Structural and electronic properties of realistic two-dimensional amorphous topological insulators

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Abstract

We investigate the structure and electronic spectra properties of two-dimensional amorphous bismuthene structures and show that these systems are topological insulators. We employ a realistic modeling of amorphous geometries together with density functional theory for electronic structure calculations. We investigate the system topological properties throughout the amorphization process and find that the robustness of the topological phase is associated with the spin–orbit coupling strength and size of the pristine topological gap. Using recursive non-equilibrium Green’s function, we study the electronic transport properties of nanoribbons devices with lengths comparable to experimentally synthesized materials. We find a $2e^2/h$ conductance plateau within the topological gap and an onset of Anderson localization at the trivial insulator phase.

1. Introduction

Topological phases of matter have gained great and increasing interest due to their outstanding properties and prospects of applications in spintronics, low energy loss devices, and quantum computing [1, 2]. Standard theoretical approaches for the search and classification of topological properties in materials are based on the analysis of the system symmetries and on topological invariants that rely on translational symmetry [3–10]. However, the statement that topological properties are robust against disorder, one of the strongest predictions of the theory, clearly indicates that translational invariance is not a requirement. Nonetheless, the demonstration that non-crystalline systems can host non-trivial topology [11] came as a surprise and opened interesting new investigation paths in the field.

Since Agarwala and Shenoy [11] have shown that a random lattice tight-binding model can display Chern insulator properties, several other non-crystalline lattice models with topological properties have been proposed [12–19]. This kind of investigation also includes an experimental realization of a two-dimensional non-crystalline system with topological properties, namely, a system of coupled gyroscopes that hosts topological chiral edge modes [20].

The classification of topological phases in non-periodic systems also offers new challenges since the standard topological insulator invariants are not applicable [21–23]. Instead, the strategies employed so far comprehend real-space topological markers [11–15, 20], response to external fields [17], modified versions of the symmetry indicators [23], Bott invariants [11, 24–28], and others [19, 29].

None of these studies has taken into account the fundamental structural properties of amorphous materials [30]. For instance, unlike random lattices, amorphous systems show short-range order. In order to address real materials, properties such as coordination number fluctuations, short-range order, formation of voids, etc. need to be properly described. Hence, overcoming the challenges posed by a realistic modeling of the electronic properties of large disordered systems is essential for advancing the theoretical understanding to help the discovery of new amorphous topological materials.

Amorphous materials recently entered the hall of synthesized topological insulators (TIs). The crystalline phase of Bi\textsubscript{2}Se\textsubscript{3} is a known 3D TI [31] and there is recent experimental evidence supporting the existence of a surface Dirac cone with helical spin-texture also in its amorphous phase [32]. Such features are a hallmark of the quantum spin Hall (QSH)
state, a topological phase protected by TRS. Two-dimensional trivial amorphous systems have also been synthesized, for instance, monolayer free-standing amorphous carbon [33] revealed an atomic arrangement with a wide distribution of both bond lengths and angles, resembling more a crystallite model [21] than a random network [34] for amorphous structures. Although metallic, this system allows us to aim for the realization of 2D amorphous topological phases with a similar structure.

There are several 2D topological materials [35–37] that are candidates to serve as platforms for amorphous topological insulators. We choose to study the properties of amorphous bismuthene, since it has been already synthesized in the pristine form and due to its remarkable properties. The experimental band gap of Bi supported by SiC(0001) surface is 0.67 eV and hosts a topologically non-trivial band structure with one of the largest reported topological band gaps [38]. The robustness of flat bismuthene is such that it withstands ~17% of vacancy concentration while retaining its topological features, this threshold depends on the energy gap and spin–orbit coupling (SOC) strength [28, 39].

In a previous work [40], some of us put forward an ab initio approach to study material-specific amorphous topological insulator properties and applied it to flat bismuthene. However, computational limitations restricted the analysis to small system sizes and amorphization steps, raising questions about robustness of the reported amorphous phase. This paper vastly expands the analysis of reference [40], confirming its main conclusions and reporting new findings.

Here, we systematically investigate the structural, electronic, and transport properties of different samples of amorphous topological insulators. Using density functional theory (DFT) [41–43] calculations combined with an amorphization scheme we obtain bismuthene amorphous structures [40, 44]. We study their topological properties by calculating the $Z_2$ topological invariant and the spin Bott index. We show that amorphization quenches the topological band gap, but does not close it. We consider a two-terminal nanoribbon geometry and using non-equilibrium Green’s functions (NEGF) [45–48] combined with DFT we calculate the system linear conductance. We show that the edge states are robust even at realistic lengths, up to 0.32 $\mu$m, with a conductance plateau of $2e^2/h$ for energies within the topological gap. Also, we consistently characterize the amorphization as a transformation that maps the pristine system into the amorphous one with the preservation of the QSH state linked to the SOC strength and size of the pristine topological band gap.

This paper is organized as follows. In section 2 we discuss the procedure used to generate the amorphous lattices. Additionally, we briefly show the standard methods we employ for the electronic structure and transport calculations. In section 3 we present our main results, namely, the topological characterization and the study of the structural, electronic, and transport properties of different realizations of amorphous bismuthene. We also show how to modify and control the material properties by breaking time-reversal symmetry. Our findings are summarized and discussed in section 4.

2. Methods

There is a vast literature on theoretical modeling of amorphous systems [30]. These works put forward different amorphization schemes and show that lattice sizes $10^4 - 10^5$ atoms with periodic boundary conditions are sufficient to describe the experimental data [49, 50]. The simulations in these studies can rely on well established empirical force models. This is not the case for 2D bismuthene. Here we perform a full DFT relaxation calculation to generate amorphous structures. From the computational point of view, this is the most severe bottleneck of our study. The details of our procedure are presented below.

We create our amorphous geometries using the bond-flipping method [44] together with density functional theory (DFT) [41–43] for structure relaxation. Figure 1 depicts the adopted procedure. Hsu et al [51] demonstrated that hydrogen half-functionalized flat bismuthene (H-bismuthene) with SiC(0001) lattice parameter (5.35 Å) essentially reproduces the same electronic structure without the computational cost of explicitly including the SiC surface. We start with a pristine flat bismuthene structure with 560 Bi and 560 H atoms. Within this geometry, the region to be transformed comprehends 400 Bi atoms and 400 H atoms, and we left pristine regions at each side so the following transport calculations can be performed. The number of bonds to be flipped is determined to result in a stable deviation of ring size distribution with the number of flipped bonds [33, 52, 53]. For the generated geometries this is achieved with 23 flipped bonds. At each amorphization step, we randomly chose and flip the bonds inside this central region. After flipping the bonds, we perform a geometry relaxation using the Vienna ab initio Simulation Package (VASP) [54, 55] until the total force on atoms was less than $10^{-2}$ eV Å$^{-1}$. The relaxations use the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) [56] functional for the electronic exchange and correlation interactions, and the projector augmented wave (PAW) [57] method for ionic core potentials.

For the optimized amorphous geometries, we calculate the electronic structure using a local basis set. The local basis is needed to obtain converged ab initio Hamiltonians and overlap matrices, which are the main ingredients for transport properties calculations. The electronic structure is obtained using the SIESTA code [58] with the Perdew–Burke–Ernzerhof
Using the off-site SOC implementation, we obtain a band gap of 0.84 eV (0.3 eV larger than observed in experiments). Hence, although the off-site implementation is usually believed to be most accurate [63], we find that the on-site SOC is better suited to describe the band structure of flat bismuthene.

(PBE) exchange and correlation functional [56, 59], real space energy grid cut-off of 350 Ry, an optimized single-c (SZ) basis set, fully relativistic norm-conserving pseudopotentials [60], and on-site self-consistent spin–orbit coupling (SOC) [61, 62]. We have verified that this framework accurately reproduces the pristine bulk band structure of flat bismuthene [51] and the experimental band gap [38].

The k-point density is set to 30 Å\(^{-1}\) in the transport direction. We add 15 Å of vacuum space to avoid spurious interactions between periodic images in non-periodic directions. The analysis of results is partially aided by the sisl code [64].

Using real space Hamiltonian obtained from SIESTA calculations, we implement the non-equilibrium Green’s function (NEGF) [45–48] method to compute the system transport properties. For this, we consider a two-terminal setup with a scattering region (S) connected to leads in thermal and electrochemical equilibrium with left (L) and right (R) electron reservoirs as displayed in figure 2. The left (L) and right (R) leads are modeled as semi-infinite armchair flat bismuthene nanoribbons.

The system Hamiltonian is written in the spin resolved local basis as a block matrix:

\[
H = \begin{pmatrix}
H_L & h_{LS} & 0 \\
h_{LS}^\dagger & H_S & h_{SR} \\
0 & h_{SR}^\dagger & H_R
\end{pmatrix},
\]

where \(H_{LR}\) is the Hamiltonian of the semi-infinite left (right) lead, \(h_{LS/SR}\) stands for the coupling matrix elements between the left (right) lead and the scattering region (S), and \(H_S\) is the scattering region Hamiltonian.

As standard [47, 48], in the limit of small bias, the retarded Green’s function reads:

\[
G_S(E) = (E^+ S - \Sigma_L - \Sigma_R)^{-1},
\]

where \(E^+ = \lim_{\delta \to 0^+} E + i\delta\), \(S\) is the local orbitals overlap matrix and \(\Sigma_L/R\) are the leads embedding self-energies given by \(\Sigma_L = h_{LS}^\dagger g_{LS} h_{LS}\) and \(\Sigma_R = h_{SR}^\dagger g_{SR} h_{SR}\). The retarded leads surface Green’s functions \(g_S(E)\) and \(g_R(E)\) are calculated following the references [65, 66].

Finally, the system linear conductance is given by the Landauer formula [47], namely,

\[
\mathcal{G} = \frac{e^2}{h} \int dE \left( -\frac{\partial f}{\partial E} \right) \mathcal{T}(E)
\]

where \(f\) is the Fermi–Dirac distribution and \(\mathcal{T}\) is the transmission [45, 46] given by:

\[
\mathcal{T}(E) = \text{Tr} [\Gamma_L G_S \Gamma_R G_S^\dagger],
\]

where \(\Gamma_{L/R} = i[\Sigma_{L/R} - \Sigma_{L/R}^\dagger]\) are the decay width matrices coupling the leads and the scattering region. At zero temperature, equation (3) is reduced to \(\mathcal{G} = \langle e^2 / h \rangle \mathcal{T}(E)\).

Using the scattering region Green’s function we can also compute the electronic density of states (DOS), namely,

\[
\text{DOS}(E) = \frac{1}{\pi} \text{Im Tr}[G_S(E)].
\]

The computation of the Green’s function \(G_S\) is a daunting task for a realistic size model system with a large basis of local orbitals \(N_T\), since equation (2) requires the inversion of a \(N_T \times N_T\) matrix. For disordered systems, where one is interested in ensemble averages, the computational time becomes even more critical. This problem is mitigated by the recursive Green’s function (RGF) methods that explore the fact that only a small fraction of the matrix elements of

Figure 1. Representation of the bond flipping method for obtaining realistic amorphous geometries. The regions with flipped bonds are colored in blue.


\[ G_S(E) \] are necessary to compute \( T \), namely the ones that are connected to the \( L/R \) leads.

The standard implementation of the RGF is to partition the scattering region into \( N \)-building blocks as shown in figure 2. Here, we consider building blocks that are sufficiently large to simulate amorphous domains (as discussed above). Such large size building blocks guarantee that only nearest neighbor partitions are coupled, allowing one to write \( H_S \) as:

\[
H_S = \begin{pmatrix}
H_{S_1} & V_{1,2} & 0 & \ldots & 0 \\
V_{1,2}^\dagger & H_{S_2} & \ldots & \ldots & \vdots \\
0 & \vdots & \ddots & \vdots & 0 \\
\vdots & \ldots & \ddots & H_{S_{N-1}} & V_{N-1,N} \\
0 & \ldots & 0 & V_{N-1,N}^\dagger & H_{S_N}
\end{pmatrix}, \tag{6}
\]

where \( H_{S_i} \) is the \( i \)th building block Hamiltonian and \( V_{ij} \) represents its coupling to the \( j \)th block. This partition scheme is depicted in figure 2. The \( V_{ij} \)'s are taken as constant and correspond to the coupling of a pristine block to its neighbors, which is guaranteed by the buffer layers, shown in figure 2.

The recursive method is used to eliminate by decimation the matrix elements of the local sites which are not coupled to the electrodes. We use the procedure put forward in reference [65] and generalized to the case of \( S \neq I \) in reference [67]. In this way, the computational cost is reduced by a factor of \( N^2 \) as compared with the full matrix inversion of equation (2).

The partition scheme also allow us to combine different sequences of amorphous supercells to build nanoribbons of arbitrary length. This strategy has been successfully applied to study the conductance of different disordered systems [65–72].

3. Results

3.1. Amorphous structures

We start by generating three amorphous H-bismuthene structures by the aforementioned bond-flip method. The corresponding obtained amorphous geometries after 23 amorphization steps are shown in figure 3(a). Each amorphous region contains 400 Bi and 400 H atoms, spanning a periodic lattice (without the vacuum layer) with 107 Å width and 46.33 Å length along the transport direction, see figure 2. We add pristine buffer layers to the amorphous geometries to properly couple the systems along the transport direction to form nanoribbons of arbitrary length. Each lead/buffer layer corresponds to a pristine armchair ribbon with 80 Bi and 80 H atoms with 9.27 Å of length. To address the structural characterization and amorphization degree of these structures, we inspect the first neighbors connectivity, the radial distribution function (RDF), ring size statistics, bond length and bond angle distributions.

In figures 3(a2)–(a4) we set the maximum bond length to 3.80 Å which is \( \approx 20\% \) larger than the pristine bond length (3.09 Å). We observe that the amorphous bismuthene structures are significantly less connected than the pristine ones. We stress that all these metastable structures are obtained by \textit{ab initio} relaxation calculations. This result indicates that the standard approach of continuous random models to consider a fixed coordination number cannot be applied to H-bismuthene. Interestingly, our simulations show the formation of voids in the amorphous structures. Their consequences to the electronic properties of the system are discussed in the next subsection.

Information regarding short and long range order is obtained through the radial distribution function (RDF) analysis [73, 74]. We computed the Bismuth RDF of the amorphous regions via the histogram method implemented in the VMD software [75]. Figure 3(b) shows that the crystalline system yields sharp and well-defined peaks at the corresponding neighbor distances of pristine flat bismuthene. In contrast, figure 3(c) shows that in the amorphous systems short-range order is characterized by two isolated peaks, one centered at the first neighbors distance at \( r \approx 3.09 \) Å, which is close to the Bi–Bi pristine bond length and the other near 5.30 Å corresponds to the second neighbors distance. As \( r \) increases the peaks become broader and undefined as a result of the absence of long range order. Figure 3(c) clearly shows
that $J(r) \propto r$ for $r/a \gg 1$ as expected for 2D amorphous materials [22, 30, 40]. We have also confirmed that the structure factor (not shown here) is isotropic, as expected. This analysis shows that the system sizes we study are large enough to describe amorphous systems.

In figure 3(d) we present the ring size distribution for the amorphous geometries [76]. The amorphization is quantified considering the standard deviation $\sigma$ from hexagons. The structures are characterized by slightly different $\sigma$, all showing a broad ring size distribution as expected for amorphous materials [22]. Figure 3(e) shows the ring size standard deviation $\sigma$ as a function of the number of flipped bonds for the amorphous realization #1, see figure 3(e). We find that the $\sigma$ tends to a constant as the number of amorphization steps is increased, indicating that the system does not undergo further significant structural modifications by continuing the amorphization process.

Figures 3(f) and (g) show the bond length and bond angle distributions. We observe a contraction in the bond lengths as the mean value for the amorphous structures is 3.06 Å, that is smaller than the pristine value. We interpret this feature as a consequence of the presence of non-connected regions (voids) inside each amorphous geometry. The mean Bi–Bi–Bi bond angle is still centered around the pristine value, which is expected since the average coordination number is close to 2.7 for all structures.

### 3.2. Electronic structure

Let us now calculate the electronic structure of the amorphous realizations and characterize their topological properties. For that, we investigate the energy levels of pristine and amorphous systems, the presence of metallic edge states at their interface with vacuum, and compute their topological indices.

For the case of periodic boundary conditions (PBC), these systems are insulators, with the band gap marked by the gray region in figures 4(a)–(d). The band gap of crystalline H-bismuthene is 0.51 eV, while the amorphous band gap ranges from 0.27 to 0.16 eV. The decrease in band gap is a result of amorphization due to the degree of structural disorder and is realization dependent. The amorphization scheme we adopt can be considered as a sequence of discrete transformations that map the pristine insulating system into an amorphous insulating phase without a band gap closure. The topological nature of these systems is confirmed by inspecting their topological invariants. The $\mathbb{Z}_2$ invariant is computed using the Wannier charge centers (WCCs) evolution method [77, 78] implemented in the Z2Pack code [79]. For the crystalline system, the non-trivial topology is characterized by $\mathbb{Z}_2 = 1$. We consider the three amorphous structures we have generated as supercells and obtain $\mathbb{Z}_2 = 1$. For non-crystalline systems, the topological nature can also be characterized by the spin Bott index ($B_s$) that gives a measure consistent with the $\mathbb{Z}_2$ invariant for sufficiently large system sizes, as discussed in references [25, 26]. Such problem is intrinsically avoided in non-crystalline systems due to the extended size of the geometries used to accommodate the amorphous phase. We implemented the calculation of the spin Bott index as in references [25, 26] using the full ab initio Hamiltonians in local basis, and obtain $B_s = 1$ for the three amorphous systems. Both results are consistent and show that
Figure 4. Energy eigenvalues versus state index for periodic (PBC) and open boundary conditions (OBC). Panel (a) corresponds to the pristine system, and (b)–(d) to the different amorphous realizations, as indicated by the insets. The gray regions stand for the topological gaps. The insets show the wavefunction probability amplitude of the states marked in green.

bismuthene keeps its pristine topological features in the amorphous state.

For open boundary conditions (OBC), the energy gap is filled. In the pristine case the states filling the topological gap are localized at the system edges. Conversely, for the amorphous systems, the distribution of these wavefunctions along the edges is significantly altered by the amorphization with respect to the crystalline case. However, we still observe strong edge localization with a variation along the edge, analogous to reference [40] and other lattice models of amorphous TIs [11–13, 20, 23, 25, 26]. The insets in figure 4 show the site-projected wavefunction of selected states.

We stress that, even though all considered structures have the same number of bonds flipped, the relaxation yields geometries with different connectivities, that directly affect the energy gap, as seen in figure 4. This effect is more dramatic for the amorphous realization #3, see figures 3(a4) and 4(d), since bulk defect-like states appear inside the energy gap pinning the Fermi level. For this realization, the lowest occupied state is localized at the void region in the bulk, and a closer analysis shows that the real energy gap is 0.16 eV. As a result, the selected mid gap state shows edge localization even though is below the Fermi energy. A similar feature has been reported in a theoretical study of vacancies and vacancy clusters in flat bismuthene [28]. In such a case, the robustness of the QSH state is proportional to the pristine energy gap and defect/disorder type. Hence the material supports the non-trivial topological state until the vacancy concentration reaches a threshold value. This observation raises the question: Does the topological gap close as one considers systems with more bond flips?

In all amorphous realizations we study, the energy gap shows an overall decrease with increasing number of amorphization steps \( N_a \) and stabilizes for \( N_a \geq 15 \) at a finite value, yielding the topological amorphous insulators presented here. This is illustrated in figure 5 that shows the gap as a function of the amorphization step for the amorphous realization #1, demonstrating the stabilization of the band gap with the number of flipped bonds. For the three amorphous realizations with full SOC strength, the \( \mathbb{Z}_2 \) is kept invariant, and there are no signs of a topological quantum phase transition. Furthermore, the standard deviation of ring size with the amorphization step number \( N_a \) shows a saturation with increasing amorphization steps (see figure 3(e)), indicating that no significant structural changes occur when introducing more bond flips. Hence, we also expect that the electronic structure is stabilized.

Next, we study the dependence of the robustness of the topological gap on the spin-orbit interaction strength. For that, we analyze the evolution of the band gap by artificially quenching the SOC strength by a factor \( \alpha (0.0 < \alpha < 1.0) \). The pristine band gap versus \( \alpha \) curve shows an inverted ‘V’ like shape (not shown here). The gap increases linearly, reaching a maximum value of 0.81 eV for \( \alpha = 0.64 \). At larger \( \alpha \) values the gap decreases, also linearly, until 0.51 eV for \( \alpha = 1.0 \). This behavior is due to a direct to indirect band gap transition. For \( \alpha < 0.64 \), a direct gap at K-point is obtained. Beyond this critical value, the conduction band minimum is shifted to the \( \Gamma \)-point. The valence band maximum persists at the K-point for all \( \alpha \) values. For \( \alpha > 0.0 \) (\( \alpha = 0 \) the system is metallic) the system is gaped and topologically non-trivial.
The result in figure 5 is obtained for the amorphous realization in figure 3 (a2) (#1). The pristine system (figure 5, amorphization step 0), shows a surprising behavior: for small to intermediate SOC strengths, the band gap increases with $\alpha$, reaching its maximum value at $\alpha \approx 0.75$. By further increasing $\alpha$, the band gap decreases to the actual value of flat bismuthene at $\alpha = 1$. This finding suggests exploring the possibility of designing novel QSHIs with increased robustness by alloying with elements with smaller SOC strength than Bi, for instance, Sb. Figure 5 shows that for large amorphization steps, the band gap stabilizes regardless of further geometry modifications. For intermediate steps the band gap decreases, reaching a minimum then increasing to its final value. This minimum is reached for 15 steps. For the QSH state to survive the amorphization the energy gap should remain open at this minimum, which is clearly dependent on the SOC strength. At this step, the energy gap converges to 0.11 eV with increasing SOC strength. For $\alpha = 0.01$, the band gap reaches a minimum of 0.02 eV indicating that a quantum phase transition may occur for this SOC strength before 15 amorphization steps. This is further supported by calculating the topological invariant. The convergence of the spin Bott index with system size also depends on the SOC strength. We have verified that when SOC is decreased to small values, the system sizes required to obtain convergence imply a prohibitive computational cost. Therefore, when studying the topological nature as a function of SOC we employ the $Z_2$ invariant. For all SOC strengths larger than 0.01, we obtain $Z_2 = 1$ throughout the amorphization procedure. For the case of $\alpha = 0.01$ SOC strength, we find $Z_2 = 1$ before the minimum energy gap is reached, while $Z_2 = 0$ after the energy gap reopens, signaling a quantum phase transition from the topologically non-trivial to the trivial system. In summary, we find that the robustness of the system topological properties against amorphization depends on the interplay between SOC strength and band gap of the pristine material. Our simulations indicate that flat bismuthene maintains its topological features for all studied amorphous realizations.

### 3.3. Electronic transport

Here, we study the effect of the non-trivial topology in the electronic conductance of amorphous bismuthene nanoribbons using the Green’s function approach described in section 2. The crystalline nanoribbons have $G_0 (2e^2/h)$ conductance inside the topological gap, which is a hallmark of the metallic edge states of QSHIs. As the energy is moved away from the topological gap, the conductance is increased in integer steps of $G_0$, due to the opening of modes corresponding to the bulk band structure of the nanoribbon geometry. See dashed lines in figure 6.

We use the three amorphous bismuthene structures obtained as discussed above to build amorphous nanoribbons. For single building blocks, the latter have a scattering region of 6.49 nm in length. Figures 6(a)–(c) show the corresponding calculated conductance as a function of the energy. The $G_0$ conductance inside the topological gap is a fingerprint of the topological edge states’ robustness and protection against back-scattering. For trivial states, outside the topological gap, the conductance is strongly suppressed with respect to the crystalline one, as expected. These results are in agreement with the results of reference [40] for amorphous H-bismuthene and defective topological systems, including stanene [80] and 2D Na$_x$Bi [81]. The insets in figure 6 show the amorphous ribbons with site-projected wavefunction probability amplitude at $E = \varepsilon_F$. These plots show that, despite being strongly affected by amorphization, the edge states preserve their key features, namely they are extended and states at opposite edges of the ribbon do not hybridize.

We now study the conductance for realistic device lengths. We use the three amorphous structures obtained above as building blocks to form arbitrarily long nanoribbons, see figure 2. First we built a system consisting of 3 building blocks in a row. The resulting scattering region is 19.46 nm long. The corresponding conductance, shown by the red line in figure 6(d), is qualitatively similar to the ones of figures 6(a)–(c). Next, we randomly combine the amorphous structures to form a sequence of 50 building blocks, that gives a nanoribbon of 324.33 nm in length. The calculated conductance, blue line in figure 6(d), shows $G = G_0$ for $-0.13 \mathrm{eV} < E < 0.10 \mathrm{eV}$, confirming the robustness of the QSH phase against amorphization, in line with the results presented in section 3.2. For energies outside this range but still within the bulk topological gap, the conductance is suppressed at few narrow energy intervals. The latter becomes
more dense as the energy approaches the bottom (or top) of the non-topological bands. For energies corresponding to trivial states, the conductance is strongly suppressed and the system becomes an insulator. We note that by taking permutations in the sequences of building blocks one can easily generate a large number of disorder realizations for a given length. We have verified that figure 6(d) is quite representative of all cases we have considered, that is, the quantized $G_0$ conductance is quite robust.

To further investigate this feature, we analyze the DOS of the systems addressed in figure 6. The dashed lines in figure 7 correspond to the DOS of a pristine bismuthene nanoribbon and serve to guide our discussion. The amorphization drives electronic states into the topological gap. When these states are isolated, they do not affect the electronic transport, an indication that they are localized. For energies close to the van Hove singularities but still in the topological gap, the density of states driven by amorphization increases and due to their overlap the conductance decreases, see figure 6. The situation is very different for energies outside the topological gap. Here, while the DOS increased significantly, the conductance is strongly suppressed and the system becomes an insulator. This behavior is characteristic of the onset of Anderson localization [82–85].

3.4. Breaking time-reversal symmetry
Let us now investigate possible mechanisms to manipulate the system conductance of the amorphous topological insulators protected by TRS. This can be accomplished by, for instance, adding to the Hamiltonian a simple exchange field expressed as an on-site term of the form $\delta H = B \cdot \sigma$. The computation of the perturbation term is done by calculating the expectation value of the Pauli matrices $\sigma_i$ ($i = x, y, z$) on the local basis, which allow us to apply this field in different directions. This field opens an energy gap in the pristine nanoribbon, as seen in figure 8(b). As expected for bismuthene armchair nanoribbons, the opened energy gap for on-site exchange fields on in-plane directions is up to two orders of magnitude larger than for out-of-plane directions [86]. The difference in gap opening is a result of the unbalanced spin-texture for the pristine nanoribbon. Figure 8(a) shows the expectation values

![Figure 6. Electronic linear conductance $G$ for different amorphous realizations and device lengths as a function of the energy. Panels (a)–(c) correspond to the different amorphous realizations #1, #2 and #3, respectively. Panel (d) correspond to a scattering region composed of randomly selected sequences of the previous amorphous realizations. The insets shows the site-projected wavefunction probability amplitude for the states with energy $E = \varepsilon_F$. The arrows indicate the transport direction.](image-url)
Figure 7. Density of states as a function of the energy. Panels (a)–(c) correspond to the different amorphous realizations #1, #2 and #3, respectively. Panel (d) correspond to a scattering region composed of randomly selected sequences of the previous amorphous realizations. The DOS in panel (d) are shifted in the y-axis for better visualization. The pristine nanoribbon is represented by the dashed line.

Figure 8. (a) Spin texture for armchair pristine H-bismuthene nanoribbon in the absence of an external magnetic field. The color bar is in units of $\hbar/2 \sigma$. (b) Armchair nanoribbon band structure for parallel ($\delta H_\parallel$) and perpendicular ($\delta H_\perp$) exchange fields. (c) Sketch of the on-site exchange field directions on armchair flat bismuthene nanoribbons.

of the spin projection operator $S = \hbar/2 \sigma$ for pristine armchair nanoribbons. The spin texture is more pronounced parallel to the system plane and perpendicular to the transport direction (y), while the out-of-plane ($z$) spin texture is only significant in a small energy range in the conduction band, right above the Fermi level. This unconventional spin-texture has been attributed to the combination of inversion asymmetry and QSH phase originated by the inverted band gap [37]. In the bulk, the valence band at the $K/K'$-points shows Zeeman-type splitting for $s_z$ and a Rashba-type spin-texture in in-plane directions. This effect is caused by strong SOC and polarization due to the functionalization [87]. Moreover, in the bulk, the states at the $K$ and $K'$ points have opposite spin-polarizations. In armchair nanoribbons, these states at $K/K'$-points mix and the spin-projection is no longer aligned with the $z$-axis [86]. These features are also observed for IV-V half-functionalized QSH phases [37] and Bi$_2$HF [87].
Figure 9 shows the conductance of the amorphous topological insulator nanoribbons for parallel ($\delta H_\parallel = B_\parallel \sigma_y$) and perpendicular ($\delta H_\perp = B_\perp \sigma_z$) field directions using the 324 nm device setup of figure 6(d). The breaking of TRS erases the topological protection of the edge states. With the opened energy gap, the mixture between spin axis enables scattering events, thus decreasing the system conductance independent of the field direction. We note that exchange fields in the out-of-plane direction (figure 9(b)) are less effective in suppressing $G$ than in-plane ones (figure 9(a)). The combination of realistic device length and exchange field induces localization effects, dramatically quenching the conductance, as shown in figure 9.

In figure 10 we show the conductance at the system Fermi energy $\varepsilon_F$ as a function of temperature, equation (3), for a parallel, figure 10(a), and perpendicular, figure 10(b), on-site exchange field. We calculate the ratio between conductance for the system without and with the in-plane exchange field ($G_{on}/G_{off}$). For the pristine and amorphous devices, this ratio is 2.02 and 15.10 at 300 K, respectively. The enhanced on/off ratio reveals that the amorphous TIs can aid the realization of QSHI-based devices at room temperature. This temperature effect is proportional to the band gap, and varies for different TIs [81, 88]. Realizing amorphous materials with topological properties is desirable to hinder the interference of bulk transport at finite temperature, screening only the transport response of topological edge states, as in figures 6(d) and 9(a). Hence, the amorphization may be used as a filtering technique for several topological systems.

4. Summary and conclusions

We have studied the realization of amorphous topological insulator materials using state of the art computational techniques to study the structural, electronic and transport properties of structure that may be obtained by standard experimental techniques before annealing.

We use a random bond flip method combined with ab initio calculations to generate flat bismuthene amorphous structures. The RDF shows that the obtained systems have short range and lack long range
order. We characterize the structure by different statistical measures and find that the ring size distribution nicely captures the degree of amorphization of our structures. We find that amorphous bismuthene has a coordination that is significantly smaller than $z = 3$, that is reflected in an average bond length smaller than the pristine one and, more interestingly, in the formation of holes.

We study the topological properties of the system by calculation the $Z_2$ invariant and the spin Bott index. As expected, these invariants reveal the non-trivial topological band structure of the material. One of the main results of this study is that the amorphization tends to suppress the band gap, but does not closes it. We find that the survival of the QSH state through the amorphization process is associated with the SOC strength of the material and the size of the bulk band gap.

Interestingly, we also find that the amorphization-induced holes host localized states at the corresponding internal edges of the system. This, not only confirms the lack of bondings in these regions, but also gives rise to new non-trivial states that deserve further investigation.

Next, we investigate the Landauer conductance for devices with realistic lengths, up to 324 nm. This is achieved by building nanoribbons composed of randomly selected sequences of the amorphous systems generated by \textit{ab initio} techniques. Using this setup we obtain that the topological helical edge states with conductance $2e^2/h$ are preserved inside the gap. For energies outside the topological gap region we find a strong suppression of the conductance, consistent with Anderson localization, a clear indication of a trivial insulator phase. Furthermore, the conductance is controllable by a simple exchange field that may be induced by a substrate or experimental probe.

Due to the robustness of such systems, amorphous H-bismuthene QSHI{s} may be the key to the experimental realization of QSHI-based devices at room temperature, not only displaying the gapless helical edge state but also hindering the bulk transport response.

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