Band Structure Engineering in Topological Insulator Based Heterostructures

T. V. Menshchikova, M. M. Otrokov, S. S. Tsirkin, D. A. Samorokov, V. V. Bebneva, A. Ernst, V. M. Kuznetsov, and E. V. Chulkov

ABSTRACT: The ability to engineer an electronic band structure of topological insulators would allow the production of topological materials with tailor-made properties. Using ab initio calculations, we show a promising way to control the conducting surface state in topological insulator based heterostructures representing an insulator ultrathin films on the topological insulator substrates. Because of a specific relation between work functions and band gaps of the topological insulator substrate and the insulator ultrathin film overlayer, a sizable shift of the Dirac point occurs resulting in a significant increase in the number of the topological surface state charge carriers as compared to that of the substrate itself. Such an effect can also be realized by applying the external electric field that allows a gradual tuning of the topological surface state. A simultaneous use of both approaches makes it possible to obtain a topological insulator based heterostructure with a highly tunable topological surface state.

KEYWORDS: Topological insulators, electronic structure, heterostructures, electric field

Topological insulators (TIs) are novel materials, demonstrating a fundamental interplay between electronic structure and topology, as well as providing a platform for potentially promising applications in spintronics. Up to date, the unique fingerprint of this class of materials, that is, spin-polarized gapless surface state with linear dispersion, has been experimentally confirmed for a number of compounds containing heavy elements like Bi, Te, Pb, and Sb. These include random alloys, binary, and ternary layered compounds, as well as the thallium-based compounds.

In the present study, we propose a new way to design the IUF/TI heterostructures, consisting of a single tetradymite-type quintuple (QL) or septuple (SL) layer blocks on top of the TI substrates. Constructed in such a way, the heterostructures are guaranteed against appearance of the trivial Shockley-type surface states due to the chemical inertness of the IUF overlayer. Using ab initio simulations, we show that depending on the relation between work functions of TI and IUF a sizable upward or downward shift of the DP occurs, allowing for the rough control of the DP position. More importantly, the deposition of the IUF on top of the TI surface can lead to a substantial increase in the number of the topological surface state (TSS) charge carriers as compared to that of the TI substrate. Moreover, we show that essentially the same effect can be achieved by applying an external electric field, which enables a gradual tuning of the TSS. A simultaneous use of both approaches makes it possible to obtain a TI-based heterostructure with a highly tunable TSS.

The compounds used as constituents of the IUF/TI heterostructures are reported in Table 1. All of them possess...
Nano Letters

Table 1. The Structural and Energetic Characteristics of the IUF/TI Pairs Given in the $X_i/X_f$ Format (except for the Lattice Mismatch, $\Delta$) with $X_i$ Being Either Experimental Lattice Parameter, $a_0$ or Calculated Work Function, $\Phi_1$, with the Indication of the Films Thicknesses, or Calculated Band Gap, $E_i$ ($i = 1, 2$) 

<table>
<thead>
<tr>
<th>IUF/TI</th>
<th>$a_0(\AA)/a_0(\AA)$</th>
<th>$\Delta$ (%)</th>
<th>$\Phi_1(eV)/\Phi_2(eV)$</th>
<th>$E_1(eV)/E_2(eV)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Sb$_2$Se$<em>2$Te]$</em>{1QL}$/[Bi$_2$Se$<em>3$]$</em>{6QL}$</td>
<td>4.105/4.114</td>
<td>−0.22</td>
<td>5.46 (1QL) / 5.42 (6QL)</td>
<td>0.66/0.30</td>
</tr>
<tr>
<td>[Sb$<em>2$Se$<em>2$Te]$</em>{1QL}$/[PbBi$<em>x$Te$</em>{1-x}$S]$</em>{6SL}$</td>
<td>4.250/4.230</td>
<td>+0.47</td>
<td>4.80 (1QL) / 4.98 (6SL)</td>
<td>0.48/0.34</td>
</tr>
<tr>
<td>[PbBi$<em>x$Te$</em>{1-x}$S]$_{1SL}$/[Sb$_2$Te$<em>3$]$</em>{6QL}$</td>
<td>4.230/4.250</td>
<td>−0.47</td>
<td>5.24 (1SL) / 4.49 (6QL)</td>
<td>0.35/0.09</td>
</tr>
<tr>
<td>[SnSb$_2$Te$<em>2$]$</em>{1SL}$/[Bi$_2$Te$<em>2$S]$</em>{6QL}$</td>
<td>4.294/4.316</td>
<td>−0.51</td>
<td>4.79 (1SL) / 5.15 (6QL)</td>
<td>0.39/0.27</td>
</tr>
<tr>
<td>[Bi$_2$Te$<em>2$S]$</em>{4QL}$/[SnSb$_2$Te$<em>2$]$</em>{6QL}$</td>
<td>4.316/4.294</td>
<td>+0.51</td>
<td>5.36 (1QL) / 4.45 (6QL)</td>
<td>0.30/0.11</td>
</tr>
<tr>
<td>[BiSb$_2$Te$<em>3$]$</em>{5SL}$/[Sb$_2$Te$<em>3$]$</em>{6QL}$</td>
<td>4.197/4.170</td>
<td>+0.63</td>
<td>4.99 (1QL) / 4.58 (6QL)</td>
<td>0.39/0.29</td>
</tr>
</tbody>
</table>

*Note that band gap values, $E_i$, are given for slab and bulk in the IUF ($i = 1$) and TI ($i = 2$) case, respectively.

A tetradymite-type structures in which QL or SL blocks are separated by the van der Waals gaps.21–27 Note that unlike the rest of the compounds listed in Table 1, Sb$_2$Se$_2$Te is topologically trivial (see Supporting Information S1). Because most of the IUFs under consideration are building blocks of three-dimensional TIs, it must be emphasized that a single QL or SL Ti compound has a gapped spectrum with no two-dimensional metallic states. The IUF/TI heterostructures were simulated within a model of repeating Ti substrates separated by the van der Waals gaps.21 Note that unlike the other heterostructures, the Dirac cone becomes much larger and, respectively, the upper part gets much smaller, see Figure 1c. To the best of our knowledge, there is no TI characterized by such a type of dispersion. For the Sb$_2$Se$_2$Te/Bi$_2$Se$_3$ heterostructure, the number of the TSS charge carriers was evaluated by calculation of the group velocity. The analysis shows that the presence of the Sb$_2$Se$_2$Te QL on top of the Bi$_2$Se$_3$ surface leads to the essential decrease in the group velocity (from $\sim 3$ eV/Å$^{-1}$ to $\sim 1.3$ eV/Å$^{-1}$) and therefore to the increase in the number of the TSS charge carriers as compared to that of Bi$_2$Se$_3$.

The inset in Figure 1c shows spin-resolved constant energy contours taken at $\sim 90$, $\sim 160$, and $\sim 250$ meV below the DP in Sb$_2$Se$_2$Te/Bi$_2$Se$_3$, that is, for the lower part of the cone. One can see that the contours have a circular shape down to $\sim 90$ meV (as in the case of Bi$_2$Se$_3$ within 90 meV above the DP, Figure 1b), while below this level the hexagonal warping appears, which can lead to intraband backscattering.5,7,28 However, it is evident that the perimeter of the Dirac cone within $\sim 90$ meV below the DP of Sb$_2$Te$_2$Se/Bi$_2$Se$_3$ is roughly two times higher than that of Bi$_2$Se$_3$ in a similar energy range above the DP. We stress that this quantity determines the number of the TSS charge carriers which in turn is directly related to the conductivity.

An interesting feature of the Sb$_2$Se$_2$Te/Bi$_2$Se$_3$ heterostructure is a significant increase in the thickness of the conducting layer as compared to that of Bi$_2$Se$_3$ (Figure 1d). It can be seen in Figure 1c that approximately 50% of the DP charge density is localized in the Sb$_2$Se$_2$Te overlayer, reaching its maximum near the Sb$_2$Se$_2$Te/Bi$_2$Se$_3$ interface. Also worth noticing is the implied throughout the paper, that the first ingredient of the IUF/TI system represents an IUF overlayer, while the second one corresponds to a TI substrate. For instance, the [Sb$_2$Se$_2$Te]$_{1QL}$/[Bi$_2$Se$_3$]$_{6QL}$ heterostructure represents the 1QL-thick Sb$_2$Se$_2$Te overlayer on top of the 6QL-thick Bi$_2$Se$_3$ slab (Figure 1a).

Figure 1 shows the Bi$_2$Se$_3$ TSS with the DP located at the Fermi level. Placing an Sb$_2$Se$_2$Te QL over the Bi$_2$Se$_3$ surface induces a fundamental modification of the spectrum: the DP shifts toward the conduction band minimum, the lower part of the Dirac cone becomes much larger and, respectively, the upper part gets much smaller, see Figure 1c. To the best of our knowledge, there is no TI characterized by such a type of dispersion. For the Sb$_2$Se$_2$Te/Bi$_2$Se$_3$ heterostructure, the number of the TSS charge carriers was evaluated by calculation of the group velocity. The analysis shows that the presence of the Sb$_2$Se$_2$Te QL on top of the Bi$_2$Se$_3$ surface leads to the essential decrease in the group velocity (from $\sim 3$ eV/Å$^{-1}$ to $\sim 1.3$ eV/Å$^{-1}$) and therefore to the increase in the number of the TSS charge carriers as compared to that of Bi$_2$Se$_3$.

The inset in Figure 1c shows spin-resolved constant energy contours taken at $\sim 90$, $\sim 160$, and $\sim 250$ meV below the DP in Sb$_2$Se$_2$Te/Bi$_2$Se$_3$, that is, for the lower part of the cone. One can see that the contours have a circular shape down to $\sim 90$ meV (as in the case of Bi$_2$Se$_3$ within 90 meV above the DP, Figure 1b), while below this level the hexagonal warping appears, which can lead to intraband backscattering.5,7,28 However, it is evident that the perimeter of the Dirac cone within $\sim 90$ meV below the DP of Sb$_2$Se$_2$Te/Bi$_2$Se$_3$ is roughly two times higher than that of Bi$_2$Se$_3$ in a similar energy range above the DP. We stress that this quantity determines the number of the TSS charge carriers which in turn is directly related to the conductivity.

An interesting feature of the Sb$_2$Se$_2$Te/Bi$_2$Se$_3$ heterostructure is a significant increase in the thickness of the conducting layer as compared to that of Bi$_2$Se$_3$ (Figure 1d). It can be seen in Figure 1c that approximately 50% of the DP charge density is localized in the Sb$_2$Se$_2$Te overlayer, reaching its maximum near the Sb$_2$Se$_2$Te/Bi$_2$Se$_3$ interface. Also worth noticing is the
emergence of the quantum well state in the conduction band local gap at ~400 meV that is the Bychkov-Rashba split\(^{29}\) and is mostly localized in the Sb\(_2\)Se\(_2\)Te overlayer. Note that the attachment of the additional Sb\(_2\)Se\(_2\)Te QL on top of [Sb\(_2\)Se\(_2\)Te\(_4\)]\(_{1\text{QL}}\)/[Bi\(_2\)Se\(_3\)]\(_{6\text{QL}}\) leads to a degradation of the surface spectrum; the DP shifts even more toward the conduction band minimum, the dispersion of the lower part of the cone becomes more anisotropic, and a trivial state appears inside the fundamental band gap (see Supporting Information S2).

The modification of the TSS upon deposition of the IUF on top of the TI is directly connected to the relation of work functions and band gaps of the corresponding TI and IUF (Table 1). It is clearly seen in Figure 1f that the valence band maxima of Bi\(_2\)Se\(_3\) and Sb\(_2\)Se\(_2\)Te QL are close to each other and that the TI band gap is built into the IUF one. The strong hybridization between the Bi\(_2\)Se\(_3\) TSS and the Sb\(_2\)Se\(_2\)Te valence band states results in the upward shift of the DP. A similar effect was found in the Sb\(_2\)Te\(_3\)/PbBi\(_2\)Te\(_2\)S (see Supporting Information S3) and SnSb\(_2\)Te\(_4\)/Bi\(_2\)Te\(_2\)S heterostructures (Figure 2) despite the fact that the DP in Bi\(_2\)Te\(_2\)S lies below the valence band maximum. In the case of SnSb\(_2\)Te\(_4\)/Bi\(_2\)Te\(_2\)S, one difference takes place: band gaps of TI and IUF do not overlap but the IUF conduction band minimum is still located significantly higher than that of TI.

Thus, our design of the Sb\(_2\)Se\(_2\)Te/Bi\(_2\)Se\(_3\), SnSb\(_2\)Te\(_4\)/Bi\(_2\)Te\(_2\)S, and Sb\(_2\)Te\(_3\)/PbBi\(_2\)Te\(_2\)S heterostructures preserves the advantages of the corresponding TI substrates leading neither to appearance of the trivial bands at the Fermi energy nor to the decrease of the fundamental band gap, as it takes place in refs 20 and 30, respectively. More importantly, a substantial increase in the numbers of the TSSs charge carriers (as compared to those of the TI substrates) is expected in these systems.

Let us now present examples of the TSS modifications characterized by even more dramatic increase in the number of charge carriers. Figure 3a shows electronic spectrum of the PbBi\(_2\)Te\(_2\)S/Sb\(_2\)Te\(_3\) heterostructure superimposed with the Sb\(_2\)Te\(_3\) bulk band structure projected onto the surface Brillouin zone. By comparing the PbBi\(_2\)Te\(_2\)S/Sb\(_2\)Te\(_3\) spectrum to that of pure Sb\(_2\)Te\(_3\) (see ref 31), one can recognize a relocation of the DP from the fundamental band gap to the local band gap of the bulk valence band. Noteworthy, for that part where the TSS dispersion is perfectly linear a maximal diameter of the TSS constant energy contour in PbBi\(_2\)Te\(_2\)S/Sb\(_2\)Te\(_3\) is almost 5 times higher than that in pure Sb\(_2\)Te\(_3\) and 1.5 times higher than that in Sb\(_2\)Se\(_2\)Te/Bi\(_2\)Se\(_3\) (Figure 1c). The charge density distributions for the selected \(k\)-points are shown in Figure 3c. As it can be seen in panels for \(k_1\) and \(k_2\) points, the part of the TSS lying in the fundamental band gap is localized in the IUF overlayer having its maximum near the heterostructure surface. Although mainly locating in the IUF SL, the \(\Gamma\)-point TSS charge density demonstrates a resonance-like behavior due to the DP proximity to the bulk continuum.

The situation very similar to that in PbBi\(_2\)Te\(_2\)S/Sb\(_2\)Te\(_3\) is observed in Bi\(_2\)Te\(_2\)S/SnSb\(_2\)Te\(_4\) (Figure 3d–f). Here, the number of the TSS charge carriers is even higher than in the case of PbBi\(_2\)Te\(_2\)S/Sb\(_2\)Te\(_3\) which correlates with deeper location of the DP in the local valence band gap. By comparing Figure 3b,e, as well as taking a look at Table 1, one may notice a similar relation between work functions and band gaps of TI and IUF for these two heterostructures. Namely, in both cases band gaps of TI and IUF do not overlap and the IUF gap lies significantly lower in energy than that of TI. Concerning Bi\(_2\)Te\(_2\)S/SnSb\(_2\)Te\(_4\), we would also like to draw attention to the trivial state locating in the SnSb\(_2\)Te\(_4\) fundamental band gap and

---

**Figure 2.** Peculiarities of the SnSb\(_2\)Te\(_4\)/Bi\(_2\)Te\(_2\)S electronic structure. (a) Surface band structure. The color coding corresponds to the one used in Figure 1c. (b) Spatial distribution of the DP charge density integrated over \((x, y)\) plane. (c) Schematic view of the band alignment of the Bi\(_2\)Te\(_2\)S substrate and the SnSb\(_2\)Te\(_4\) SL.

**Figure 3.** Peculiarities of the electronic structures of PbBi\(_2\)Te\(_2\)S/Sb\(_2\)Te\(_3\) and Bi\(_2\)Te\(_2\)S/SnSb\(_2\)Te\(_4\). (a,d) Surface band structures of PbBi\(_2\)Te\(_2\)S/Sb\(_2\)Te\(_3\) and Bi\(_2\)Te\(_2\)S/SnSb\(_2\)Te\(_4\), respectively. The color coding corresponds to that in Figure 1c. (b,e) Schematic view of the band alignment of the SnSb\(_2\)Te\(_4\) substrate and the PbBi\(_2\)Te\(_2\)S SL (b) as well as of the SnSb\(_2\)Te\(_4\) substrate and the Bi\(_2\)Te\(_2\)S QL (e). (c,f) Spatial distributions of the TSS charge density for \(\Gamma\), \(k_1\), and \(k_2\) points as integrated over \((x, y)\) planes of PbBi\(_2\)Te\(_2\)S/Sb\(_2\)Te\(_3\) and Bi\(_2\)Te\(_2\)S/SnSb\(_2\)Te\(_4\), respectively. The \(k_1\) and \(k_2\) points are respectively marked by green and black triangles in panels (a) and (d).
crossing the Fermi level. Despite having quite characteristic shape, this state is not of the Bychkov–Rahsba-type because it remains almost unchanged upon switching-off the spin–orbit coupling. This state is essentially the second band of the free Bi\textsubscript{2}Te\textsubscript{2}S QL conduction band and appears in the heterostructure spectrum as a consequence of the specific band alignment of the SnSb\textsubscript{2}Te\textsubscript{4} substrate and the Bi\textsubscript{2}Te\textsubscript{2}S QL. The presence of trivial states at the Fermi level of the TI-based heterostructure can have negative consequences for the topological transport. Below we offer an efficient way of the Fermi level clearance from such states.

Apart from two considered cases of the IUF/TI band alignment, there is another important scenario: the IUF conduction band minimum is situated near the TI valence band maximum. If this takes place, there is not any signification. The presence of trivial states at the Fermi level of the TI-based heterostructure can have negative consequences for the topological transport. Below we offer an efficient way of the Fermi level clearance from such states.

Let us now demonstrate that a gradual tuning of the DP position within the fundamental or local band gap can also be realized by means of the transverse electric field in the dual-gate geometry.\textsuperscript{32,33} Within the model employed, applying an external electric field breaks the inversion symmetry thereby lifting the degeneracy of the TSS, which is manifested in the energy separation of the DPs belonging to different sides of the slab, as illustrated for Sb\textsubscript{2}Se\textsubscript{2}Te/Bi\textsubscript{2}Se\textsubscript{3} in Figure 5a. Since the bulklike states remain almost unaffected by the applied field, this separation means the change of the DP position inside the fundamental band gap. In case when the DP of the IUF/TI heterostructure resides in the local band gap of the bulk valence band, the application of the electric field results in a similar separation of the DPs. Noteworthy, we find that the energy separation of the DPs increases linearly with the strength of electric field (not shown). Therefore, the latter appears as a very efficient tool for the gradual tuning of the DP inside the bulk band gap. It is worth emphasizing that the TSS shift induced by the external electric field is rigid and therefore the linear dispersion of the TSS is preserved.

In the limit of thick TI films (six and more QLs) when the TSSs belonging to the different sides of the slab are decoupled, one can think about the manipulation not with two, but one DP. Indeed, the two TSSs shown in blue and red in Figure 5a can be considered as being located at the very same surface but corresponding to the different directions of the electric field, that is, to $E_{\text{ext}} \parallel z$ and $E_{\text{ext}} \parallel z$, respectively. Thus, depending on the electric field direction, one can induce either upward or downward shift of the DP. This situation is rather similar to that of the DP shift induced by the deposition of the IUF overlayer on top of the TI surface. However, unlike the latter case, the use of the electric field allows a gradual tuning of the DP whose shift can be controlled in real time by changing the gate voltage. Moreover, by applying an external electric field of a corresponding strength and direction one can efficiently remove undesirable trivial surface states from the Fermi level. Indeed, as it can be seen in Figure 5b, where the spectrum of the gated Bi\textsubscript{2}Te\textsubscript{2}S/SnSb\textsubscript{2}Te\textsubscript{4} is shown, the application of the electric field antiparallel to the surface normal ($E_{\text{ext}} \parallel z$) shifts trivial states toward the TI conduction band, cf. Figure 3d.

Thus, we have studied the electronic spectra of various heterostructures made of a single tetrahedrite-type quintuple or septyte layer blocks and topological insulator substrates. We have shown that depending on the relation of band gaps and

---

**Figure 4.** Peculiarities of the BiSbTe\textsubscript{2}S/Sb\textsubscript{2}Te\textsubscript{2}S electronic structure. (a) Surface band spectrum. The color coding corresponds to that in Figure 1c. (b) Spatial distribution of the DP charge density integrated over (x, y) plane. (c) Schematic view of the band alignment of the Sb\textsubscript{2}Te\textsubscript{2}S substrate and the BiSbTe\textsubscript{2}S QL.

---

**Figure 5.** The effect of electric field on the electronic spectra of TI-based heterostructures. (a,b) Electronic spectra of Sb\textsubscript{2}Se\textsubscript{2}Te/Bi\textsubscript{2}Se\textsubscript{3} (a) and Bi\textsubscript{2}Te\textsubscript{2}S/SnSb\textsubscript{2}Te\textsubscript{4} (b) subjected to the external electric fields $E_{\text{ext}} = (0.0 \pm 0.03)$ V/nm and $E_{\text{ext}} = (0.0 \pm 0.01)$ V/nm, respectively. The size of blue (red) circles corresponds to the weight of the state in the top (bottom) IUF QL of the IUF/TI slab. In the alternative treatment, the bands highlighted by blue and red circles respectively correspond to the $E_{\text{ext}} \parallel z$ and $E_{\text{ext}} \parallel x$ cases (see text).
work functions of the topological insulator substrate and the insulator ultrathin film overlayer two scenarios are expected. The first one is characterized by a substantial modification of the topological surface state leading to a significant increase in the number of the surface state charge carriers as compared to that of the substrate. Such a modification stems from sizable shift of the Dirac point arising upon bringing the topological insulator in contact with the insulator ultrathin film and is accompanied by a partial or almost complete relocation of the topological surface state from the substrate to the overlayer. We stress that such a scenario is equally possible for the topological insulators with the Dirac point lying both above and below the bulk valence band maximum. In the second case, the topological surface state appears to be almost unchanged in the energy-momentum space, while in the real space it likewise relocates from the substrate to the overlayer. Furthermore, we have shown that applying transverse electric field it is possible to gradually change the Dirac point position across the topological insulator band gap, which can be done in real time. Finally, we have demonstrated that electric field can even be efficiently used to largely move trivial states from the Fermi level, which appear in some heterostructures due to specific overlayer/substrate band alignment. Combining the advantages of the two approaches described, one can obtain a topological insulator based heterostructure with a highly tunable topological surface state.

**Methods.** Electronic structure calculations were carried out within the density functional theory using the projector augmented-wave method as implemented in the VASP code. The exchange-correlation energy was treated using the generalized gradient approximation. The Hamiltonian contained the scalar relativistic corrections and the spin–orbit coupling was taken into account by the second variation method. In order to correctly describe the van der Waals interactions we made use of the DFT-D2 approach.

**ASSOCIATED CONTENT**

* Supporting Information

Atomic structure, bulk and surface electronic spectra of the trivial insulator $Sb_xSe_yTe_2$ peculiarities of the electronic structure of $[Sb_xSe_yTe_2]_{10Q}/[Bi_2Te_3]_{13QL}$, $[Sb_xTe_y]_{13QL}/[PbBi_2Te_3S_2]_{38QL}$, and $[BiSbTeS_2]_{15QL}/[Sb_2Te_3S_2]_{40QL}$. This material is available free of charge via the Internet at http://pubs.acs.org.

**AUTHOR INFORMATION**

*E-mail: menshikova_t@mail.ru.

**Author Contributions**
The calculations were performed mainly by T.V.M. with contributions by M.M.O., S.S.T., D.A.S., and V.V.B. The idea of the study was proposed by E.V.C., who is the supervisor of the project, and A.E. All authors contributed to discussion, data analysis, and manuscript editing. T.V.M., M.M.O., V.M.K., and E.V.C. wrote the manuscript.

**Notes**
The authors declare no competing financial interest.

**ACKNOWLEDGMENTS**
We acknowledge support by the Ministry of Education and Science of the Russian Federation (state task No. 2.8575.2013), the Federal Targeted Program “Scientific and scientific-pedagogical personnel of innovative Russia in 2009-2013” (No. 14.B37.21.1164) and Russian Foundation for Basic Research (Grant 13-02-12110 ofi m). A.E. acknowledges funding by the German Research Foundation (DFG Grants ER 340/4-1 and the Priority Program 1666 “Topological Insulators”). Calculations were performed on the SKIF-Cyberia supercomputer of Tomsk State University. The authors also would like to thank Dr. S. V. Eremeev for useful discussion.

**REFERENCES**


(26) Zhukova, T. B.; Zaslavskii, A. I. Crystal structures of the compounds PbBi$_4$Te$_7$, PbBi$_2$Te$_4$, SnBi$_4$Te$_7$, SnBi$_2$Te$_4$, SnSb$_2$Te$_4$, and GeBi$_2$Te$_4$. Sov. Phys. Crystallogr. 1972, 16, 796–800.


(30) Zhang, Q.; Zhang, Z.; Zhu, Z.; Schwingenschlögl, U.; Cui, Y. Exotic Topological Insulator States and Topological Phase Transitions in Sb$_2$Se$_3$-Bi$_2$Se$_3$ Heterostructures. ACS Nano 2012, 6, 2345–2352.


