Strain Effects in Topological Insulators: Topological Order and the Emergence of Switchable Topological Interface States in Sb$_2$Te$_3$/Bi$_2$Te$_3$ heterojunctions

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We investigate the effects of strain on the topological order of the Bi$_2$Se$_3$ family of topological insulators by ab-initio first-principles methods. Strain can induce a topological phase transition and we present the phase diagram for the 3D topological insulators, Bi$_2$Te$_3$, Sb$_2$Te$_3$, Bi$_2$Se$_3$ and Sb$_2$Se$_3$, under combined uniaxial and biaxial strain. Their phase diagram is universal and shows metallic and insulating phases, both topologically trivial and non–trivial. In particular, uniaxial tension can drive the four compounds into a topologically trivial insulating phase. We propose a Sb$_2$Te$_3$/Bi$_2$Te$_3$ heterojunction in which a strain-induced topological interface state arises in the common gap of this normal insulator–topological insulator heterojunction. Unexpectedly, the interface state is confined in the topologically trivial subsystem and is physically protected from ambient impurities. It can be switched on or off by means of uniaxial strain and therefore Sb$_2$Te$_3$/Bi$_2$Te$_3$ heterojunctions provide a topological system which hosts tunable robust helical interface states with promising spintronic applications.

I. INTRODUCTION AND MOTIVATION

Topological insulators (TIs) are a novel quantum phase of matter characterised by a topological invariant that exhibit topologically protected states at the boundary with a trivial insulator. In particular, the Bi$_2$Se$_3$ family of three–dimensional (3D) TIs has been extensively studied during the last few years as paradigmatic TIs that show an inverted band gap due to a strong spin–orbit coupling (SOC). At the surface, these materials exhibit a Dirac cone–like helical state with a circular skyrmionic spin texture, and the topological protection ensures the robustness of these states against disorder scattering as long as time–reversal symmetry is maintained.

Fundamental interest and potential applications have driven the search of external and internal agents such as stress, electromagnetic fields, chemical substitution or stacking defects to engineer and manipulate the band structure of TIs. In particular, strain can be exploited to control the topological order. Several works have already assessed the importance of purely uniaxial strain in these materials and its influence on their topological character. For bulk materials, it was predicted that the topological phase can be effectively manipulated by strain. Uniaxial strain can be induced by the chemical intercalation of zerovalent non–magnetic metals in the van der Waals (vdW) gaps. This technique has already been experimentally demonstrated and developed by Koski et al. in Bi$_2$Se$_3$ to effectively enhance the c lattice parameter without disrupting the ionic or electronic configuration. In addition, Bi$_2$Se$_3$ films under tensile stress along the c–axis have been recently grown via a self–organized order method and significant changes of the Fermi level and band gap of those films have been measured. Topological state shifts at the strained grain boundaries in Bi$_2$Se$_3$ films have also been reported. To our knowledge, no study has systematically addressed the combined effect of both uniaxial and biaxial strain in the topology of the Bi$_2$Se$_3$ family. Being the four compounds narrow gap semiconductors, small strain fields can strongly affect their electronic properties, and, consequently, their topological nature. In this work we study the role of combined uniaxial and biaxial tension on the Bi$_2$Se$_3$ family of compounds, namely Bi$_2$Te$_3$, Sb$_2$Te$_3$, Bi$_2$Se$_3$, and Sb$_2$Se$_3$.

We show how uniaxial and biaxial strain can tune several properties of the topological states and how the combined effect of both kinds of strain can drive the four systems into a metallic phase or two topologically distinct insulating phases. We calculate the phase diagram for the four materials in terms of uniaxial and biaxial strain, and we show the band inversion process that governs their topology. Furthermore, we predict the emergence of strain induced topological interface states in Sb$_2$Te$_3$/Bi$_2$Te$_3$ heterojunctions. The article is structured as follows: in Section III we describe the methods employed for the calculations along with the crystal structure of the Bi$_2$Se$_3$ family of compounds. Section III is devoted to the effect of uniaxial and biaxial strain in bulk and thin films of the studied compounds. Next, we propose two topologically distinct heterojunctions of Bi$_2$Te$_3$ and Sb$_2$Te$_3$ and address their special electronic properties in Section IV. Finally, Section V includes a summary of the results and conclusions.

II. METHODS AND CRYSTAL STRUCTURE

Bismuth dichalcogenides show a rhombohedral crystal structure with a five atom basis that constitute a quintuple layer (QL) –see Figure 1. The four compounds forming the Bi$_2$Se$_3$ family studied in this work belong to the $R3m$ ($D_{3d}^5$) crystallographic group. Along the [111] direction each atomic layer contains only one element and is hexagonally compact. The stacking pattern along this direction is ...AbCaB... where capital (small) letters in-
Fig. 1. (a) Rhombohedral unit cell of the four studied compounds. Lattice constants \(a\) and \(c\) are indicated in the figure. (b) The corresponding bulk Brillouin Zone along with its projection along the [111] direction (purple shaded area).

dicate the position of Se or Te (Bi or Sb) atoms. Within a QL, interactions among the atoms are strong, while inter–QL bonding is of the weaker vdW kind.

To model the systems we employed the Vienna \textit{ab-initio} simulation package (VASP)\textsuperscript{17} density functional theory (DFT) code for the atomic relaxations and electronic structure calculations of bulk materials. The SIESTA code\textsuperscript{18}, through its implementation in the GREEN package\textsuperscript{19}, was additionally used for electronic structure calculations of the Bi\textsubscript{2}Te\textsubscript{3}–Sb\textsubscript{2}Te\textsubscript{3} heterojunctions. In all the calculations we used the Perdew–Burke–Ernzerhof\textsuperscript{20} implementation of the generalized gradient approximation (GGA). The semi–empirical pair–potential vdW correction of Grimme\textsuperscript{21} was used in the atomic relaxations as implemented in the VASP code to correctly account for the weak inter-QL interaction. The spin–orbit coupling was included self–consistently in both VASP\textsuperscript{22} and SIESTA–GREEN\textsuperscript{23} calculations. A 340 eV energy cut–off was employed for the plane wave basis set in VASP calculations, while a double \(\zeta\)-polarized scheme with confinement energies of 100 meV was used for the numerical atomic orbital basis set in SIESTA. Three–center integrals in SIESTA were computed using an hyperfine mesh cut–off of 1200 Ry, equivalent to a real space grid resolution below 0.05 Å\textsuperscript{3}. Biaxial (uniaxial) strain was taken into account by elongating or contracting lattice parameter \(a\) (\(c\)) –see Figure 1– and allowing the internal coordinates of the ions to relax. Biaxial and uniaxial strain (\(\epsilon_a\) and \(\epsilon_c\) respectively) of a particular compound with lattice parameters \(a, c\) are given by:

\[
\begin{align*}
\epsilon_a &= \frac{(a - a_{eq})}{a_{eq}} \\
\epsilon_c &= \frac{(c - c_{eq})}{c_{eq}}
\end{align*}
\]

where \(a_{eq}\) and \(c_{eq}\) are the equilibrium values of the in–plane and out–of–plane lattice parameters respectively.

Fig. 2. Total energy calculations using GGA+vdW in VASP for (a) Bi\textsubscript{2}Te\textsubscript{3}, (b) Sb\textsubscript{2}Te\textsubscript{3}, (c) Bi\textsubscript{2}Se\textsubscript{3} and (d) Sb\textsubscript{2}Se\textsubscript{3}. Each curve shows the energy versus \(c\) for a fixed value of \(a\) (see legend at the right). Symbols marked in black indicate the equilibrium configuration. The exact values of the equilibrium lattice parameters are given in Table I.

III. UNIAXIAL AND BIAXIAL TENSION

A. Bulk Materials

To address the effects of biaxial tension, we first calculated the total energy of the Bi\textsubscript{2}Se\textsubscript{3} family of compounds for different values of the lattice constants using GGA+vdW with the VASP code. In this way, we obtain the relaxed geometry for a fixed value of the in–plane lattice parameter \(a\). Figure 2 shows the total energy of Bi\textsubscript{2}Te\textsubscript{3}, Sb\textsubscript{2}Te\textsubscript{3}, Bi\textsubscript{2}Se\textsubscript{3} and Sb\textsubscript{2}Se\textsubscript{3} for different values of \(a\) as a function of the out–of–plane lattice constant \(c\). The equilibrium lattice parameters \(a_{eq}\) and \(c_{eq}\) were also calculated, and are given in Table I. In Figure 3 we show the band structure of fully relaxed Bi\textsubscript{2}Se\textsubscript{3} for both bulk and thin film geometries as a reference. As shown in Figure 3 for compressive in–plane biaxial strains (\(\epsilon_a < 0\)) lattice parameter \(c\) tends to increase, while for tensile strains (\(\epsilon_a > 0\)) \(c\) decreases with respect to its equilibrium value. In fact, we can estimate the value of the Poisson ratio \(\nu\) from our calculations with the following
in–plane biaxial strains in any tor (TI), with $Z_3$ topological invariant 0 – and a topologically non–trivial phase – topological insulator (TI), with $Z_3$ topological invariant 1 –. The metallic phase is obtained for large in–plane biaxial strains in any direction. This is due to the fact that a high compressive in–plane strain enhances the bandwidth of the $p_x$ and $p_y$ orbitals in the valence band (VB), which eventually crosses the Fermi level and makes the system metallic. For high tensile in–plane biaxial strains, the conduction band (CB) undergoes an analogous process, leading also to a metallic system. For moderate in–plain strains (below ~ 10% in absolute value) the systems remain insulating. In this range, the topological behavior of these systems is governed by the band inversion between the Se and Bi $p_z$ bands, and a topological phase transition (TPT) can be induced by out–of–plane strain. Starting from an inverted phase, for $\epsilon_e < 0$ the bandwidth of the $p_z$ bands is enhanced, which in turn makes the gap bigger at first, until eventually the gap becomes indirect, starts to decrease and at a certain large compressive out–of–plane strain the system becomes metallic again. On the other hand, tensile out–of–plane strain ($\epsilon_e > 0$) tends to diminish the gap until it closes when the energies of the Bi and Se $p_z$ bands at the $\Gamma$ point become equal. Further tensile strain reopens the gap, turning the system into a topologically trivial insulator. Figure 5 shows the behavior of the gap with out–of–plane strain for Bi$_2$Se$_3$ at $a=4.20$ Å. The band gap closing and reopening is evident from the crossing between the Bi and Se $p_z$ bands, which have opposite parity and are responsible for the topological nature of the Bi$_2$Se$_3$ family of compounds.

For $\epsilon_a=0$, the critical uniaxial strain driving the TPT for Sb$_2$Se$_3$, Bi$_2$Se$_3$, Sb$_2$Te$_3$ and Bi$_2$Te$_3$ is 3%, 6%, 6% and 12% respectively. This trend is in turn related to the crystal structure and the strength of the SOC in each system, being largest in Bi$_2$Te$_3$, smallest in Sb$_2$Se$_3$ and intermediate in Bi$_2$Se$_3$ and Sb$_2$Te$_3$. Note that this values are given for zero biaxial in–plane strain, and the TPT will occur at different values of $\epsilon_e$ for $\epsilon_a \neq 0$ (see Figure 4). Other studies have shown similar TPTs for Bi$_2$Se$_3$–like systems under purely uniaxial strain of 6–10%[13][14], which is in good agreement with our results.

Recent studies have revealed the importance of quasiparticle correction[23][24] and temperature effect[25] which lead to a renormalization of the single-particle bands. However, according to those studies the band inversion persists and the value of the $Z_2$ invariant remains unchanged. Therefore, the inclusion of both effects could slightly modify the values of the critical strains, but our results should remain qualitatively correct. In fact, although DFT is known to underestimate band gaps, we find very good agreement between our computed band gaps and experimental data[13][14].

The universal phase diagram for the Bi$_2$Se$_3$ family of 3D TIs under the combined effect of uniaxial and biaxial strain is sketched in Figure 6. To our best knowledge, no other previous work has systematically addressed the effects on the topology of combined uniaxial and biaxial strain. Moreover, as the four systems show a positive Poisson ratio, pure compressive biaxial strain induces an expansion in the $c$ direction which could, in principle, drive the system into the normal insulating phase. Nevertheless, if no additional uniaxial strain is applied, we find that the four systems undergo a TI to metallic phase transition with both tensile and compressive biaxial...

### Table I. Calculated values of the equilibrium lattice parameters of the Bi$_2$Se$_3$ family of compounds.

| Compound   | $a_{eq}$ (Å) | $c_{eq}$ (Å) |
|------------|---------------|---------------|
| Bi$_2$Te$_3$ | 4.40 (4.383)  | 30.5 (30.487) |
| Sb$_2$Te$_3$ | 4.25 (4.25)   | 30.9 (30.35)  |
| Bi$_2$Se$_3$ | 4.17 (4.138)  | 28.4 (28.64)  |
| Sb$_2$Se$_3$ | 4.04 (-)      | 28.7 (-)      |

TABLE I. Calculated values of the equilibrium lattice parameters of the Bi$_2$Se$_3$ family of compounds. Relaxations were carried out with VASP in the GGA+vdW approximation. Values in parentheses correspond to experimental data from Ref. [25]. No experimental data was available for Sb$_2$Se$_3$ in the rhombohedral phase.
FIG. 4. (a) Band gap (in color code shown on the right) for Bi$_2$Te$_3$ for different values of lattice constants $a$ and $c$. The ionic configurations were allowed to relax for every single calculation. Negative gaps (purple) indicate that the energy of Bi $p_z$ orbital is lower than the Se $p_z$ orbital, i.e., the system is topologically non–trivial. (b), (c) and (d) show equivalent diagrams for Sb$_2$Te$_3$, Bi$_2$Se$_3$ and Sb$_2$Se$_3$ respectively. These phase diagrams show the regions in phase space where the system is a normal insulator (orange), a TI (purple) or a metal (gray). The equilibrium position is marked with a black square and the thicker line corresponds to the relaxed $c$ lattice parameter for a fixed value of $a$ for each system.

Our results predict unstrained Sb$_2$Se$_3$ to be a topologically non–trivial insulator in the $R3m$ phase. Nevertheless, the region of parameter space in which Sb$_2$Se$_3$ is a TI is small and therefore minor variations of the lattice parameters result in a trivial insulator. Previous calculations have reported this material to be a normal insulator under no strain. Comparing with Refs. 5 and 32, we obtain slightly smaller lattice constants ($a=4.04$ Å, $c=28.7$ Å) versus 4.076 Å, 29.83 Å for Ref. 5, and similar values for Ref. 32, probably due to the inclusion of vdW corrections in our calculations. With their lattice constants our calculations also predict Sb$_2$Se$_3$ to be a narrow gap NI –see Figure 4 (d)–. In Ref. 13 they obtain lattice parameters closer to ours ($a=4.026$ Å, $c=28.732$ Å) within the GGA+vdW approximation, but decide to set the equilibrium (unstrained) configuration at the plain GGA relaxed parameters (without the vdW correction, $a=4.078$ Å, $c=29.92$ Å), yielding again a NI phase. Recent calculations by other group$^{13}$ estimate smaller values of lattice parameters for rhombohedral Sb$_2$Se$_3$ ($a=4.004$ Å, $c=28.553$ Å) and seem to predict an inverted band structure for antimony selenide –see the curvature of the bands around the $\Gamma$ point in Figure 2 (d) of Ref. 33, but do not elaborate on its topological nature. Unfortunately, experimental data for Sb$_2$Se$_3$ is only available for its more stable orthorhombic phase ($Pnma$)$^{34}$. We recently became aware of another work$^{35}$ in which DFT+vdW calculations predict rhombohedral Sb$_2$Se$_3$ to be topologically non–trivial.

The Sb$_2$Se$_3$ compound

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B. Thin Films

Now we investigate the effect of pure biaxial in–plane strain along with low dimensional effects on thin films of Bi$_2$Se$_3$–like systems. Our starting points are bulk calculations in which, for a fixed amount of biaxial strain, the lattice parameter $c$ was allowed to fully relax along with the atomic coordinates. These bulks correspond to the equilibrium systems for each value of the in–plane strain.
FIG. 5. Projected density of states (PDOS) in the $\Gamma$ point around the energy gap for bulk Bi$_2$Se$_3$ with lattice parameter $a$ fixed to 4.20 Å and different values of $c$ (left axis). The equilibrium configuration is marked with a thicker frame. Black and red lines show the contribution of Bi $p_z$ and Se $p_z$ orbitals respectively. The magenta and blue lines indicate the Bi and Se $s$ contributions, while the gray and green lines depict the Bi and Se $p_x + p_y$ weight. At $c \sim 30$ Å the bulk band gap closes and the system undergoes a topological phase transition, so that for $c > (\approx) 30$ Å the bands are uninverted (inverted) and the system is topologically trivial (non–trivial). The different behavior of the Se and Bi $p_z$ bands with uniaxial strain is apparent in the figure.

The behavior with both compressive and tensile biaxial strain of Bi$_2$Se$_3$ thin films is in clear analogy with the bulk behavior. Nevertheless, they show distinct features induced by strain. Under compressive biaxial strain the size of the Bi$_2$Se$_3$ bulk gap acquires a smaller value than that of the unstrained system, and therefore the penetration depth of the surface states is enlarged and a larger number of layers is needed to close the hybridization gap. Moreover, the "M"–shaped feature in the VB around the $\bar{\Gamma}$ point is smoothed out and consequently the linear dispersion of the TSS is extended to a larger energy region in the VB. On the other hand, applying tensile biaxial strain also tends to close the bulk gap, but the "M"–shaped feature becomes more pronounced and hence the DP in the films is shifted inside the VB (see the 6 QL series in Figure 7). A sharp enough "M"–shaped VB detaches the DP from the Fermi level and consequently induces an $n$–type doping of the surface states. This result explains the shift in the DP observed in Ref. [14], as well as the different behavior, gap opening or $n$–doping, observed at the grain boundaries in Bi$_2$Se$_3$ films, in regions under compressive or tensile strain, respectively.

Moreover, a small decrease in the Fermi velocity with tensile strain is also apparent. The penetration depth of the TSS also varies with strain, and the closer in the phase diagram to the critical Metal–TI lines the more QLs are needed to close the hybridization gap (see for instance the 2 QL series in Figure 7, in which compressive or tensile biaxial strain takes the system closer to a critical line in the phase diagram, and the TSS are gapped but for $a = 4.20 \approx a_{eq}$), in agreement with the results displayed in Ref. [8]. Higher compressive biaxial strain drives the thin films into a metallic state due to the upward shift in energy of the valence band maximum (see for example Figure 16 in the appendix), while for a critical tensile biaxial strain the bulk–like CB crosses the Fermi level and the thin films become metallic again (see Figure 18).

Strain can therefore turn the Bi$_2$Se$_3$ family of compounds insulating or metallic, and allows for engineering of the gap, the orbital character of the bands, the Fermi velocity, DP energy and thus also the doping of the TSSs. The table–like figures for the four systems are displayed so that they can be used for determining what kind of band dispersion is expected when a bismuth dichalcogenide of a certain thickness is grown on a substrate with a particular lattice parameter.
FIG. 7. Band dispersion diagrams close to the $\bar{\Gamma}$ point along the $\bar{M}$-$\bar{\Gamma}$-$\bar{K}$ directions for Bi$_2$Se$_3$ slabs under biaxial strain. Each column corresponds to a fixed value of the in–plane lattice parameter labeled on top and the corresponding out–of–plane $c$ parameter. The calculated equilibrium in–plane lattice parameter of unstrained Bi$_2$Se$_3$ bulk is 4.17 Å. The five rows correspond to different slab thicknesses: 1, 2, 3, 4 and 6 QLs from top to bottom. The horizontal dashed lines indicate the Fermi level, whereas the vertical dashed lines show the $\bar{\Gamma}$ point.

IV. STRAINED HETEROJUNCTIONS

When two distinct TIs are faced to one another, an interesting problem arises. If both materials belong to the same Z$_2$ topological class, no interface state is guaranteed by the bulk–to–boundary correspondence, as the change in topological invariant is zero. Therefore, a topological surface state can be annihilated by placing another TI on top, even if both bulk gaps align in a straddling gap configuration. Still, topologically trivial interface states may arise regardless of the topological invariants. Moreover, in broken gap heterojunctions (without a common gap) no topologically protected interface state may appear since the system will no longer be an insulator. In this section we will study interfaces of Bi$_2$Te$_3$ and Sb$_2$Te$_3$ both in superlattices and in slab geometry. Among the four members of the Bi$_2$Se$_3$ family of compounds, we have chosen these two so that the difference in electronegativity, $\chi$, between the A and B elements in the A$_2$B$_3$ compounds is as small as possible, in order to obtain a straddling gap at the heterojunction and minimize the band bending along the system. Table II shows the Pauling and Allen electronegativities ($\chi_P$ and $\chi_A$) for Bi, Sb, Te and Se. The first two elements have an almost equal value of the electronegativity—in fact $\chi_P$(Bi) < $\chi_P$(Sb) while $\chi_A$(Bi) > $\chi_A$(Sb). On the other hand, Se and Te show a bigger difference in their $\chi$ values. Opposite doping for Se- and Te-based materials is expected, and we have additionally calculated Bi$_2$Se$_3$/Bi$_2$Te$_3$ heterojunctions which exhibit a broken gap alignment, thus leading to a metallic phase where the Z$_2$ invariant is ill-defined and no topological interface states can exist.

A. TI/TI interfaces

We have chosen Sb$_2$Te$_3$/Bi$_2$Te$_3$/Sb$_2$Te$_3$ trilayers with equal number of QLs of Sb$_2$Te$_3$ at both sides so that inversion symmetry is preserved, making the analysis sim-
FIG. 8. Geometry of the $m$-Sb$_2$Te$_3$/n-Bi$_2$Te$_3$/m-Sb$_2$Te$_3$ trilayer with $m=3$ and $n=6$. The in-plane lattice parameter $a$ is fixed to that of Sb$_2$Te$_3$ under no strain. Interfaces are shown as dashed lines as a guide to the eye. The whole system follows the AbCaB stacking pattern analogous to an fcc (111) crystal, which ensures inversion symmetry is preserved. Superlattices are constructed by imposing periodic boundary conditions on this and similar trilayers, which will also preserve inversion symmetry.

pler, as both interfaces will be equivalent. We calculated $m$-Sb$_2$Te$_3$/n-Bi$_2$Te$_3$/m-Sb$_2$Te$_3$ trilayers, where $m$ and $n$ are the number of QLs of Sb$_2$Te$_3$ and Bi$_2$Te$_3$ respectively. In the superlattice geometry, due to periodic boundary conditions, the trilayer turns into a $2m$-Sb$_2$Te$_3$/n-Bi$_2$Te$_3$/m-Sb$_2$Te$_3$ structure repeated in the [111] direction. We still call it a $m$-Sb$_2$Te$_3$/n-Bi$_2$Te$_3$/m-Sb$_2$Te$_3$ superlattice to emphasize the centrosymmetric nature of the system. We fixed $n=6$, for which the surface–surface interaction in Bi$_2$Te$_3$ is negligible and a gapless Dirac cone (DC) develops at the surface—see Fig. 8(a)—, while the number of Sb$_2$Te$_3$ QLs at both sides is varied from $m=1$ to 3. The AbCaB stacking sequence of the pristine subsystems is preserved along the interfaces and in the superlattices in order to preserve inversion symmetry. The $C_3$ rotation axis and the three vertical mirror planes of the pristine systems are also preserved in the heterojunction. We fix the in-plane lattice vector $a$ to that of Sb$_2$Te$_3$ in equilibrium, $a_{eq}=4.25$ Å, and the $c$ lattice parameter for each subsystem is set to its relaxed value for a fixed to the aforementioned value, that is 30.9 Å for Sb$_2$Te$_3$ and 32.0 Å for Bi$_2$Te$_3$ (see Fig. 2). The ionic coordinates within each subsystem are fixed to their relaxed bulk values, and the vdW gap between Sb$_2$Te$_3$ and Bi$_2$Te$_3$ is taken as the average vdW gap between both subsystems. This setup could correspond to a 6 QL thick Bi$_2$Te$_3$ slab grown on a $m$–QL Sb$_2$Te$_3$ substrate, and another $m$–QL Sb$_2$Te$_3$ thick film grown on top of it. Figure 8 depicts the geometry for the $m=3$ case. According to the phase diagram calculated in Fig. 4 both the Sb$_2$Te$_3$ and Bi$_2$Te$_3$ subsystems show an inverted gap in the bulk. This means that the existence of an interface state is not guaranteed, since the change in the $Z_2$ invariant across the interface is zero as both materials are topological insulators.

We start by analyzing the electronic structure of the isolated subsystems, depicted in Figure 9. Bi$_2$Te$_3$ under small biaxial strain remains a TI, and so it develops surface states when truncated in the [111] direction. For a 6 QL slab (as shown in the figure), surface–surface interaction is already negligible and the linearly dispersive DCs at the $\Gamma$ point emerge. In contrast with Bi$_2$Se$_3$ or Sb$_2$Te$_3$, the DP of the Bi$_2$Te$_3$ surfaces is not at the Fermi level and lies below the VB maximum. This is in agreement with previous results, and can be attributed to the larger curvature of the VB along the $\Gamma$–$M$ direction. Sb$_2$Te$_3$ in this system presents neither uniaxial nor biaxial strain, and it is therefore also in the topologically non–trivial phase. In Figure 9 the electronic structure of unstrained 1, 2, 3, 4 and 6 QL thick Sb$_2$Te$_3$ films is also shown—panels (b) to (f)–. Antimony telluride presents a topological surface state being the DP at the Fermi level for 6 QLs. The penetration depth is $\sim 2$ QLs, so that a gap opens in thin films of less than 5 QLs due to surface–surface hybridization.

The bulk structures of the periodic superlattices are shown in Figure 10 (a) to (c) for $m=1$, 2 and 3, and those corresponding to the trilayer slabs in Figure 10 (d) to (f). The former –(a), (b) and (c)– present a band gap of $\sim 0.1$ eV, being the VB (CB) offset of $\sim 0.1$ (0.05) eV between both subsystems, with the VB (CB) of Sb$_2$Te$_3$ lying at a higher energy. The small band staggering at the heterojunction can be attributed to the small deviation in the values of the electronegativity for Bi and Sb. Figs. 11 (a), (b) and (c) represent the atomic orbital decomposed partial density of states (PDOS) at $\Gamma$ in the energy region displayed in Fig. 10. They evidence the band inversion in both Sb$_2$Te$_3$ and Bi$_2$Te$_3$ slabs and the similar band alignment for the three superlattices, $m=1$, 2 and 3. The top of the VB is dominated by Sb and Bi $p_z$ orbitals with positive parity, being the former at higher energy, while the Te $p_z$ orbitals with negative parity are located at the bottom of the CB region. The interaction between the CB Te orbitals of both compounds is weak, particularly for the wider superlattices. Hence, in the superlattice both subsystems present an inverted band structure.

The bulk–to–boundary correspondence predicts no topologically protected interface state at the junction, and although trivial interface states could develop, our results show that this is not the case. We therefore conclude that this Sb$_2$Te$_3$/Bi$_2$Te$_3$ heterojunction is insulating with no interface states whatsoever, but will develop surface states when truncated. This is proved in the thin film geometry—Figure 10 (d), (e) and (f)–, where surface states that span the whole bulk band gap appear at both ends. The DP of these TSSs is pinned at the Fermi level irrespective of the thickness of the Sb$_2$Te$_3$ layers. In fact, even for the $m=1$ and 2 for which the thickness of the Sb$_2$Te$_3$ subsystem is below the penetration depth of the surface states—see Figure 9 (b) and (c)–, there is no energy gap and the spectrum of the trilayer slab still exhibits a semimetallic character. The corresponding atomic orbital PDOS are shown in Fig. 11 (d) to (f). The three trilayers exhibit a sharp peak at $\Gamma$, associated with the TSSs. They have a predominant contribution of the Sb$_2$Te$_3$ orbitals, mostly of Sb $p_z$.

This orbital contribution is consistent with the TSS
FIG. 9. Band structure of the different isolated subsystems involved in the TI/TI/TI trilayers –top row, (a) to (f)– and in the NI/TI/NI trilayers –bottom row and (a)–. (a) corresponds to a 6 QL Bi$_2$Te$_3$ thin film under biaxial compressive strain so that its in–plane lattice parameter matches that of equilibrium Sb$_2$Te$_3$ (4.25 Å). (b) to (f) show the band dispersion for unstrained Sb$_2$Te$_3$ slabs of 1, 2, 3, 4 and 6 QLs respectively, which show a TSS according to their topologically non–trivial nature, although for thicknesses below ∼ 5 QL a gap opens in the TSSs due to surface–surface interaction. (g) to (k) show the electronic structure of uniaxially elongated Sb$_2$Te$_3$ slabs of 1, 2, 3, 4 and 6 QLs respectively. In these cases the system is clearly in the normal insulating regime, since no TSS appears for thicknesses as large as 6 QL.

FIG. 10. Band structure of the TI/TI/TI heterojunctions considered, both in superlattice –(a) to (c)– and slab –(d) to (f)– geometries. (a), (b) and (c) show the band dispersion for the trilayers in a superlattice with $n = 6$ and $m = 1, 2, 3$ respectively. As all the constituents of the superlattice are topologically non–trivial, there are no interfaces between subsystems with different value of the $Z_2$ topological invariant, and no interface state exists. (d), (e) and (f) correspond to slab geometries with $n = 6$ and $m = 1, 2, 3$ respectively. In these three cases a surface state develops irrespective of the number of Sb$_2$Te$_3$ layers, but no interface state is present.

FIG. 11. (a) to (f) show the PDOS in $\bar{\Gamma}$ close to the Fermi level of the studied TI/TI heterojunctions. Blue and black lines show the contribution of Bi $p_z$ and Sb $p_z$ orbitals respectively. The green and red lines indicate the Te $p_z$ contributions from the Te atoms in the Bi$_2$Te$_3$ and Sb$_2$Te$_3$ subsystems respectively. (a) to (c) –(d) to (f)– depict the PDOS for superlattices –slabs– with $m = 3$ to 1. Both subsystems show an inverted band structure in all cases. The 2D averaged Hartree potential profile for the $m = 3$ TI/TI slab is shown in (g), along with the average Hartree potential in each QL (horizontal straight solid lines).

Localization shown in Figure [12] (a), for the three different slabs. The surface state is strongly confined in the Sb$_2$Te$_3$ subsystem, with a penetration depth of ≈ 2 QLs, although for the $m = 1$ case the state strongly localizes at the surface-most QL. Fig. [11] (g) displays the 2D averaged Hartree potential profiles –including the ionic contribution– along the [0001] direction for the $m = 3$ slab. It reflects the chemical difference between both Sb$_2$Te$_3$ and Bi$_2$Te$_3$ compounds and the potentials are almost identical for the finite trilayers and the superlattice (not shown), differing only on the potential step at the surface of the slab. Therefore, our results corroborate the fact that unstrained Sb$_2$Te$_3$ is a TI even for ultrathin films,
and support the idea that the TI/TI \( \text{Sb}_2\text{Te}_3\)-\( \text{Bi}_2\text{Te}_3 \) heterojunction behaves as a homogeneous TI and does not confine neither topological nor trivial states at the interface.

### B. NI/TI interfaces

Now we will discuss the effect of applying uniaxial tensile strain to \( \text{Sb}_2\text{Te}_3 \) in the system presented in the previous subsection. The systems considered are again \( m\)-\( \text{Sb}_2\text{Te}_3/n\)-\( \text{Bi}_2\text{Te}_3/m\)-\( \text{Sb}_2\text{Te}_3 \) trilayers in either a slab geometry (thin film) or a superlattice. The in–plane lattice parameter is again fixed to \( a=4.25 \) Å and \( c \) is set to 32.0 Å for \( \text{Bi}_2\text{Te}_3 \), but now the \( \text{Sb}_2\text{Te}_3 \) subsystem is expanded to \( c=34.0 \) Å, corresponding to an uniaxial tensile strain of \(-10\%\). According to the phase diagram shown in Figure 9 (a) and (g) to (k), \( \text{Sb}_2\text{Te}_3 \) will now be in a normal insulating phase, so that at the interface of \( \text{Sb}_2\text{Te}_3 \) and \( \text{Bi}_2\text{Te}_3 \) the topological \( Z_2 \) invariant will increase from 0 to 1. The TPT on \( \text{Sb}_2\text{Te}_3 \) can be induced by external uniaxial tensile strain or via the chemical intercalation of zerovalent non–magnetic metals in the vdW gap,\(^\text{53}\) as stated in a previous section.

The electronic structure of the different isolated constituents is shown in Figure 9 (a) and (g) to (k). \( \text{Sb}_2\text{Te}_3 \) under such out–of–plane strain shows no band inversion in the bulk, and this is reflected in the thin film electronic structure. In contrast with the previously analyzed systems, \( \text{Sb}_2\text{Te}_3 \) now shows no surface state since it is in the NI phase. The gap is of 0.4 eV for the 1 QL slab –Figure 9 (g)– and decreases down to 0.2 eV for the 6 QL thin film –Figure 9 (k)–. On the other hand, the 6 QL \( \text{Bi}_2\text{Te}_3 \) slab under purely biaxial strain is a TI which develops TSSs with no gap, and its DP lies below the Fermi level –Figure 9 (a)–. When the two subsystems are brought together, the bulk–to–boundary correspondence dictates that topologically protected interface states must develop in the gap. The band structures of the junctions are shown in Figure 13–(a) to (f).

For periodic boundary conditions –panels (a) to (c) of Figure 13–, and in contrast to the TI/TI superlattices analyzed in subsection IV A, a topological interface state (TIS) develops that spans the bulk band gap. Unexpectedly, the interface topological state localizes in the normal insulator \( \text{Sb}_2\text{Te}_3 \) (see Figure 14), as opposed to TSSs, which always localize in the topological insulator. In this heterojunction a hybridization gap opens in the spectrum for thicknesses of the 2\( m\)-\( \text{Sb}_2\text{Te}_3 \) layer below \( m=2 \) QLs –Figure 13 (b)– since the two opposed interfaces are closer than twice the penetration depth of the TISs. The TISs show no doping in contrast with the TSS of 6 QL \( \text{Bi}_2\text{Te}_3 \) –see Figure 13 (f)–, opening a new way of tuning the DP energy of the topological states.

To understand the fundamental difference between the TI/TI and NI/TI heterojunctions, we analyze the atomic orbital PDOS at \( \bar{\Gamma} \) in Figs. 11 and 15. While the Bi\( _2 \text{Te}_3 \) shows band inversion in both cases, the \( \text{Sb}_2\text{Te}_3 \) subsystem exhibits opposite traits in the two different sets of heterojunctions. In the TI/TI systems, as discussed previously, there is band inversion, while in the NI/TI there is not. In the NI/TI case the Te \( p_z \) orbital of the \( \text{Bi}_2\text{Te}_3 \) with negative parity occupies the top of the VB region, while the Bi \( p_z \) orbital with positive parity is located at the CB just above the Te derived bands of Bi\( _2 \text{Te}_3 \). Therefore, the \( \text{Sb}_2\text{Te}_3 \) remains in the trivial state. Nevertheless, the topological interface states are mainly formed from the orbitals closest to the energy gap, namely from the Te orbitals of \( \text{Sb}_2\text{Te}_3 \). This feature explains why the TISs are located predominantly in the non-topological slab. Furthermore, due to their spatial localization, there is a strong interaction between the TISs at both interfaces for \( m=1 \) and 2, and a gap opens up.

For the trilayer slab configurations shown in panels (d) to (f) of Figure 13, the system shows a common bulk gap of \( \sim 0.15 \) eV and a gapless interface state with the DP at the Fermi level. This topological interface state is also undoped and develops irrespective of the thickness of the non-topological \( \text{Sb}_2\text{Te}_3 \) layers, and analogously to the emergent TISs in the SLs, it is not strictly localized at the interface. Instead, the state at the gap is confined in the \( \text{Sb}_2\text{Te}_3 \) subsystem, with more weight at the interfacemost QL of \( \text{Sb}_2\text{Te}_3 \), but exceeding the expected \( \sim 2 \) QL penetration depth of the TSSs in an isolated \( \text{Bi}_2\text{Te}_3 \) slab –see Figure 12 (b)–. Moreover, the orbital distribution in the VB and CB, and hence that of the TIS, is similar in the NI/TI superlattices and trilayers (see Fig. 15). The main difference between the superlattice and the trilayer TISs lies in the lack of interaction in the trilayer geometry due to the localization in the \( \text{Sb}_2\text{Te}_3 \) subsystem. Thus, all the trilayers remain semimetallic. On the other hand, only minor differences between the averaged Hartree potential of NI/TI and TI/TI heterostructures of equivalent TI/TI geometry –see Fig. 11 (g) and Fig. 15– are observed.

Our findings are in agreement with previous results,\(^\text{35,41}\) in which similar TISs with large penetration depths appear in NI/TI junctions localized in the NI. We additionally checked that in NI/TI/NI heterojunctions of \( m\)-\( \text{Sb}_2\text{Te}_3/n\)-\( \text{Bi}_2\text{Te}_3/m\)-\( \text{Sb}_2\text{Te}_3 \) with \( n \) as low as 1 QL, the TISs are always gapless in slab configuration, and remain gapless in superlattice geometries as long as \( m \geq 2 \). Note that Bi\( _2 \text{Te}_3 \) here is the TI, and 1 QL Bi\( _2 \text{Te}_3 \) thin films show a relatively large Dirac gap due to surface–surface hybridization. Therefore, capping Bi\( _2 \text{Te}_3 \) with uniaxially strained \( \text{Sb}_2\text{Te}_3 \) leads to a closing of the Dirac gap in the topological states, since the latter localizes in the normal insulating \( \text{Sb}_2\text{Te}_3 \). In addition, although the development of TISs in NI/TI junctions is dictated by topology, their spatial location is determined by the orbitals dominating the edges of the valence and conduction band of the heterostructures, and thus by the relative alignment of the bands of both subsystems.
V. SUMMARY AND CONCLUSIONS

We have shown the combined effects of uniaxial and biaxial strain on Bi$_2$Te$_3$, Sb$_2$Te$_3$, Bi$_2$Se$_3$, and Sb$_2$Se$_3$, both in bulk and slab geometries. A phase diagram for the four systems was computed and analyzed, demonstrating that topological phase transitions, either to a metal or to a trivial insulator, can occur for different combinations of both kinds of strains, and a universal behavior was found for the four compounds. We showed how strain can engineer the DP energy, the Fermi velocity, the metallic character and the topology of the four compounds, thus offering a wide tunability regarding strainedtronics. We have also calculated the electronic structure of Sb$_2$Te$_3$/Bi$_2$Te$_3$/Sb$_2$Te$_3$ trilayers, in which Sb$_2$Te$_3$ was driven into the topologically trivial insulating regime by applying uniaxial strain. For the TI/TI systems no trivial nor topological interface state is found, and the superlattice shows a straddling gap of $\sim 0.1$ eV. In the NI/TI heterojunctions, topologically protected interface states are predicted and characterized. Since the TIS spatial location is determined by the relative band alignment of the two compounds forming the heterostructures, we find TISs to localize in the NI both in slab configurations and periodic superlattices, thus opening a route to closing hybridization gaps in topological states of ultrathin films of the Bi$_2$Se$_3$ family by capping the system with NI layers. Our results for the NI/TI heterojunctions also indicate a way to avoid interactions of the topological states with undesired ambient impurities while preserving the bulk band gap of the system, and thus maintaining the topological protection of the states. Uniaxial strain on the Sb$_2$Te$_3$ subsystem can additionally turn the interface conducting channel on or off, thus the system hosts a switchable topological interface state irrespective of the thickness of the TI layer.

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Appendix: Band dispersion tables for Bi$_2$Te$_3$, Sb$_2$Te$_3$ and Sb$_2$Se$_3$
FIG. 12. Layer projected density of states (LDOS) of the topological states in \( m\)-Sb\(_2\)Te\(_3\)/n-Bi\(_2\)Te\(_3\)/\( m\)-Sb\(_2\)Te\(_3\) trilayer slabs for \( m=1 \) (red line at the bottom), \( m=2 \) (magenta line in the middle) and \( m=3 \) (blue line at the top). The LDOS was computed at \( k=(5, 0) \cdot 10^{-3} \text{Å}^{-1} \), along the \( \Gamma-\bar{K} \) direction and close to the \( \bar{\Gamma} \) point for the electron–like TSSs. The trilayer is centered at the middle of the 6 QL \( \text{Bi}_2\text{Te}_3 \) layer. Vertical dashed lines depict the boundaries of each QL. The gray shaded region corresponds to the \( \text{Sb}_2\text{Te}_3 \) subsystem, while white regions belong to the \( \text{Bi}_2\text{Te}_3 \) subsystem and the vacuum is shaded with a cyan pattern. (a) shows the TI/TI/TI trilayer for which TSSs localize at the surfacemost QL of the \( \text{Sb}_2\text{Te}_3 \) which is in the topological insulating phase. In (b) the LDOS of the NI/TI/NI trilayer is shown. In this case TISs localize at both interfacial QLs, one in the \( \text{Bi}_2\text{Te}_3 \) subsystem and the other in the \( \text{Sb}_2\text{Te}_3 \) subsystem, being the latter in the NI phase. The extension of the TISs spans the whole trivial \( \text{Sb}_2\text{Te}_3 \) subsystem. All the topological states shown are degenerate due to inversion symmetry, and only one of the two-fold degenerate states is shown in each case (being always the other state localized at the opposite surface or interface).
FIG. 13. Band structure of the NI/Tl/NI heterojunctions considered, both in superlattice –(a) to (c)– and slab –(d) to (f)– geometries. (a), (b) and (c) show the band dispersion for the superlattices with \( n=6 \) and \( m=1, 2, \) and 3 respectively. As the Sb\(_2\)Te\(_3\) subsystem has been driven to the normal insulating phase by applying uniaxial tensile tension, topologically protected states localized at the interface appear, according to the bulk-to-boundary correspondence. A gap in the spectrum opens for \( m \) below \( \sim 2 \) due to interface–interface interaction (note that the total thickness of the Sb\(_2\)Te\(_3\) subsystem is \( 2m \) QLs in the superlattices). (d), (e) and (f) correspond to slab geometries with \( n=6 \) and \( m=1, 2, \) and 3 respectively. In these three cases a topological interface state (TIS) develops irrespective of the number of Sb\(_2\)Te\(_3\) layers.
FIG. 14. LDOS of the TISs in $m$-$\text{Sb}_2\text{Te}_3$/$n$-$\text{Bi}_2\text{Te}_3$/$m$-$\text{Sb}_2\text{Te}_3$ superlattices for $m=1$ (red line at the bottom), $m=2$ (magenta line in the middle) and $m=3$ (blue line at the top) –note that the total thickness of the $\text{Sb}_2\text{Te}_3$ subsystem is $2m$ QLs–. The LDOS was computed at $k=(5, 0) \cdot 10^{-3}\text{Å}^{-1}$, along the $\Gamma$–$K$ direction and close to the $\Gamma$ point for the electron–like TISs. The system is centered at the middle of the 6 QL $\text{Bi}_2\text{Te}_3$ layer. Vertical dashed lines depict the boundaries of each QL. The gray shaded region corresponds to the $\text{Sb}_2\text{Te}_3$ subsystem, while white regions belong to the $\text{Bi}_2\text{Te}_3$ subsystem. TISs of N1/TI superlattices exhibit strong hybridization with the opposite interface for thicknesses of the $2m$–$\text{Sb}_2\text{Te}_3$ layer below $m=2$ QLs, while for the $m=3$ QLs the TISs are already decoupled. All three TISs shown are degenerate due to inversion symmetry, and only one of the two–fold degenerate states is shown in each case.

FIG. 15. (a) to (f) show the PDOS in $\Gamma$ close to the Fermi level of the studied N1/TI heterojunctions. Blue and black lines show the contribution of Bi $p_z$ and Sb $p_z$ orbitals respectively. The green and red lines indicate the Te $p_z$ contributions from the Te atoms in the $\text{Bi}_2\text{Te}_3$ and $\text{Sb}_2\text{Te}_3$ subsystems respectively. (a) to (c) –(d) to (f)– depict the PDOS for superlattices –slabs– with $m=3$ to 1. The $\text{Bi}_2\text{Te}_3$ subsystem shows band inversion, while the $\text{Sb}_2\text{Te}_3$ subsystem is uninvited. The 2D averaged Hartree potential profile for the $m=3$ N1/TI slab is shown in (g), along with the average Hartree potential in each QL (horizontal straight solid lines).
**FIG. 16.** Same as Figure 7 for Bi$_2$Te$_3$.

**FIG. 17.** Same as Figure 7 for Sb$_2$Te$_3$.
FIG. 18. Same as Figure 7 for Sb$_2$Se$_3$. 

\[ a (\text{Å}) = 4.00 \ 4.10 \ 4.20 \ 4.30 \ 4.40 \]

\[ \# \text{QLS} \]

\[ \bar{M} \leftarrow \Gamma \rightarrow \bar{K} \]

E-E$_F$ (eV)