

Article

Switching Topological States via Uniaxial Strain in 2D Materials

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Abstract

In topological materials, dissipationless edge currents are protected against local defect scattering by the bulk inverted band structure and band gap. We propose that large uniaxial strain can effectively switch a 2D Chern insulator to a topologically trivial state. Further, we suggest that the boundary between strained and unstrained regions of a sample can act as a new edge for dissipationless current flow. Using density functional theory (DFT) calculations we demonstrate the strain-tunability of the monolayer $\text{MnBi}_2\text{S}_2\text{Te}_2$ band structure and the switching of the Chern number. We combine uniaxial and biaxial strain results to map out the strain-tuned topological phase diagram.

Keywords: topological materials; 2D magnets; strain; electronic structure; chern insulator

1. Introduction

In a topological insulator, electronic bands of distinct symmetry cross and hybridize, which opens an inverted bulk band gap. A consequence of this mixed-symmetry band gap is the formation of chiral spin-polarized metallic bands localized at the boundaries of the inverted region, which results in conductive edge modes. The bulk band gap protects these edge modes against scattering, allowing a current to flow with zero dissipation. This topological protection of the edge mode conductivity is a hallmark of these materials, and has generated great interest for potential energy-efficient device applications. However, it is inherently difficult to externally tune the edge current as it requires changing the topological state of the entire inverted volume, potentially limiting its utility in practical devices. In this work we use DFT to show how mechanical strain can tune the edge mode conduction of a specific subclass of topological insulators, namely those with intrinsic ferromagnetic order (often called quantum anomalous Hall insulators or Chern insulators), though our results are applicable to other systems such as nonmagnetic topological insulators and topological crystalline insulators.

In a topological insulator, the spin-momentum locking of the edge bands results in spin-up and spin-down electrons propagating in opposite directions around the boundary of a material. The propagation direction for a particular spin species is determined by the slope of the edge band. When both spin edge bands are equally occupied, no net charge current flows along the boundary.

A Chern insulator is defined by the Chern number C , which is the difference between the number of right- and left-propagating edge modes at the Fermi level. A nonzero value of C arises from the magnetization of the material, which pushes edge bands for spins



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anti-parallel to the magnetization to higher energy and leaves only parallel spin edge bands populated at the Fermi level. This results in a net charge current along the boundary, with the edge conductivity given by the transverse conductivity equation $\sigma_{xy} = \frac{e^2}{h}C$. Therefore, the transverse conductivity can be modified by flipping the magnetization direction (which flips the sign of the Chern number) and by changing the net number of the edge bands (which changes the integer value of the Chern number).

Topologically protected edge modes must exist at the boundary between any two regions of space with different values of C [1]. The simplest such boundary is between the physical edge of a sample and the vacuum ($C = 0$). This was first demonstrated experimentally in magnetically doped $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ thin films [2–4], and later in few-layer samples of MnBi_2Te_4 [5–9]. A second type of boundary exists along the domain walls between regions of net spin-up ($C > 0$) and spin-down ($C < 0$) magnetization within a single sample. Control over the direction of edge currents was demonstrated by using an external magnetic field to “write” areas of a sample into spin-up or spin-down states [10]. A third type of boundary is found between areas of different thickness within a single sample. For instance, in MnBi_2Te_4 , the boundary between a four-layer ($C = 1$) and a six-layer ($C = 2$) region was shown to support one edge mode [11]. These preceding examples demonstrate the diversity of approaches to generating topological boundaries in Chern insulators.

While the previous examples demonstrate boundaries defined by discrete quantities (magnetization direction, layer number), a boundary could also be formed by a continuous tuning parameter. For instance, consider a material with a doping gradient such that the heavily doped side hosted ferromagnetism ($C = 1$) while the lightly doped side did not ($C = 0$). Then, there would be a path somewhere in the middle of the sample along which the inverted band gap must close and a conductive edge mode must form. The existence of this closed band gap path is a strict requirement of the topological nature of the inverted band structure [1].

Here we introduce another type of topological boundary, which can form between regions of a sample experiencing different amounts of mechanical strain. We posit that in some Chern insulator systems, uniaxial strain may be able to close and reopen a band gap, and in doing so change the value of the Chern number. In that case, the boundary between regions of different strain will host conductive edge modes. We first discuss this process schematically for an idealized system with the desired topological strain tunability. Then, we discuss DFT calculations for several 2D Chern insulating materials.

We show that a realistic value of uniaxial strain can indeed reverse the band gap in $\text{MnBi}_2\text{S}_2\text{Te}_2$, suggesting that control of edge modes across a strain boundary is feasible experimentally.

We consider a $C = 1$ Chern insulator with a strain-tunable band gap, where increasing tensile strain causes the topological band gap to close and reopen as a trivial gap as shown in Figure 1a. In a sample experiencing a large strain gradient, the low-strain region will maintain an inverted band gap ($C = 1$), while the high-strain region will have a trivial band gap ($C = 0$). The critical strain ϵ_c where the band gap closes marks the boundary between regions of different Chern number. At this boundary a conductive edge mode must form.

Such a strain-tunable material could be used in a device where applied uniaxial strain controls the flow of dissipationless current. We discuss two strain-tunable topological circuit elements, diagrammed in Figure 1b,c. A topological transistor is formed by straining a large region of a sample, such that the total current flow between two contacts can be turned on and off by straining the sample between the $C = 1$ and $C = 0$ states. A topological current switch is formed by straining a narrow width between two contacts on

a sample, controlling whether the unidirectional current flows around the whole sample or through the middle of the sample.

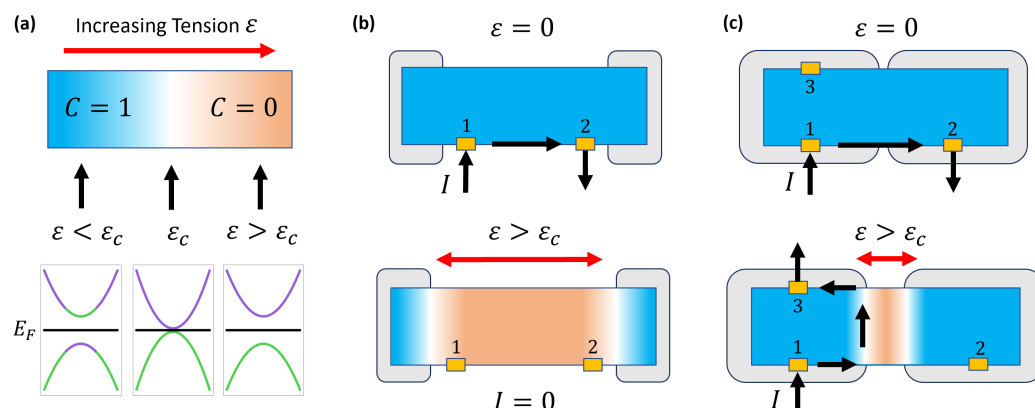


Figure 1. (a) Conceptual schematic of a Chern insulator with a strain-tunable band gap under a large strain gradient. Regions of low-strain inverted band gap ($C = 1$, blue) and high-strain topologically trivial band gap ($C = 0$, orange) are separated by a narrow width at the critical strain ϵ_c where the band gap is closed (white). (b,c) Strain-switchable topological circuit elements. The sample bar is clamped to substrate plates (gray) which can move and apply strain to the sample. Black arrows indicate dissipationless edge current flow. (b) Topological transistor. Under zero strain, edge current flows from contact 1 to contact 2. Under large applied tension, the device is reduced to a trivial insulator and no current flows. (c) Topological current switch. Under zero strain, current flows from contact 1 to contact 2. Under large applied strain, the current follows the internal boundary between strained and unstrained regions and is received at contact 3.

More broadly, our work illustrates how uniaxial strain can serve as a continuous tuning parameter for Chern numbers in polar Janus monolayers. Experimentally realized Janus transition-metal dichalcogenides such as MoSSe already demonstrate robust out-of-plane dipoles and broken mirror symmetry [12–14], while a growing set of magnetic and topological Janus compounds has been proposed theoretically [15–17]. The strain-driven switching mechanism we establish for $\text{MnBi}_2\text{S}_2\text{Te}_2$ should therefore be relevant across a broader Janus materials landscape, and provides design principles for future experimental and device-level studies.

2. Results

First-principles calculations were performed to investigate the possibility of inducing a topological phase transition with uniaxial strain (see the Methods Section for details). We first explored the effect of tunable strain on MnBi_2Te_4 in one- and three-layer samples (the latter in both ferromagnetic and antiferromagnetic configurations), with initial magnetic moments of $5\mu_B$ onto the Mn atoms in each layer. We were unable to identify a strain-induced switching between a Chern insulating and a trivial insulating state in these analyses; instead, a metalization transition usually occurred. We also investigated uniaxial strain-tuning of V_2WS_4 , a quantum anomalous Hall insulator candidate material [18], and again found a metalization transition. These results are presented in the Supplementary Materials (SM).

We then performed calculations on a monolayer of $\text{MnBi}_2\text{S}_2\text{Te}_2$, which has the same structure as MnBi_2Te_4 but with half of the Te atoms replaced with S (Figure 2a). Previous first-principles studies have predicted that this material hosts a doubly inverted band gap [16]. Under biaxial tension, $\text{MnBi}_2\text{S}_2\text{Te}_2$ was shown to undergo two topological transitions, from $C = 2$ to $C = -1$, and then to $C = 0$ (note that the change in sign of C comes from a change in slope of the edge band with strain tuning and not from a

reversal of the magnetization). In this work, we were able to identify a uniaxial strain-mediated transition from the $C = 2$ phase to $C = 1$, $C = 0$, and metallic phases, discussed below. Throughout, we keep the Mn spins ferromagnetically aligned along the out-of-plane axis by construction, as appropriate for the quantum anomalous Hall regime of interest (see Discussion).

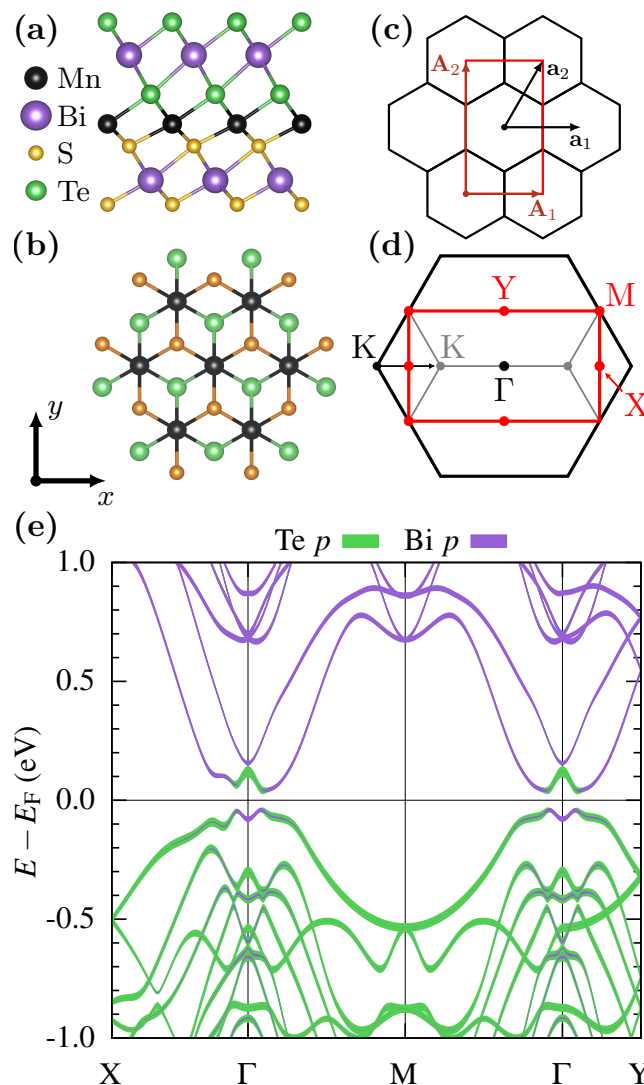


Figure 2. (a) Crystal structure of monolayer $\text{MnBi}_2\text{S}_2\text{Te}_2$. (b) In-plane crystal structure showing the Mn layer and its surrounding S and Te layers. Note the inequivalence of the x and y directions. (c) Real space and (d) reciprocal space diagrams of the hexagonal conventional cell (black) and the rectangular supercell (red) used for strain calculations. The reflected K point is shown in light gray. (e) Orbital-projected band structure of $\text{MnBi}_2\text{S}_2\text{Te}_2$ under zero strain. The Te and Bi p orbital projections are shown in green and purple, respectively.

$\text{MnBi}_2\text{S}_2\text{Te}_2$ has a hexagonal crystal lattice with C_3 rotational symmetry, meaning the crystal structure is distinct along the perpendicular x and y directions. Here we take x to be the “zig zag” direction and y to be the “armchair” direction, and explore strain tuning along both. In order to model uniaxial strain, a rectangular $1 \times \sqrt{3}$ supercell was constructed and superimposed over the hexagonal lattice; see Figure 2c. The lattice was stretched or compressed in one direction, and the orthogonal lattice vector was scaled by a Poisson ratio of -0.3 , a typical value for 2D materials. More precisely, we apply a prescribed axial strain of ε_{xx} or ε_{yy} to one in-plane lattice vector, rescale the perpendicular lattice vector using a fixed in-plane Poisson ratio $\nu = -0.3$, and then fully relax all internal atomic coordinates at

fixed cell angles; all strain values quoted in this work refer to the axial components ε_{xx} and ε_{yy} (see Methods for justification of the chosen ν).

The rectangular supercell results in zone folding of the hexagonal Brillouin zone (BZ) in momentum space (Figure 2d). The K and K' points at the corners of the hexagonal BZ map to identical points within the rectangular BZ between the X point and the Γ point. The M point at the midpoint of the edge of the hexagonal BZ becomes the corner of the rectangular BZ.

We first calculated the electronic structure of $\text{MnBi}_2\text{S}_2\text{Te}_2$ under zero strain (Figure 2e), and our results are in agreement with the previous report [16]. At the Γ point, the valence band is primarily of Te p_{xy} character, while the conduction band is primarily of Bi p_z character. The band gap itself shows two points of band inversion, which results in an expected Chern number of $C = 2$ (discussed below).

We then calculated the electronic structure as a function of tensile and compressive uniaxial strain up to 8% along the x axis and up to 10% along the y axis; other 2D materials such as graphene and transition-metal dichalcogenides have previously been demonstrated to withstand such large strain values [19,20].

We first compare results for the zero- and tensile-strain cases (Figure 3). Under tensile strain, we observed that the band gap closes and reopens at around 3% strain along the x direction and at 3.5% strain along the y direction. This results in a band gap with only one point of inversion along x (Figure 3d) and a topologically trivial band gap for y (Figure 3g). Orbital-projected “fat-band” plots (SI) confirm that, for $\varepsilon_{xx} > 0$, only one of the two Bi- p /Te(S)- p inversions present at zero strain is removed, whereas for $\varepsilon_{yy} > 0$ both inversions are lifted, consistent with the Chern numbers discussed below. We then calculated the edge electronic band structure. The presence of one or two edge modes in the fundamental band gap indicates the QAH phase, while the gapped edge spectrum indicates a topologically trivial edge state. Under zero strain, we found two right-moving edge states that cross the Fermi level, indicating a Chern number of $C = 2$ (Figure 3b). For tensile strain along x , this was reduced to a single edge state ($C = 1$) (Figure 3e), while for tensile strain along y the edge states vanish ($C = 0$) (Figure 3h). Finally, we calculated the transverse conductivity (Figure 3c,f,i), and find peaks (or no peak) in the in-plane transverse conductivity σ_{xy} corresponding to the expected quantized conductivity equation $\sigma_{xy} = \frac{e^2}{h} C$. Numerically, the $\sigma_{xy}(E)$ plateaus lie very close to the ideal values Ce^2/h ; the small deviations are attributable to finite k -mesh sampling and the finite energy broadening used in the Kubo formula, rather than to any intrinsic non-quantization.

In Figure 4a–d, we present DFT results at very large strain values for both tension and compression along x and y . In all cases, a metalization transition occurs when a side band rises in energy to eventually cross the Fermi level. Then, the total conduction includes a non-dissipative source from edge conduction, and a dissipative source from regular metallic bulk conduction. Combining our results for uniaxial strain with previous results for biaxial strain [16], we can construct a partially-explored strain-tuned phase diagram for $\text{MnBi}_2\text{S}_2\text{Te}_2$ (Figure 4e). In this diagram, filled symbols denote points calculated in this work (uniaxial strain, PBE+ U with $U_{\text{eff}} = 3$ eV), while open symbols denote biaxial-strain results taken directly from Ref. [16]; in particular, the $C = -1$ region and its boundaries are reproduced from Ref. [16] and are not independently recomputed here. In regions not explicitly sampled we avoid drawing sharp phase boundaries and regard the interpolated lines as schematic. These results show clearly that the edge conduction of $\text{MnBi}_2\text{S}_2\text{Te}_2$ is strongly strain-tunable, and transitions from the $C = 2$ state to any of $C = 1$, $C = 0$, $C = -1$, or a metallic phase, can be obtained by choice of strain axis and symmetry. In all $\text{MnBi}_2\text{S}_2\text{Te}_2$ calculations we employ a PBE+ U description of the Mn $3d$ states with $U_{\text{eff}} = 3$ eV (see Methods), so that all band gaps and critical strain values quoted below

should be regarded as PBE+ U -level estimates; previous comparisons of PBE(+ U) and hybrid functions in $\text{MnBi}_2\text{S}_2\text{Te}_2$ and closely related Janus $\text{MnBi}_2\text{X}_2\text{Te}_4$ systems indicate that such treatments primarily renormalize the gap size while leaving the band inversion pattern and Chern sequence intact [16,17]. Within this theoretical framework we show that uniaxial strains in the order of a few percent can reverse the band gap in monolayer $\text{MnBi}_2\text{S}_2\text{Te}_2$ and change its Chern number, implying that control of edge modes across a strain boundary should in principle be possible if a Janus Chern insulator of this type can be realized and strained within its mechanical stability window.

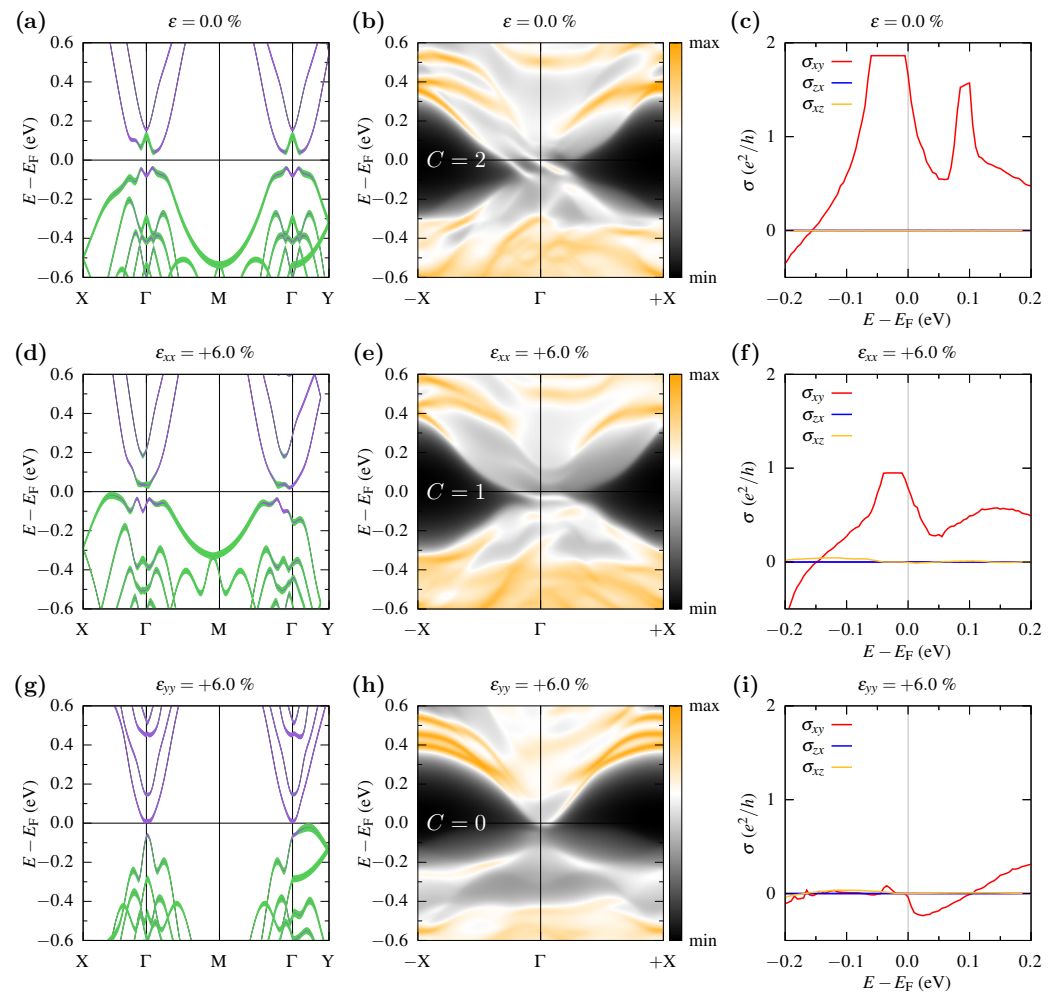


Figure 3. Comparison of $\text{MnBi}_2\text{S}_2\text{Te}_2$ under zero strain (a–c), $\epsilon_{xx} = 6\%$ tensile strain (d–f), and $\epsilon_{yy} = 6\%$ tensile strain (g–i). (a,d,g) Band structure calculations. (b,e,h) Calculated edge states. The number of Fermi level-crossing edge modes (and corresponding Chern number C) changes from two ($C = 2$) under zero strain, to one ($C = 1$) for $\epsilon_{xx} = 6\%$, to zero ($C = 0$) for $\epsilon_{yy} = 6\%$. (c,f,i) Quantum anomalous Hall conductivity calculations. Plateaus for the in-plane transverse conductivity σ_{xy} occur near the expected quantized conductivity values for the $C = 2$ and $C = 1$ cases, and is nearly zero for the $C = 0$ case.

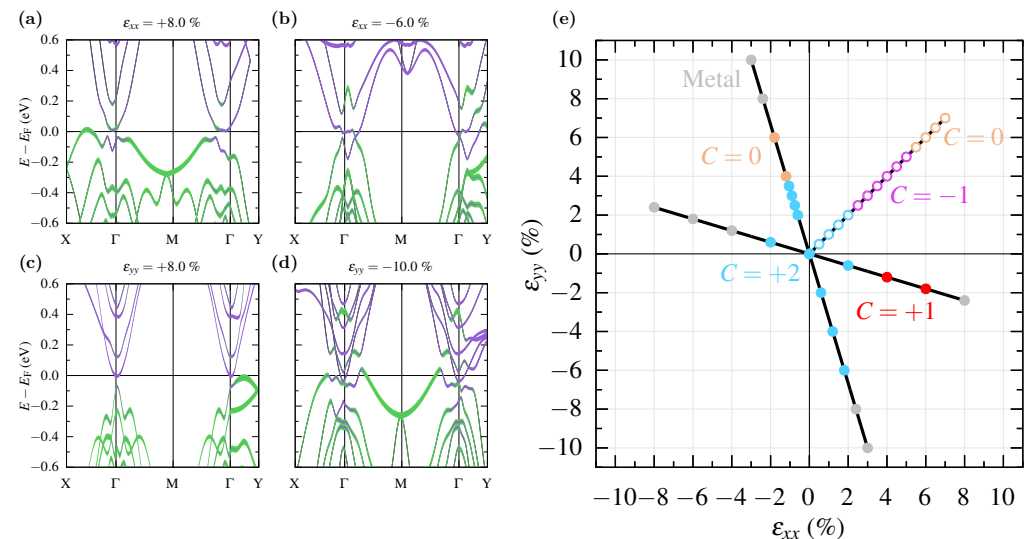


Figure 4. (a–d) Orbital-projected band structures under large tensile and compressive uniaxial strain along (a,b) x and (c,d) y . (e) Topological phase diagram of MnBi₂S₂Te₂ as a function of strain in the x and y directions. The $C = +2, +1, 0$, and -1 phases are shown in blue, red, orange, and magenta, respectively, and the metallic phase is shown in gray. The filled circles represent calculations from this work, and the empty circles represent calculations from Ref. [16].

3. Discussion

In MnBi₂Te₄, strong SOC induces band inversion and nontrivial topology in multilayers [21]. Switching on SOC results in a very small gap about the Fermi level, with significant band inversion between the Bi and Te p states. After exploring the possibility of inducing a topological phase transition in pure MnBi₂Te₄ [5–7], we found that the band inversion could not be undone through the application of biaxial or uniaxial strain. The gap and band inversion was found to be robust against biaxial strain. Upon application of uniaxial strain, the gap closed (insulator–metal transition), but did not reopen again as a trivial insulator. One possible reason for the persistence of the topological state (avoided crossing), is the combination of symmetries here. Biaxial strain preserves both inversion symmetry and C_3 symmetry, which may be protecting the band inversion and avoided crossing. Uniaxial strain breaks rotation symmetry but not inversion symmetry, which may be enough to remove the avoided crossing, but not enough to induce a topological phase transition (we have a topological $\rightarrow$ metal transition). This is in fact a common occurrence in attempts to realize topological insulators [22]. These MnBi₂Te₄ calculations were carried out at the same PBE+ U level as our MnBi₂S₂Te₂ study, so the contrast between the two systems underscores the crucial role of inversion-symmetry breaking in enabling a clean, strain-tunable topological transition.

In MnBi₂S₂Te₂, the inequivalence of the Bi–Te and Bi–S layers surrounding the Mn layer classifies it as a Janus material. This naturally breaks inversion symmetry, which may be the necessary condition that enables external structural tuning to cleanly uninvert the band gap, as seen for both biaxial and uniaxial strain. Janus materials have been gaining interest for their additional complexity over centrosymmetric 2D materials [23,24]. Like other Janus materials, MnBi₂S₂Te₂ likely exhibits a c -axis spontaneous electrical polarization [25] due to the different electronegativities of the Bi–Te and Bi–S layers. It remains unexplored how this may interact with the topological features of the system. Thus, the $C = 2 \rightarrow 1$ vs. $C = 2 \rightarrow 0$ behavior of ϵ_{xx} and ϵ_{yy} reflects how directional strain couples to the anisotropic bonding and orbital character of the two inversion points in the Janus MnBi₂S₂Te₂ monolayer. From the electronic-structure point of view, the built-in polar field shifts the relative on-site energies of the p orbitals on the Te-terminated and S-terminated sides and is therefore

one of the ingredients that splits and stabilizes the multiple inversion points in the band structure. Although we have not computed the polarization or its strain dependence explicitly, our results suggest that this internal field works together with SOC to separate the inverted states and to make them particularly sensitive to anisotropic in-plane distortions. In principle, external control of this polarization—for example, by an out-of-plane electric field or asymmetric substrates—could provide an additional tuning parameter alongside strain, and a combined strain-plus-electric-field phase diagram for Janus Chern insulators would be a natural extension of the present work.

Another salient feature of the phase diagram is the asymmetry between tensile and compressive strain. Compressive in-plane strain preserves the $C = 2$ phase over a wider range before metallization than tensile strain does. Qualitatively, compression enhances Bi- p /Te(S)- p orbital overlap and tends to increase the SOC-induced splitting that stabilizes the inverted gap at Γ , while pushing the side bands that eventually drive metallization away from the Fermi level. Under tension, reduced overlap weakens the inverted splitting and simultaneously brings other conduction or valence bands closer to E_F , causing the gap to close and metallic states to appear at relatively small tensile strains. This picture is consistent with the band-structure evolution in Figure 4 and explains why the $C = 2$ phase occupies a broader window on the compressive side. The inequivalence of the two surfaces also is expected to result in a difference in the interlayer coupling to a substrate [25,26], which could affect the degree of strain transmission to the sample. While an attempt to grow crystals of $\text{MnBi}_2\text{S}_2\text{Te}_2$ does not appear to have been reported in the literature thus far, there have been several successful attempts at growing Janus transition-metal dichalcogenides [24], and several growth methods could be pursued.

Throughout this work we assume a ferromagnetic ground state with magnetization along the out-of-plane axis for $\text{MnBi}_2\text{S}_2\text{Te}_2$, in line with prior first-principles studies of MnBi_2Te_4 -family and Janus MBT-type monolayers at zero strain [16,27–29]. In our calculations this magnetic configuration is enforced at all strain values, allowing us to isolate the effect of strain on the electronic topology. Our strain–topology phase diagram should therefore be interpreted as conditional on the persistence of out-of-plane ferromagnetism over the insulating portions of the diagram.

Similarly, we do not attempt a full mechanical-stability analysis of $\text{MnBi}_2\text{S}_2\text{Te}_2$ under strain, nor do we include defects, disorder, substrate coupling, or finite-temperature effects. The strain range considered here (up to $|\epsilon| \lesssim 10\%$) is motivated by experiments on other two-dimensional materials such as graphene and transition-metal dichalcogenides that can sustain comparable strains before fracture. Whether $\text{MnBi}_2\text{S}_2\text{Te}_2$ itself remains structurally and magnetically stable throughout this window is an open question that calls for future phonon, elasticity, and finite-temperature simulations once this or closely related Janus Chern insulators become experimentally accessible. Our proposed “topological transistor” and “current switch” geometries in Figure 1 should therefore be viewed as schematic illustrations of how strain-defined boundaries between regions with different Chern numbers could route dissipationless edge currents. By the bulk–boundary correspondence, any interface between regions whose Chern numbers differ by ΔC must host $|\Delta C|$ chiral channels, as already demonstrated experimentally for interfaces defined by thickness and magnetization in MnBi_2Te_4 -based Chern insulators [11,30]. A quantitative device-level description, including realistic strain profiles and transport simulations based on the Wannier Hamiltonian, is an important direction for future work.

Beyond $\text{MnBi}_2\text{S}_2\text{Te}_2$, we expect the strain-driven switching mechanism demonstrated here to be broadly relevant across the rapidly expanding landscape of Janus two-dimensional materials. On the nonmagnetic side, experimentally realized Janus transition-metal dichalcogenides such as MoSSe and related MXY monolayers combine strong spin–

orbit coupling with robust out-of-plane dipoles and piezoelectric response, providing a natural arena in which strain and built-in polarization can jointly tune band topology [12,13]. Polar Rashba semiconductors such as BiTeI and epitaxial Janus BiTeCl/BiTeBr layers likewise exploit broken inversion symmetry and strong spin–orbit coupling to generate giant Rashba splitting and pronounced nonlinear optical effects, and could offer complementary platforms for strain- and field-control of spin–momentum locked states [14,31]. On the magnetic side, theoretical studies of Janus $\text{MnBi}_2\text{S}_2\text{Te}_2$, $\text{MnBi}_2\text{S}_2\text{Te}_2$, and $\text{MnSbBi}_2\text{S}_2\text{Te}_2$ monolayers already indicate that internal polarization, electric fields, and biaxial strain can stabilize quantum anomalous Hall phases and drive topological phase transitions in MnBi_2Te_4 -family materials [15–17]. Our results on uniaxial-strain control of Chern number in $\text{MnBi}_2\text{S}_2\text{Te}_2$ therefore fit into a wider Janus context and suggest that combining directional strain, electric gating, and heterostructure engineering across this materials space could enable a versatile toolbox for reconfigurable topological circuitry.

In conclusion, we have demonstrated the feasibility of using realistic values of applied uniaxial strain to switch off the spontaneous edge conduction in a quantum anomalous Hall material. This provides a path towards creating electronic devices with switchable topological states. Our result adds to the growing body of work exploring the structural tunability of topological materials [16,32,33].

4. Methods

Density functional theory calculations were performed using the VASP code [34], PBE exchange–correlation function [35], and projector augmented wave (PAW) pseudopotentials [36] with 13, 15, and 6 valence electrons for the Mn, Bi, and Te/S atoms, respectively. For $\text{MnBi}_2\text{S}_2\text{Te}_2$ we employed the rotationally invariant PBE+*U* scheme in the Dudarev formulation with an effective on-site Hubbard parameter $U_{\text{eff}} = 3$ eV applied to the Mn 3*d* orbitals [37], consistent with previous studies of MnBi_2Te_4 -family and Janus $\text{MnBi}_2\text{S}_2\text{Te}_2$ -type compounds [27].

For all three materials studied we employed a plane-wave energy cutoff of 520 eV as well as the zero-damping DFT-D3 van der Waals correction [38]. Forces on each atom were reduced below 0.01 eV/Å during structural relaxations, and we used a Γ -centered $15 \times 15 \times 1$ k-point grid for the final self-consistent calculations. Spin–orbit coupling was included self-consistently in all $\text{MnBi}_2\text{S}_2\text{Te}_2$ calculations.

Uniaxial strain was applied by rescaling one in-plane lattice vector by a prescribed axial strain ϵ_{xx} or ϵ_{yy} , while the perpendicular in-plane lattice vector was rescaled using a fixed in-plane Poisson ratio $\nu = -0.3$ [39,40]. After rescaling the lattice vectors, all internal atomic coordinates were fully relaxed at fixed cell angles. Throughout the manuscript the quoted strain values refer to these axial components, ϵ_{xx} and ϵ_{yy} ; the choice of ν only affects the transverse response and does not change the qualitative sequence of phases.

The maximally localized Wannier transformations [41,42] were performed using the Wannier90 code [43], with initial projections onto the *p* orbitals of the Bi and Te(S) atoms. For $\text{MnBi}_2\text{S}_2\text{Te}_2$ we used an outer disentanglement window of $[-8, 10]$ eV around the Fermi level, chosen to include all bands relevant to the topological gap. The resulting maximally localized Wannier functions have spreads in the range $[2, 6]$ Å² for the Bi-*p* and Te(S)-*p* orbitals and were checked to be stable with respect to the disentanglement parameters. These maximally localized Wannier functions (MLWFs) were then used to build a tight-binding model using the WANNIERTOOLS code [44].

Surface (edge) states were obtained using the semi-infinite slab Green's-function method in WannierTools, with a (100) surface and slab parameters NumSlabs = 20 and NP = 2. Unless otherwise stated, the ribbons are oriented along the *x* direction. The anomalous Hall conductivity $\sigma_{xy}(E)$ and the Chern numbers *C* were calculated from the same tight-

binding Hamiltonian using the Berry-curvature-based Kubo formula [45] as implemented in WANNIERTOOLS [44]. We evaluated $\sigma_{xy}(E)$ and C on a Γ -centered 100×100 k-mesh, and verified that increasing N further does not change the integer Chern numbers and only slightly refines the shape of the $\sigma_{xy}(E)$ curves. In all cases, the values of C quoted in the text and in Figure 4e are taken from this Berry-curvature integration, while the edge spectra and σ_{xy} plateaus are used as illustrative consistency checks.

Previous work on $\text{MnBi}_2\text{S}_2\text{Te}_2$ and related $\text{MnBi}_2\text{X}_2\text{Te}_4$ Janus monolayers has shown that moderate values of U_{eff} in the 2–5 eV range, benchmarked against hybrid functionals, primarily renormalize the band gap while leaving the band inversion pattern and Chern numbers unchanged [16,17]. In $\text{MnBi}_2\text{S}_2\text{Te}_2$, the states that form the topological gap near the Fermi level are dominated by Bi and Te(S) p orbitals, whereas the Mn d states lie several eV away, so a moderate U_{eff} mainly adjusts the position of these deeper d levels and the quantitative size of the gap without changing the ordering of the p -derived bands that determine the Chern number. We therefore expect the strain-driven sequence of Chern phases reported here to be robust against reasonable variations of U_{eff} and of the in-plane Poisson ratio used to parametrize the transverse response, even though the absolute gap sizes and critical strain values are quantitatively approximate. All phase boundaries in Figure 4e should thus be viewed as PBE+ U -level estimates. The integer Chern numbers shown there are obtained from Berry-curvature integration over the two-dimensional Brillouin zone using the Wannier tight-binding Hamiltonian, and we have checked that they are converged with respect to k -mesh density and Wannier disentanglement windows (see Methods). The edge spectra and $\sigma_{xy}(E)$ plateaus serve as independent, qualitative checks that the number of gap-crossing edge modes matches the computed C .

Supplementary Materials: The following supporting information can be downloaded at <https://www.mdpi.com/article/10.3390/ijt3030014/s1>. File S1: Density Functional Theory Calculations of 2D Materials Under Strain.

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