHIs, are computed by considering open boundary conditions in the previously discussed tight-binding models. First, we confirm the presence of edge states preserving the TR symmetry, i.e., anti-propagating spin current in each edge. Before including the electric field effects, the spin is forced to be perpendicular to the mirror plane to preserve this symmetry, i.e., oriented along the z-axis (x-axis) in Na3Bi (HF-hexagonal) compounds, as shown in Fig. 2 and 3. This suggests that external perturbations breaking the mirror symmetry could induce spin-polarization components parallel to the mirror plane, as we show below by considering an external electric field.

In the Na3Bi compound, a perpendicular electric field
model describing the Rashba effect in inversion symmetry can be understood using the phenomenological out-plane spin-polarization, as represented in Fig. 3. We find that this field induces a non-zero term, i.e., \( \tilde{N} \) of the Bi atoms in a nanoribbon formed by an external electric field breaking the mirror symmetry, leading to in-plane spin-polarization components in the bulk band structure of a nanoribbon 33.6 nm width armchair terminated for (top) \( E_0 = 0 \) V/Å and (bottom) \( E_0 = 2.67 \times 10^{-2} \) V/Å. Here, \( E_0 \) is an external electric field breaking the mirror symmetry \( M_z \) (blue plane). The color code stands for the spin orientation. The spin texture is also schematically represented in a transistor model: a nanoribbon connected to two ferromagnetic contacts (FM). This structure is deposited in a substrate (gray area). States with eigenvalue symmetry operator \( \pm i \), which are only defined if the electric field is zero, are represented by purple and green, respectively.

breaks the symmetry \( M_z \), as previously discussed. This field induces a helical spin-texture in the bulk band structure, leading to in-plane spin-polarization components in the edge states, i.e., parallel to \( M_z \), as represented in Fig. 2. The edge states are still protected by the TR-symmetry and the electric field provides a mechanism to change the spin-polarization orientation.

An external electric field breaking the mirror symmetry \( M_z \) can be introduced by modifying the on-site term, i.e., \( \tilde{e}_n(\tilde{k}) = e(\tilde{k}) + naeE_0/N \), where \( n \) is the index of the Bi atoms in a nanoribbon formed by \( N \) unit cells along the \( x \)-axis, \( a \) is the lattice constant, and \( e \) is the electron charge. We find that this field induces a non-zero out-plane spin-polarization, as represented in Fig. 3.

The effect of an electric field breaking the mirror symmetry can be understood using the phenomenological model describing the Rashba effect in inversion symmetry breaking systems: the electric field \( \tilde{E} \) induces a momentum-dependent Zeeman energy \( \tilde{\phi}_{\text{eff}} = \mu_B \tilde{B}_{\text{eff}} \cdot \sigma \) with \( \tilde{B}_{\text{eff}} = \tilde{E} \times h\tilde{k}/m_e c^2 \) \([43, 44]\). This odd-in-\( k \) effective field, i.e., \( \tilde{B}_{\text{eff}}(\tilde{k}) = -\tilde{B}_{\text{eff}}(-\tilde{k}) \), preserves the Tr-symmetry and only appears when the mirror symmetry is broken, in the same way that the Rashba effect depends on the inversion symmetry breaking \([44, 45]\). Analogous to the generic helical edge states \([46, 47]\), this field changes the direction of the spin polarization, as observed in Fig. 2 and 3. Specifically, in arm-chair nano-ribbons, the momentum carried by the electrons at the edge is oriented along the \( y \)-axis. In HF-hexagonal compounds, the external electric field is transverse (perpendicular) to the nanoribbon \( \tilde{E} = E_0 \tilde{x} \) (\( \tilde{E} = E_0 \tilde{z} \)), resulting in an effective field along the \( z \)-axis (\( x \)-axis), \( \tilde{B}_{\text{eff}} = (\mu_B/m_e c^2)E_0k_y \).

The mirror symmetry protection in HF-hexagonal materials implies that states spatially localized in different edges have the same momentum and spin direction. Thus, the spin-flip is required in scattering processes involving these states. This spin texture has also been observed in curve QSHIs \([48]\). In zigzag nanoribbons, the mirror symmetry is intrinsically broken and hence, the spin is not only oriented along the \( x \)-axis \([31]\). Although giant Rashba-splitting coexists with surface states in the 3D TIs due to the band bending and structural inversion asymmetry \([49–51]\), the consequences of the Rashba effect and transverse electric fields in surface states have not been widely explored \([52]\). Based on the tight-binding model proposed in Ref. 53, we verify that spin-polarization can also be controlled in 3D TIs with DTC (See supplemental material). The spin-polarization control proposed in this letter is different from the dynamic spin-orbit torque in anti- and ferromagnetic 2D and 3D TIs \([54–58]\), since the effective field \( \tilde{B}_{\text{eff}} \) appears for the equilibrium carrier spin density configuration and does not require magnetic order.

The change of spin orientation suggests that a simple transistor model can be constructed. If the armchair nano-ribbon of HF-honeycomb materials (Na\( _3 \)Bi) is connected to ferromagnetic electrodes, the electrons in the edge states are not detected by a drain whose magnetic moment is perpendicular to the \( x \)-axis (\( z \)-axis), as schematically represented in Fig. 3. This corresponds to the Off of the transistor. If an electric field perpendicular to the mirror plane is turned on, the electrons in the edge states have a non-zero probability of being detected by the electrode (See Fig. 3). Different from the transistors based on TCIs, in DTC insulators, the switch is not defined by the band-gap opening, but the spin-polarization direction.

Summarizing, we proposed a transistor model using the spin-direction as a switch. We showed that in systems simultaneously protected by the TR and mirror symmetries, the spin-polarization is always perpendicular
to the mirror plane protecting the metallic edge states. We demonstrated that an external electric field breaking the mirror symmetry induces a spin-polarization parallel to the mirror plane. Since the electric field does not break the TR-symmetry, the metallic edge states are still protected by this symmetry, which allows the control of the spin-polarization preserving the Dirac cone formed by these states. We constructed tight-binding models for Na$_3$Bi and HF-honeycomb materials. Using this model we computed the mirror Chern number, predicting the DTC in HF-honeycomb materials and verifying this behavior in the Na$_3$Bi compound, which are protected by the mirror plane $M_x$ and $M_z$, respectively. In order to illustrate that the proposed spin-polarization control does not depend on the mirror plane orientation, we study this effect in both materials, the only two-dimensional systems predicted to exhibit a DTC. In light of recent advances in the application of electric fields in the 2D Na$_3$Bi [59], the practical realization of the proposed device is feasible.

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* acosta@if.usp.br

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