Nearly perfect spin-filtering in curved two-dimensional topological insulators

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The spintronic properties of curved nanostructures derived from two-dimensional topological insulators (2DTIs) are explored theoretically with density functional theory-based (DFT) calculations and tight-binding models. We show that curved geometries make it possible to manipulate electron spins in ways that are not available for planar 2DTI devices. We predict that, unlike planar 2DTI devices, curved 2DTI-related nanostructures can function as highly effective two-terminal spin filters even in the absence of magnetic fields. We construct a generalization to curved geometries of our previous tight binding model of the wide band gap planar 2DTI bismuthene on SiC. The resulting model, applied to an ideal dome geometry with a free edge, is shown to exhibit quantum spin Hall physics, including spin polarized edge states. The model predicts nearly perfect spin filtering by the dome for a particular two-terminal geometry in the absence of magnetic fields. Our DFT calculations predict a Bi\textsubscript{105}Si\textsubscript{105}H\textsubscript{15} dome of bismuthene with adsorbed silicon and hydrogen atoms to be stable. Our tight binding model, adjusted to match density of states given by DFT calculations, predicts that the Bi\textsubscript{105}Si\textsubscript{105}H\textsubscript{15} dome should exhibit quantum spin Hall physics and very effective spin filtering in a two-terminal arrangement.

I. INTRODUCTION

In two-dimensional topological insulators (2DTIs) electron transport occurs via edge states when the Fermi level is located in the bulk band gap\textsuperscript{1–10}. These edge states exhibit locking between the electron momentum and spin which results in a quantum spin Hall (QSH) effect\textsuperscript{11–16} i.e., the electric current is carried by spin polarized electrons with opposite spin orientations at the opposite edges of the sample. The 2D QSH systems considered to date have been planar\textsuperscript{7–10}. curved 2D QSH systems have received little if any attention theoretically or experimentally. In this paper we initiate the exploration of the physics of curved 2D QSH systems theoretically by constructing tight binding models of finite nanostructures based on 2DTIs with curved geometries and examining their properties. We find that curved geometries offer additional degrees of freedom for manipulating the orientations of the spins of QSH edge states that are not available for planar 2DTIs. In particular, while the spin orientation of an electron traveling along the edge of a planar 2DTI nanostructure remains fixed, we show that the spin orientation of an electron traveling along the edge of a suitably curved 2DTI can vary as a function of the position along the edge. Thus while the spin orientations induced by an electric current on the opposite edges of planar 2DTIs are always antiparallel, our work reveals that, for suitable curved geometries, the spin orientations on opposite edges of the 2DTI can be tailored so as to vary continuously from antiparallel to parallel depending on the locations where the spin orientations are measured. From the perspective of potential applications, it follows that appropriately contacted curved 2DTIs can function as 2-terminal spin filters in the absence of magnetic fields whereas in order to achieve spin filtering at zero magnetic field in a planar 2DTI at least a 3-terminal device is required.

II. CURVED BISMUTHENE NANOSTRUCTURES

Recent theoretical and experimental work has provided strong evidence that monolayer bismuthene on SiC is a wide gap 2DTI\textsuperscript{11–19}. Tight binding models of the bismuthene monolayer employing basis sets consisting only of the valence orbitals of the bismuth atoms but parameterized so as to take into account the influence of the SiC substrate on the bismuthene have been constructed\textsuperscript{12–18}. These simple models have succeeded in capturing the essential topological insulator and QSH physics of this planar system\textsuperscript{12–18}.

Whether curved bismuthene monolayers chemically modified by suitable adsorbates can also exhibit topological insulator and QSH physics is unknown at present. However, theoretical studies have suggested that approximately spherical and cylindrical bismuthene nanostructures may be stable\textsuperscript{20–23}. Also, bismuth nanotubes have been synthesized\textsuperscript{24–31}.

We have investigated curved bismuthene-based nanostructures further by means of density functional theory (DFT) computer simulations as implemented in the GAUSSIAN 16 package with the B3PW91 functional and Lan12DZ effective core potential and basis sets\textsuperscript{32}. The electronic energy and ionic forces of our optimized geometries were converged within 10\textsuperscript{−5} eV and 0.0008 eV/Å, respectively. Our simulations indicate that an approximately spherical bismuthene fullerene structure consisting of 180 Bi atoms comprised of Bi hexagons and 12 symmetrically arranged Bi pentagons should be stable and that a similar 180 Bi atom fullerene with 180 Si atoms in its interior, one Si atom bound to each Bi atom, should also be stable. We attribute the stability of the latter structure to the fact that for it the distance between nearest neighbor Si atoms is similar to the nearest neighbor distance in crystalline silicon; we find that bismuthene fullerenes decorated with Si atoms but having very different nearest neighbor Si-Si distances tend to be unstable. We also find that spherical domes of bismuthene are unstable, being prone to collapse into compact clusters of Bi atoms. However, interestingly, we find that a particular bismuthene dome can be...
stabilized by the addition of Si and H atoms. In Fig. 1 we show such a stable structure of 105 Bi and 105 Si atoms obtained by relaxing a truncated 180 Bi-Si atom spherical fullerene. A Si atom is bound to each Bi atom on the concave surface of the dome; the dome has a zigzag edge. The edge Si atoms are passivated with hydrogen atoms. We refer to this nanostructure as a Bi$_{105}$Si$_{105}$H$_{15}$ dome. This suggests that making a curved monolayer bismuthene nanostructure with a free edge may be possible.

Whether such stable curved nanostructures based on monolayer bismuthene or other 2DTI’s and having a free edge can be realized experimentally remains an open question. Never the less it is of interest to explore the properties of such prospective systems theoretically. Here we initiate this theoretical work by constructing and studying potentially relevant tight binding models. We construct a generalization of our tight-binding Hamiltonian of planar bismuthene (modified chemically by SiC)\textsuperscript{15} to curved bismuthene nanostructures. We show that for an ideal 105 Bi atom spherical dome geometry this basic model exhibits spin polarized edge states, a QSH effect and nearly perfect spin filtering in a two terminal arrangement.

We then modify this basic model in such a way as to reproduce approximately the partial density of states on the Bi atoms obtained by our DFT calculations for the relaxed Bi$_{105}$Si$_{105}$H$_{15}$ dome shown in Fig. 1. We find that the electronic structure and transport properties of this realistic curved bismuthene-based nanostructure are more complex, being strongly affected by both edge and bulk states, but that it also exhibits a pronounced QSH effect and very effective spin filtering in a two terminal arrangement.

III. GENERALIZATION OF THE TIGHT BINDING MODEL OF INFINITE MONOLAYER BISMUTHENE ON SiC TO CURVED GEOMETRIES

The bismuth atoms of planar monolayer bismuthene on SiC form a honeycomb lattice.\textsuperscript{11,12} For bismuthene in the $x$-$y$ plane, the main contributions to the low energy electronic states are those of the Bi $6p_x, 6p_y$ and $6s$ atomic valence orbitals.\textsuperscript{12} The tight binding models of bismuthene on SiC have to date have employed basis sets consisting of only these bismuth valence orbitals. In bismuthene on SiC the Bi $6p_z$ valence orbital is shifted away from the Fermi level because of the interaction with the SiC substrate.\textsuperscript{12} For this reason it has been omitted in most tight binding models of planar bismuthene on SiC. However, for curved bismuthene geometries the Bi $6p_z$ orbital should be included in the theory. We do this as follows.

Our generalized tight binding model Hamiltonian is of the form

$$H_{\alpha s,i}^\alpha_{\alpha's,i'} = H_{\alpha s,i}^\alpha_{\alpha's,i'} + H_{\alpha s,i}^\alpha_{\alpha's,i'} + H_{\alpha s,i}^\alpha_{\alpha's,i'} + H_{\alpha s,i}^\alpha_{\alpha's,i'}$$

(1)

where $\alpha$ and $\alpha'$ denote the Bi $6p_x, 6p_y, 6p_z$ and $6s$ valence orbitals of atoms $i$ and $i'$, $s$ and $s'$ are spin indices, $H_{\alpha s,i}^\alpha_{\alpha's,i'}$ is the onsite orbital part of the Hamiltonian matrix for atom $i$ omitting the spin-orbit and Rashba contributions, $H_{\alpha s,i}^\alpha_{\alpha's,i'}$ is the Hamiltonian matrix element between orbital $\alpha'$ on Bi atom $i'$ and orbital $\alpha$ on Bi atom $i$ that is a nearest neighbor of atom $i'$, $H_{\alpha s,i}^\alpha_{\alpha's,i'}$ is the atomic spin-orbit interaction and $H_{\alpha s,i}^\alpha_{\alpha's,i'}$ is the Rashba Hamiltonian. Following the reasoning in Ref. 12 only the intra-atomic matrix elements of $H_{\alpha s,i}^\alpha_{\alpha's,i'}$ and $H_{\alpha s,i}^\alpha_{\alpha's,i'}$ are considered here.

The onsite orbital Hamiltonian matrix elements $H_{\alpha s,i}^\alpha_{\alpha's,i'}$ are given in Table I. $H_{\alpha s,i}^\alpha_{\alpha's,i'}$ has energy eigenvalues $E_x$ and $E_y$ corresponding to the orbital states $|6s\rangle$ and $|6p_\alpha\rangle = a|6p_x\rangle + b|6p_y\rangle + c|6p_z\rangle$, respectively, where $x = (a, b, c)$ is the unit vector normal to the surface of the curved topological insulator at Bi atom $i$. The other two eigenvalues of $H_{\alpha s,i}^\alpha_{\alpha's,i'}$ correspond to the $6p$ states that are orthogonal to $|6p_\alpha\rangle$ and are both zero. Thus $|6p_\alpha\rangle$, the $6p$ orbital whose symmetry axis is parallel to the local normal to the surface of curved topological insulator, is shifted in energy relative to the other $6p$ orbitals by an amount $E_x$, emulating the shift of the $6p_z$ orbital relative to $6p_x$ and $6p_y$ for planar bismuthene on SiC.\textsuperscript{12}

The nearest neighbor Hamiltonian matrix elements $H_{\alpha s,i}^{\alpha\alpha'}_{\alpha's,i'}$ are given in Table II. For $\delta = 0$ they have been fitted to the band structure\textsuperscript{12} of planar bismuthene on SiC. For geometries other than that of planar bismuthene on SiC, they are assumed to depend on the Bi-Bi bond orientations as in the Slater-Koster model\textsuperscript{34} and to scale with the bond lengths as in extended Hückel theory.\textsuperscript{35}

The intra-atomic matrix elements of the spin-orbit Hamiltonian can be approximated as\textsuperscript{36,37}

$$H_{\alpha s,i}^{\alpha\alpha'}_{\alpha's,i'} = \zeta \frac{(C_\alpha S|S\cdot L|C_{\alpha'} S')}{\hbar^2}$$

(2)

where $S$ and $L$ are the spin and orbital angular momentum operators, and $C_\alpha$ is the cubic harmonic that corresponds to...
Table I. The onsite orbital part $H_{i,\alpha'}^{\delta}$ of the model Hamiltonian matrix for atom $i$ in Eq. 1. Here $\hat{r} = (a, b, c)$ is the unit vector normal to the surface of the curved topological insulator at Bi atom $i$. The parameter values are $E_x = -10.22$ eV and $E_y = -5.0$ eV.

| $H_{i,\alpha'}^{\delta}$ | $6s^l$ | $6p_x^l$ | $6p_y^l$ | $6p_z^l$ |
|-------------------------|--------|----------|----------|----------|
| $6s$                    | $E_x$  | 0        | 0        | 0        |
| $6p_x$                  | $a^l$  | $b^l$    | $c^l$    | $d^l$    |
| $6p_y$                  | $e^l$  | $f^l$    | $g^l$    | $h^l$    |
| $6p_z$                  | $i^l$  | $j^l$    | $k^l$    | $l^l$    |

orbital state $\alpha$. $\zeta$ is the spin-orbit interaction strength and $l$ is the orbital angular momentum quantum number. The matrix $\langle C_{\alpha,s}^l | \mathbf{S} \cdot \mathbf{L} | C_{\alpha',s'}^l \rangle / \hbar^2$ is given in Table III. $\zeta$ is regarded here as a model fitting parameter with value $\zeta = 1.8$ eV for the Bi $6p$ valence orbitals.

Rashba phenomena are due to spin-orbit coupling in systems whose symmetry is broken by the presence of a surface or interface. The form of the intra-atomic Rashba Hamiltonian matrix elements $H_{\alpha,s,\alpha',s'}^{R}$ for the present system can be deduced by considering a contribution to $\nabla V(\mathbf{r})$ in the general spin-orbit Hamiltonian of Ref. 44.

where the electron transmission probability through the nanostructure at the Fermi energy is

$$T(E_F) = \sum_{\alpha,i,\beta,j} |t_{\beta,j,\alpha,i}(E_F)|^2 \frac{v_{\beta,j}}{v_{\alpha,i}}.$$ (4)

Here $t_{\beta,j,\alpha,i}$ is the amplitude for electron scattering at the Fermi energy from state $\alpha$ of 1D lead $i$ connected to the electron source to state $\beta$ of 1D lead $j$ connected to the electron drain reservoir. $v_{\alpha,i}$ and $v_{\beta,j}$ are the corresponding subband Fermi velocities.

In order to study the spin Hall effect and spin filtering, we consider spin-unpolarized electrons entering the device through the electron source contact and calculate the spin resolved probabilities $T_{\uparrow}$ and $T_{\downarrow}$ of spin up and spin down electrons exiting through the drain contact at the Fermi energy. $T_{\uparrow}$ and $T_{\downarrow}$ are obtained by restricting the sum over $\beta$ in Eq. (4) to spin up and spin down states, respectively, while including both the spin up and spin down states in the sum over $\alpha$. The axis of quantization is the $z$-axis.

The scattering amplitudes $t_{\beta,j,\alpha,i}$ are obtained by solving numerically the Lippmann-Schwinger equation

$$|\psi\rangle = |\phi_0^{\alpha,i}\rangle + G_0(E)|\psi\rangle.$$ (5)

Here $|\phi_0^{\alpha,i}\rangle$ is an eigenstate of the $i^{th}$ ideal 1D lead that is decoupled from the nanostructure consisting of the quantum dot and conducting contacts (if those are present), $G_0(E)$ is the sum of the Green’s functions of the nanostructure and 1D leads if they are decoupled from the nanostructure, and $|\psi\rangle$ is the corresponding exact scattering eigenstate of the coupled system. $\psi$ is the coupling Hamiltonian between the nanostructure and the ideal 1D leads. A methodology for numerically solving Lippmann-Schwinger equations such Eq. (5) within a tight-binding framework is described in Appendix A of Ref. 44.

In the present work the ideal leads are represented by 1D tight binding chains. Each site of each chain is assumed to have 6 orbitals, including spin. The on-site energies of these chain orbitals are the same as the corresponding atomic orbital energies $H_{i,\alpha}$ of the $6p_x, 6p_y$, and $6p_z$ orbitals of the Bi atoms described by the Hamiltonian Eq. (1). Only nearest neighbor Hamiltonian matrix elements between like orbitals of the 1D chains and between the chains and adjacent Bi atoms of the nanostructure are assumed to be non-zero. For simplicity, all of these nearest neighbor Hamiltonian matrix elements are assumed to have the same value $t = -2.0$ eV.

V. RESULTS

A. Predictions of model of Section III for ideal Bi$_{105}$ dome

The predictions of the tight binding model described in Section III for a curved topological insulator whose structure is that of an ideal 105 atom bismuthene fullerene dome formed by truncating a 180 atom bismuthene sphere without any subsequent relaxation of the atomic geometry are shown in Figs.
vice from the source electrode are initially spin- 
rectly by either the source or drain. The electrons entering the de-
tron source (drain). Dark blue atoms are not contacted di-
Light blue (chartreuse) atoms are edge atoms connected directly to
atom spherical bismuthene fullerene without subsequent relaxation.
atom bismuthene dome with zigzag edge formed by truncating a 180
Figure 2. (Color online). View of the concave side of an ideal 105
induced by the electric current on the bismuth atoms at the
However, as is seen in Fig. 2, strong spin polarizations are
large, is not sufficient to close the topological gap in planar
similar origin (the Bi-Si interaction) in our model system as in
As has been discussed by Sheng et al., it is possible for a
strong Rashba coupling to close the topological gap in some
systems. However, it has been well established both theo-
retically and experimentally that the Rashba term, although
large, is not sufficient to close the topological gap in planar
bismuthene on SiC.11-19 Since the Rashba effect has a sim-
lar origin (the Bi-Si interaction) in our model system as in
the planar bismuthene on SiC, it is reasonable to expect the
Rashba effect not to close the topological gap in the present
system either.

When contacts are attached to the 105 atom bismuthene
fullerene dome as shown in Fig. 2 and an electric current
flows, the calculated electron spin polarizations induced on
the Bi atoms by the electric current are shown by red arrows
in Fig. 2. Here the Fermi energy is at 0.4 eV above the valence band edge of bulk
bismuthene on SiC. The black arrow is the z-axis. Image prepared
using Macmolplt software.33

2 and 3. The geometry considered is shown in Fig. 2 where the
electron source (drain) electrode is attached to the light
blue (chartreuse) colored bismuth edge electrode.

The calculated electronic spectrum of this structure when
the bismuthene is decoupled from the contacts is shown in
the inset of Fig. 3. The states in the spectral gap of the 180
atom bismuthene fullerene (marked in red) are edge states that
are confined to the vicinity of the edge of the 105 atom bis-
muthene fullerene dome.

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Rashba effect not to close the topological gap in the present
system either.

When contacts are attached to the 105 atom bismuthene
fullerene dome as shown in Fig. 2 and an electric current
flows, the calculated electron spin polarizations induced on
the Bi atoms by the electric current are shown by red arrows
in Fig. 2. Here the Fermi energy is at 0.4 eV in the inset of
Fig. 3, i.e., within the spectral gap of the complete 180 atom
spherical bismuthene fullerene. The electrons entering the de-
vice from the source electrode are initially spin-une
polarized. However, as is seen in Fig. 2, strong spin polarizations are
induced by the electric current on the bismuth atoms at the
edges of the 105 Bi atom dome between the source and drain
electrodes, as is expected for the spin polarization induced by
electric currents carried by edge states in quantum spin Hall
systems.

Notice that in Fig. 2 the spin polarizations point radially
outward from the center of the dome for electrons traveling
counterclockwise along the edge of the dome from source
to drain but radially inward for electrons traveling clock-
wise along the edge. Because of this, for the arrangement
of electrodes shown in Fig. 2, the spin polarizations of
both the clockwise and counterclockwise-moving edge states
point in approximately the same direction (i.e., the negative z-
direction) where these two edges feed into the drain electrode.
In other words, both of the edge states feed spin down elec-
trons into the drain contact. Thus all of the electrons entering
the drain electrode have approximately spin down polarization.
Consequently, this two-terminal curved topological insulator
device functions as a nearly perfect spin filter.

This can be seen quantitatively in Fig. 3 where for Fermi
energies throughout most of the spectral gap of the 180 atom
bismuthene fullerene the spin down transmission T↓ of
the 105 bismuth atom dome is close to 2 while the spin up trans-
mision T↑ is close to zero. The maximum value of spin
polarization of the electrons entering the drain (defined as
T↓/(T↑+ T↓)) is ~ 0.99 in Fig. 3. [More sophisticated mea-
sures of the spin polarization are in general possible, as de-
scribed, for example, by Nikolić et al. However, in this paper
our objective is to show that the curved topological insulators
can function as nearly perfect spin filters. For this purpose it
is sufficient to demonstrate that T↓/(T↑ + T↓) is close to 1 (in
some range of Fermi energy values) since this implies that the

Figure 2. (Color online). Spin-resolved Landauer transmission
probabilities T↑ and T↓ of spin up and spin down electrons exiting
through the drain contact of the device shown in Fig. 2 at the Fermi
energy assuming that spin unpolarized electrons enter from the elec-
tron source. Inset: Histogram of eigenstates of the Hamiltonian of
the device shown in Fig. 2 when it is decoupled from the leads. The
band gap predicted by the present model for planar bismuthene on
SiC is shown in blue. The spectral gap predicted by the model for
the spherical 180 atom bismuthene fullerene geometry is shown in
red. The states in the spectral gap are edge states.
z-component of the spin polarization of electrons entering the drain is much larger than the other components. Our calculations accomplish this.

By contrast, a planar 2D two-terminal bismuthene on SiC topological insulator device does not exhibit such spin filtering in a two-terminal arrangement because for it edge states traveling on opposite edges always have opposite spin polarizations and the directions of those spin polarizations can not become aligned.

The structure of the bismuthene dome considered in Figs. 2 and 3 is idealized, being an unrelaxed truncated portion of the 180 atom bismuthene fullerene sphere. Also the tight binding model used (that described in Section III) is a generalization of the tight-binding models of infinite 2D bismuthene on SiC; no adjustment of the tight binding parameters due to the presence of the edge is included in that model.

B. Predictions of improved model for Bi\textsubscript{105}Si\textsubscript{105}H\textsubscript{15} dome

We now consider the more realistic Bi\textsubscript{105}Si\textsubscript{105}H\textsubscript{15} dome nanostructure shown in Fig. 1, taking into account the relaxed geometry as well as the influence of the Si and H on the electronic structure of the bismuthene. We also provide an improved treatment of the Bi\textsubscript{105}Si\textsubscript{105}H\textsubscript{15} dome’s edge electronic structure. We accomplish this by modifying the tight binding model described in Section III so as to bring the bismuthene density of states (DOS) that the model predicts near the Fermi level (in the absence of the spin-orbit and Rashba terms of the Hamiltonian, Eq. 1) into agreement with that predicted by our tight binding hopping parameters including the onsite energies of all of the atomic orbitals of all of the 45 Bi atoms closest to the edge of the structure upshifted by 1.4 eV and the hopping parameters do not require adjustment appear to require substantial modification. The physical reasons why the hopping parameters do not require adjustment appear to require substantial modification. The physical reasons why

Figure 4. (Color online). Calculated bismuth density of states vs. energy measured from the Fermi level ($E = 0$) for the relaxed Bi\textsubscript{105}Si\textsubscript{105}H\textsubscript{15} dome shown in Fig. 1. (a): Black curve: Prediction of density functional theory (B3PW91 functional with Lanl2DZ effective core potential and basis sets). Red curve: Prediction of the tight-binding model described in Section III omitting the spin-orbit and Rashba terms from the Hamiltonian, Eq. 1. (b): Black curve: As in (a). Red curve: Prediction of the tight-binding model described in Section III omitting the spin-orbit and Rashba terms from the Hamiltonian, Eq. 1, but with the onsite energies of all of the orbitals of the 45 Bi atoms closest to the edge of the structure upshifted by 1.4 eV. (c) Red curve: As in (b) but including the spin-orbit and Rashba terms in the Hamiltonian.
Bi valence orbitals in addition to the \( p_x \) and \( p_y \) orbitals that are sufficient to describe planar bismuthene on SiC. (ii) The Slater-Koster type dependence of the hopping parameters on the Bi-Bi bond orientation implemented in Table I appears to be adequate for this system, and (iii) The onsite Hamiltonian as parameterized in Table I succeeds in capturing appropriately the Bi \( p \)-orbital level splitting induced by the coupling between the neighboring Bi and Si atoms even for the curved bismuthene geometry.

Reintroducing the spin-orbit and Rashba terms of Eq.1 into the modified tight-binding model yields the DOS shown in red in Fig.4(c). That the spin-orbit and Rashba terms have resulted in the presence of electronic states in the energy range of the spectral gap of Fig.4(b) is not surprising since the magnitude of the spin orbit coupling parameter \( \zeta_1 = 1.8\,\text{eV} \) in Eq. 2 substantially exceeds the size of the spectral gap in Fig.4(b). Never the less we regard the modification of the tight-binding model prompted by our comparison between the DOS of DFT and the model in the absence of spin orbit coupling as a significant improvement of the model as applied to the Bi\(_{105}\)Si\(_{105}\)H\(_{15}\) dome and especially the properties of its edge. This becomes apparent when one considers spin filtering by the Bi\(_{105}\)Si\(_{105}\)H\(_{15}\) dome, as will be explained next.

In Fig.5(a) the blue curve shows the calculated spin polarization of electrons injected into the drain electrode from the Bi\(_{105}\)Si\(_{105}\)H\(_{15}\) dome at the Fermi energy \( E \) in the linear response regime, assuming that the electrons entering the dome from the source electrode are spin unpolarized. The source and drain electrodes are connected to the bismuth atoms of the dome as in Fig. 2. The energies of the Hamiltonian eigenstates of the dome when it is disconnected from the leads are shown by the red ticks at the top of Fig.5(a). The eigenstates that are edge states are marked by asterisks (*). Values of the spin polarization as high as \( T_\downarrow/(T_\downarrow + T_\uparrow) \sim 0.93 \) can be seen in Fig.5(a). The mechanism responsible for the largest values of the spin polarization is similar to that illustrated in Fig.2, i.e., the spin polarizations associated with the electric currents carried by the edge states point radially outward from the dome for electrons traveling counterclockwise along the edge of the dome from source to drain but radially inward for electrons traveling clockwise along the edge. Because of this, the spin polarizations of the clockwise and counterclockwise-moving edge become approximately aligned where these two edges feed into the drain electrode and the dome functions as a nearly perfect spin filter. The eigenstates of the Hamiltonian that are not edge states (indicated in Fig.5(a) by red ticks without asterisks) do not support this spin filtering mechanism. Thus when the Fermi level is close in energy to any of these non-edge states the value of the spin polarization of the electrons entering the dome is sharply reduced. Notice that unlike in Fig.3 where all of the states in the bulk spectral gap are edge states, in Fig.5(a) the edge states are interspersed with non-edge states that are in fact the majority. However, since the non-edge states have very small amplitudes on the bismuth atoms at the edge of the dome, they couple very weakly to the electrodes and consequently the transport resonances associated with them are narrow. Because of this the influence of the edge states and the strong spin filtering associated with them predominates at energies between the spin polarization dips associated with the non-edge states even at energies between non-edge states where there is no edge eigenstate.

This is further clarified by considering the calculated conductance \( G \) = \( (T_\downarrow + T_\uparrow) e^2/h \) of the Bi\(_{105}\)Si\(_{105}\)H\(_{15}\) dome vs. Fermi energy \( E \) shown by the red curve in Fig.5(b). This plot shows sharp conductance resonances or antiresonances at the energies of the non-edge Hamiltonian eigenstates. However, no such features in the conductance are visible at the energies of the edge eigenstates. This is due to the very strong coupling of the edge eigenstates to the leads that results in very strong broadening of the edge eigenstates. This in turn means that the edge eigenstates influence the spin transport strongly over wide energy ranges that are interrupted by narrow regions where the effects of the non-edge eigenstates are crucial.

**VI. SUMMARY**

We have investigated theoretically the properties of curved nanostructures derived from 2D topological insulators, a topic that has not previously received experimental or theoretical attention. We have shown that curved geometries make it possible to manipulate the spin polarizations of electron edge states in ways that are not possible for planar systems, opening the way for the realization of previously unanticipated devices. In particular, we have shown that it is possible to bring the spin polarizations of electron edge states traveling along opposite edges of curved nanostructures into alignment and thus to realize nearly perfect two-terminal spin filters operating in the absence of magnetic fields.

![Figure 5](image_url)
Our study has combined the construction and application of appropriate tight-binding models and density functional theory-based calculations. We generalized our previous tight binding model of the wide band gap planar topological insulator bismuthene on SiC to curved geometries. Our transport calculations based on the resulting tight binding model applied to an ideal spherical bismuthene dome with a free zigzag edge showed this model system to exhibit quantum spin Hall physics: We showed this model to support edge states propagating along the edge of the dome within the bulk band gap of planar bismuthene on SiC. These edge states have radially oriented spin polarizations that point towards or away from the center of the dome, depending on whether the edge state travels in the clockwise or counter-clockwise direction. Thus, unlike for planar 2D topological insulators (for which the directions of the spin polarizations of the edge states are fixed), the directions of spin polarizations of the edge states of the curved structure can vary, controlled by the nanostructure’s geometry. Because of this it is possible for the spin polarizations of the clockwise and counter-clockwise edge states traveling from the electron source electrode to the drain to be parallel where the edge states enter the drain. Thus we predict that nearly perfect two terminal spin filters operating in the absence of magnetic fields can, in principle, be constructed from curved topological insulators.

Our density functional theory-based calculations have addressed the question whether chemically modified bismuthene domes exhibiting such spintronic properties can be stable. We find that a bismuthene dome of 105 bismuth atoms with a zigzag edge can be stabilized by the adsorption of a silicon atom to each bismuth atom on the concave surface of the dome if the edge silicon atoms are passivated with hydrogen. We have carried out density functional theory based calculations of the bismuth density of states of this Bi$_{105}$Si$_{105}$H$_{15}$ structure and have modified our tight binding model so that its predicted density of states approximately matches the corresponding density functional theory based result. We find that the resulting modified tight binding model of Bi$_{105}$Si$_{105}$H$_{15}$ exhibits both edge states and non-edge states at energies in the bulk band gap of planar bismuthene on SiC. However, our transport calculations for this system predict the influence of the edge states and the strong spin filtering mechanism associated with them to predominate for several ranges of the Fermi energy, including some Fermi energy ranges lying between the energies of consecutive non-edge states.

The results of our investigation show that curved nanostuctures based on 2D topological insulators should have spintronic properties that differ qualitatively from those of planar 2D topological insulators and that these distinctive properties may have important practical applications. We have identified a nanostructure that we predict to be stable and to exhibit these properties. Based on our work, it is clear that experimental and theoretical studies exploring this topic further are warranted and would be of considerable interest.

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Table II. Nearest neighbor Hamiltonian matrix elements $H_{\alpha,i',\alpha'}^{NN}$ in Eq. 1. In terms of the coordinates of the primed and unprimed neighboring atoms $d = ((x' - x)^2 + (y' - y)^2 + (z' - z)^2)^{1/2}; l = (x' - x)/d; m = (y' - y)/d; n = (z' - z)/d$. Fitting parameter values are $\Sigma = -0.81(1 - 1.583\delta + 0.821\delta^2)$eV, $\Sigma'' = -1.00(1 - 1.087\delta + 0.313\delta^2)$eV, $\Sigma''' = -1.635(1 - 0.509\delta - 0.187\delta^2)$eV, $\Pi = 0.55(1 - 1.361\delta + 0.634\delta^2)$eV and $\delta = d - 3.089\AA$.

$$
\begin{array}{cccccc}
\hline
H_{\alpha,i',\alpha'}^{NN} & 6s' & 6p_x' & 6p_y' & 6p_z' \\
\hline
6s & \Sigma & -\Sigma & i\alpha & i\alpha & i\alpha \\
6p_x & \Sigma' & \Sigma'' + \Pi(1 - l'^2) & (\Sigma'' - \Pi)lm & (\Sigma'' - \Pi)ln \\
6p_y & \Sigma' & \Sigma'' + \Pi(1 - m'^2) & \Sigma'' m'' + \Pi(1 - m'^2) & (\Sigma'' - \Pi)mn \\
6p_z & \Sigma' & \Sigma'' + \Pi(1 - n'^2) & \Sigma'' n'' + \Pi(1 - n'^2) & \\
\hline
\end{array}
$$

Table III. Matrix elements of $\frac{\text{sL}}{\hbar^2}$ that enter the intra-atomic spin-orbit Hamiltonian matrix, Eq. 2. All matrix elements involving the atomic $s$ orbital are zero.

$$
\begin{array}{cccccccc}
\langle C_{\alpha,i} | \text{sL} | C_{\alpha',i'} \rangle & 6p_x' & 6p_y' & 6p_z' & 6p_y' & 6p_z' & 6p_x' & 6p_z' \\
\hline
6p_x & -i/2 & 0 & 0 & 0 & 0 & 0 & 0 \\
6p_y & 0 & -i/2 & 0 & 0 & 0 & 0 & 0 \\
6p_z & 0 & 0 & -i/2 & 0 & 0 & 0 & 0 \\
6p_x & 0 & 0 & 0 & -i/2 & 0 & 0 & 0 \\
6p_y & 0 & 0 & 0 & 0 & -i/2 & 0 & 0 \\
6p_z & 0 & 0 & 0 & 0 & 0 & -i/2 & 0 \\
\hline
\end{array}
$$

Table IV. Matrix elements of the intra-atomic Rashba Hamiltonian $H_{\alpha,i',\alpha'}^{R}$, Eq. 1. Here $\hat{r} = (a, b, c)$ is the unit vector normal to the surface of the curved topological insulator at Bi atom $i$. The fitting parameter value is $R = 0.395$eV.

$$
\begin{array}{cccccccc}
\hline
H_{\alpha,i',\alpha'}^{R} & 6s' & 6s' & 6p_x' & 6p_y' & 6p_z' & 6p_y' & 6p_z' \\
\hline
6s & 0 & 0 & -iRb & Rc & iRa & -iRc & 0 & iR(b + ia) \\
6p_x & iRb & -Rc & 0 & 0 & 0 & 0 & 0 & 0 \\
6p_y & -iRa & Rc & 0 & 0 & 0 & 0 & 0 & 0 \\
6p_z & iRa & -Rc & 0 & 0 & 0 & 0 & 0 & 0 \\
6p_x & 0 & -iR(b + ia) & 0 & 0 & 0 & 0 & 0 & 0 \\
6p_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6p_z & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
\end{array}
$$