Topological insulators (TI) are new states of matter with a bulk gap and robust gapless surface states protected by time-reversal symmetry. When time-reversal symmetry is broken, the surface states are gapped, which induces a topological response of the system to electromagnetic field—the topological magneto-electric effect. In this paper we study the behavior of topological surface states in heterostructures formed by a topological insulator and a magnetic insulator. Several magnetic insulators with compatible magnetic structure and relatively good lattice matching with topological insulators Bi₂Se₃, Bi₂Te₃, and Sb₂Te₃ are identified, and the best candidate material is found to be MnSe, an anti-ferromagnetic insulator. We perform first-principles calculation in Bi₂Se₃/MnSe superlattices and obtain the surface state bandstructure. The magnetic exchange coupling with MnSe induces a gap of ~54 meV at the surface states. In addition we tune the distance between Mn ions and TI surface to study the distance dependence of the exchange coupling.

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which are aligned to each other in each layer parallel to the surface, but staggering in the perpendicular direction, it provides the same form of ferromagnetic exchange coupling as a ferromagnetic insulator does. In fact, the best candidate material found in our search is an anti-ferromagnetic insulator, MnSe, which is a better candidate than ferromagnetic insulators such as EuS since the latter has magnetism from f-electrons and has a weaker exchange coupling with the p-electrons in TI compared with the d-electrons in MnSe. We present ab initio calculation in MnSe/Bi$_2$Se$_3$ superlattices, from which we obtain the surface state gap and also describe it in a surface state effective model. In addition we tune the distance between Mn ions and TI surface to study the distance dependence of the exchange coupling. Then we conclude by discussing the band-bending effect caused by the interface charge at the TI/MI junction, which is the main experimental challenge that needs to be addressed in future works.

Criteria and candidate materials

The topological insulators Bi$_2$Se$_3$, Bi$_2$Te$_3$, and Sb$_2$Te$_3$ have layered structure, and the 2-dimensional lattice within each layer has triangular symmetry. The 2D lattice constants of Bi$_2$Se$_3$, Bi$_2$Te$_3$, and Sb$_2$Te$_3$ are 4.1355 Å, 4.395 Å, and 4.264 Å, respectively. We look for candidate MI materials with 2D crystal plane of compatible symmetry to TI layers, i.e. hexagonal lattice. The other criteria for the candidate MI materials include similar lattice constant, and ferromagnetic moments in the 2D hexagonal interface atomic plane.

A list of candidate MI materials is shown in Table I. EuO, EuS, EuSe, and MnSe have the cubic rocksalt structure, of which the atoms in the (111) plane form triangular lattice, with compatible lattice constant to the TIs. Both EuO and EuS are ferromagnetic insulators, which meets the requirement of correct magnetic configuration, however the lattice constant of EuO is too small for good lattice matching with the common 3D topological insulators. EuSe has a complex magnetic phase diagram, and it also becomes FM under suitable pressure range. Magnetism in EuO, EuS and EuSe originates from the half-filled 4f orbitals of the Eu$^{+2}$ ions. MnSe has the type-II (G-type) anti-ferromagnetic structure, of which the magnetic moments in each (111) atomic planes are ferromagnetic. MnTe is chemically similar to MnSe, although it has a hexagonal lattice. Mn moments in MnTe also have an AFM configuration, formed of alternating hexagonal (0001) FM planes. Magnetism in MnSe and MnTe comes from the high-spin $d^5$ orbitals of the Mn$^{+2}$ ions. RbMnCl$_3$ is also in hexagonal structure, with the Mn sites forming alternating (0001) FM planes. Although its hexagonal plane has a much larger lattice constant, it matches the $\sqrt{3} \times \sqrt{3}$ reconstruction of the in-plane lattice of Bi$_2$Se$_3$. Thus RbMnCl$_3$ is a potential candidate material, although the magnetic coupling would be weaker because only 1/3 of the atomic sites of the TIs will be in contact with the Mn sites.

In the candidate materials listed in Table I we carried ab initio calculations to several of them including MnSe/Bi$_2$Se$_3$, MnTe/Bi$_2$Se$_3$, MnTe/Sb$_2$Te$_3$, EuS/Bi$_2$Se$_3$ and EuSe/Bi$_2$Se$_3$. Among these heterostructures, we find MnSe/Bi$_2$Se$_3$ to be the best one, with relatively strong exchange-coupling and simple surface state band structure. In the following we will focus on the results of MnSe/Bi$_2$Se$_3$ heterostructure, and present the results on MnTe/Sb$_2$Te$_3$ and MnTe/Bi$_2$Se$_3$ in the appendix as a comparison.

Bi$_2$Se$_3$/MnSe interface

We study the Bi$_2$Se$_3$/MnSe interface by constructing a superlattice composed of Bi$_2$Se$_3$ slab and MnSe slab. The supercells employed in the first-principles calculations are required to have inversion symmetry, and the Mn atoms at the top and bottom surfaces of Bi$_2$Se$_3$ slab have parallel spin orientation. The thickness of the Bi$_2$Se$_3$ slab is chosen to be 4 QLs, the MnSe slab is determined to have a thickness of 6n+1 (7, 13, 19, ...) layers, in order to meet the requirements of inversion symmetry and parallel spin orientations. To simulate the physical system of a MnSe film deposited on top of a bulk Bi$_2$Se$_3$, the in-plane lattice constant of the MnSe is fixed to that of Bi$_2$Se$_3$, and the out-of-plane lattice constant is determined by energy optimization. The 4-7 supercell structure (composed of 4 QLs of Bi$_2$Se$_3$ and 7 layers of MnSe) is shown in fig. 1(b). First-principles density functional theory (DFT) calculations are performed to optimize the supercell structure and to obtain the electronic band structure. We used the Hohenberg-Kohn density-functional theory with the generalized-gradient approximation (GGA) and the projector augmented-wave method as implemented in VASP. The Mn 3d orbitals are treated with the GGA plus Hubbard $U$ (GGA+$U$) method and typical values of correlation parameters are used: $U = 5.0$ eV, and $J = 1.0$ eV.

If not noted otherwise (as when tuning the separation distance between Bi$_2$Se$_3$ and MnSe slabs), the atomic

FIG. 1: (color online). (a) Schematic picture of a MnSe film deposited on the surface of Bi$_2$Se$_3$. (b) Crystal structure of the supercell structure in the first-principles calculations.
coordinates of the superlattice are optimized as in the following. The middle part of the Bi$_2$Se$_3$ slab is fixed to the experimental structure, while the atomic coordinates of the whole MnSe slab together with the first Bi and Se atomic planes of Bi$_2$Se$_3$ at the interface are optimized according to the forces from first-principles calculations. 

**Bandstructure.** We first investigate the 4-13 Bi$_2$Se$_3$/MnSe superlattice, with Mn spins along [001] direction. The bandstructure from first-principles calculations is shown in fig. 2. By projecting the bands to the Bi and Se atoms of the top and bottom surfaces, shown in fig. 2(a), we identify the Dirac cone feature located about 0.4 eV below the bulk gap of Bi$_2$Se$_3$ as surface states of Bi$_2$Se$_3$. Further analysis on the spin directions of the states around Γ point confirms it to be the topological surface state. A small gap appears at the Dirac point, and both the lower and upper Dirac cones show spin related energy splitting in the vicinity of Γ point, indicating the magnetic interaction with MnSe.

The band gap of MnSe is much larger than that of Bi$_2$Se$_3$. In order to obtain a clearer picture of the electronic states of the two materials forming the superlattice, we project the bands separately to the Bi$_2$Se$_3$ slab and the MnSe slab in the superlattice, shown in fig. 2(b). The bulk gap of Bi$_2$Se$_3$, as well as the Dirac cone states, are located in the band gap of MnSe, which makes it possible to realize a fully gapped system and observe the TME effect.

**Effective model fitting.** To gain better understanding of the exchange coupling experienced by the surface states, we introduce an effective Hamiltonian $H_{\text{eff}}$ for the Dirac fermion surface states of the topological insulator thin film coupled with the exchange field $H_{\text{ex}}$. 

$$H_{\text{eff}} = Dk^2 I + \left( \frac{\hbar v_F (\sigma_x k_y - \sigma_y k_x)}{tI} + M \cdot \sigma \right),$$

where $\sigma_i$ ($i = x, y, z$) are the Pauli matrices, and $I$ the identity matrix. $M$ and $t$ correspond to the effective magnetic field acting on the Dirac fermion surface states and the inter-edge interaction between the two surfaces. The other parameters in the model are: $D$, the quadratic term, and $v_F$ the Fermi velocity.

The four eigen-energies of the model Hamiltonian can be solved analytically,

$$E = Dk^2 \pm \sqrt{k^2 + M^2 + t^2 \pm 2 \sqrt{M^2 t^2 + (M_x k_y - M_y k_x)^2}},$$

here we set $\hbar v_F = 1$. We note that at Γ point ($k = 0$), the four eigen-energies are $E = \pm (M \pm t)$. In the case of strong magnetic coupling and weak inter-edge interaction where $M > t$, the zone-center eigen-energies (from low energy to high energy) and the corresponding spin orientations are: $-M - t$ (spin down), $-M + t$ (spin down), $M - t$ (spin up), and $M + t$ (spin up). In the opposite case where $M < t$, the zone-center eigen-energies and spin orientations are: $-M - t$ (spin down), $M - t$ (spin up), $-M + t$ (spin down), and $M + t$ (spin up). In both cases, an energy gap $\Delta$ forms at the original Dirac point, $\Delta = 2|M - t|$.

The Dirac fermion bandstructure obtained from first-principles calculations is fitted to the model solution in

### Table I: A list of candidate magnetic insulators and their properties.

| Materials | Structure | Lattice matching | Magnetic phase | Comments |
|-----------|-----------|------------------|----------------|----------|
| EuO       | rocksalt, | 5.145/√2        | FM             | 4f electrons |
|           | $a = 5.145$ Å | = 3.64 Å       | weak coupling  |          |
| EuS       | rocksalt, | 5.98/√2        | FM             | 4f electrons |
|           | $a = 5.98$ Å | = 4.23 Å       | weak coupling  |          |
| EuSe      | rocksalt, | 6.192/√2        | complex,       | 4f electrons |
|           | $a = 6.192$ Å | = 4.38 Å       | FM under P     |          |
| MnSe      | rocksalt, | 5.464/√2        | type-II AFM,   | 3d electrons |
|           | $a = 5.464$ Å | = 3.86 Å       | FM (111) planes | stronger coupling |
| MnTe      | hexagonal, | 4.1497 Å       | AFM,           | 3d electrons |
|           | $a = 4.1497$ Å |           | FM (0001) planes | stronger coupling |
| RbMnCl$_3$ | hexagonal, | 7.16/√3        | AFM,           | only 1/3 of |
|           | $a = 7.16$ Å | = 4.13 Å       | lattice points  |          |
FIG. 2: (color online). Bandstructure of the Bi$_2$Se$_3$/MnTe superlattice. The two panels show the projection of the wavefunctions to the Bi and Se atoms at the top and bottom surfaces (a), and that to the two materials Bi$_2$Se$_3$ and MnSe (b). The calculation is done for the superlattice structure composed of 4 quintuple layers of Bi$_2$Se$_3$ and 13 layers of MnSe, with Mn spins along [001] direction.

For the superlattice structure composed of 4 quintuple layers of Bi$_2$Se$_3$ and 13 layers of MnSe with Mn spins along [001] direction, the calculated Dirac fermion surface states around Γ point for crystal momentum along $k_x$ (Γ-M) direction are fitted satisfactorily to the model solution, as shown in figure 3(a). The fitting parameters are: $M = 28.2$ meV, $t = 17.6$ meV, $D = 9.8$ eVÅ$^2$, and $v_F = 2.66\times10^5$ m/s. Fitting the model solution to the calculated band dispersion along $k_y$ (Γ-K) direction results in very similar parameters, $D = 9.9$ eVÅ$^2$, and $v_F = 2.70\times10^5$ m/s.

**Distance dependence of parameters $t$ and $M$.** To understand the behavior of large physical system, we investigate the dependence of the effective magnetic field $M$ and inter-edge interaction $t$ on the thickness of the MnSe slab in the superlattice structure. First-principles band structure calculations of the 4-7 (composed of 4 QLs of Bi$_2$Se$_3$ and 7 layers of MnSe), 4-13, and 4-19 Bi$_2$Se$_3$/MnSe superlattices were fitted to the model solution using equation 2. The fitting parameters $M$ and $t$ are plotted as a function of the MnSe layer number, as shown in fig. 3(b). The effective magnetic field $M$ does not vary strongly as the number of MnSe layers increases, consistent with the fact that it is mostly due to the magnetic exchange coupling between the MnSe and the surface states of Bi$_2$Se$_3$ at the interface. In contrast, the inter-edge interaction $t$ decreases rapidly as the number of MnSe layers increases. This indicates that the inter-edge interaction in smaller superlattices are mediated mostly through the MnSe slab, instead of within the Bi$_2$Se$_3$ layers. The strong effective magnetic field ($M \sim 27$ meV) at this interface results in a large gap open-
ing ($2M \sim 54 \text{ meV}$) in realistic experimental setup with thicker MnSe slab, which holds promise for magnetic manipulation of TI surface states at room temperature.

In our calculation a perfect interface between MnSe and Bi$_2$Se$_3$ is assumed. In reality, the interface will probably contain impurities and defects, so that the coupling between Mn and Se across the surface is weaker. To see how the magnetic exchange coupling is affected by the distance between Mn and Se atoms, we now keep fixed the atomic coordinates within the Bi$_2$Se$_3$ and MnSe slabs, but varying the separation $d$ between the Bi$_2$Se$_3$ and MnSe slabs, as shown in fig. 3(c). As the effective magnetic field $M$ is mostly due to the exchange coupling between MnSe and Bi$_2$Se$_3$ across the interface, we expect a strong dependence of $M$ on the separation distance $d$. For the 4-13 Bi$_2$Se$_3$/MnSe superlattice, the effective magnetic field $M$ is plotted in fig. 3(d), showing a strong dependence of $M$ as a function of the separation $d$ between Bi$_2$Se$_3$ and MnSe. This result indicates that the magnetic exchange coupling at the TI-MI interface could be tuned by applying external pressure.

**Surface charge and band bending**

Although the Dirac cone is in the bulk gap of MnSe, from the band structure shown in Fig. 2 we see some additional hole-type bands coexisting with the massive Dirac cone. These bands can be understood as a consequence of the band bending occurring at the heterostructure. Band bending at a heterojunction is common. In MnSe, Mn$^{2+}$ and Se$^{2-}$ ions carry positive and negative charge, respectively. Consequently, the Mn terminated surface considered here carries a finite positive charge density. Since the Bi$_2$Se$_3$ is a covalent material and has no surface charge, the net charge of the heterojunction between these two materials is positive, leading to a trap for the surface electrons. Therefore the bands bend down around the interface, as is illustrated in Fig. 4(a), leading to the additional surface state bands.

We studied the band bending effect by calculating the electronic density-of-states projected to individual atomic planes. The projected density-of-states (PDOS) of the Mn-Se atomic planes are shown in red curves in fig. 4(b), while the PDOS for the top and bottom Bi-Se atomic planes in the Bi$_2$Se$_3$ slab are shown in black curves. It is clear that very little band bending exists in MnSe, while there is significant shift between the states of the first and second QLs in Bi$_2$Se$_3$. The electronic states in the first QL of Bi$_2$Se$_3$ is shifted down in energy compared to the second QL, consistent with the direction of the interface electric dipole moment shown in fig. 4(a).

The additional surface states lead to difficulty in opening a full gap at the surface, the solution of which is the main open question we leave for future theoretical and experimental works. Possible solutions include screening the surface charge by a top gate, or by proper chemical doping at the junction.

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1. J. E. Moore, Nature 464, 194 (2010).
2. M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
3. X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
4. X.-L. Qi, T. Hughes, and S.-C. Zhang, Phys. Rev. B 78, 195424 (2008).
5. A. M. Essin, J. E. Moore, and D. Vanderbilt, Phys. Rev. Lett. 102, 146805 (2009).
6. A. Karch, Phys. Rev. Lett. 103, 171601 (2009).
7. J. Maciejko, X.-L. Qi, H. D. Drew, and S.-C. Zhang, Phys. Rev. Lett. 105, 166803 (2010).
8. A. H. M. Wang-Kong Tse, Phys. Rev. Lett. 105, 057401 (2010).
9. X.-L. Qi, R. Li, J. Zang, and S.-C. Zhang, Science 323, 1184 (2009).
10. G. Rosenberg and M. Franz, Phys. Rev. B 82, 035105 (2010).
11. G. Rosenberg, H.-M. Guo, and M. Franz, Phys. Rev. B 82, 041104 (2010).
12. T. Yokoyama, J. Zang, and N. Nagaosa, Phys. Rev. B 81, 241140 (2010).
13. K. Nomura and N. Nagaosa, Phys. Rev. B 82, 161401(R) (2010).
14. R. V. Aguilar, A. Stier, W. Liu, L. Bilbro, D. George, N. Bansal, J. Cerne, A. Markelz, S. Oh, and N. Armitage, *The response and colossal magneto-electric effect in the topological insulator Bi$_2$Se$_3*, e-print arXiv:1105.0237 (2011).
15. A. D. LaForge, A. Frenzel, B. C. Pursley, T. Lin, X. Liu, J. Shi, and D. N. Basov, Phys. Rev. B 81, 125120 (2010).
16. A. B. Sushkov, G. S. Jenkins, D. C. Schmadel, N. P. Butch, J. Paglione, and H. D. Drew, Phys. Rev. B 82, 125110 (2010).
17. G. S. Jenkins, A. B. Sushkov, D. C. Schmadel, N. P. Butch, P. Syers, J. Paglione, and H. D. Drew, Phys. Rev. B 82, 125120 (2010).
18. Q. Liu, C.-X. Liu, C. Xu, X.-L. Qi, and S.-C. Zhang, Phys. Rev. Lett. 102, 156603 (2009).
19. R. Yu, W. Zhang, H. J. Zhang, S. C. Zhang, X. Dai, and Z. Fang, Science 329, 61 (2010).
20. Y. L. Chen, J.-H. Chu, J. G. Analytis, Z. K. Liu, K. Igarashi, H.-H. Kuo, X. L. Qi, S. K. Mo, R. G. Moore, D. H. Lu, et al., Science 329, 659 (2010).
21. S.-Y. Xu, M. Neupane, C. Liu, D. M. Zhang, A. Richardella, L. A. Wray, N. Alidoust, M. Leanderson, T. Balasubramanian, J. Sachez-Barriga, et al., *Mag-
netically induced spin reorientation and magnetic transition on the surface of a topological insulator, e-print arXiv:1206.2090.

22. M. Liu, J. Zhang, C.-Z. Chang, Z. Zhang, X. Feng, K. Li, K. He, L.-L. Wang, X. Chen, X. Dai, et al., Phys. Rev. Lett. 108, 036805 (2012), URL http://link.aps.org/doi/10.1103/PhysRevLett.108.036805

23. C.-Z. Chang, J.-S. Zhang, M.-H. Liu, Z.-C. Zhang, X. Feng, K. Li, L.-L. Wang, X. Chen, X. Dai, Z. Fang, et al., Carrier-independent ferromagnetism and giant anomalous hall effect in magnetic topological insulator, e-print arXiv:1108.4754 (2011).

24. C. Pérez Vicente, J. L. Tirado, K. Adouby, J. C. Jumas, A. Abba Touré, and G. Kra, Inorg. Chem. 38, 2131 (1999).

25. Y. Feutelais, B. Legendre, N. Rodier, and V. Agafonov, Mater. Res. Bull. 28, 591 (1993).

26. T. L. Anderson and H. B. Krause, Acta Cryst. B30, 1307 (1974).

27. D. B. McWhan, P. C. Souers, and G. Jura, Phys. Rev. 143, 385 (1966).

28. M. Palazzi and E. Breetey, Mater. Res. Bull. 24, 695 (1989).

29. K. Westerholt and H. Bach, Phys. Rev. B 31, 7151 (1985).

30. A. J. Jacobson and B. E. F. Fender, J. Chem. Phys. 52, 4563 (1970).

31. S. S. A. Noor, J. Appl. Phys. 61, 3549 (1987).

32. E. M. Ali and A. A. Felimban, Aust. J. Phys. 42, 307 (1989).

33. J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).

34. P. E. Blöchl, Phys. Rev. B 50, 17953 (1994).

35. G. Kresse and J. Furthmüller, Phys. Rev. B 54, 11169 (1996).

36. G. Kresse and D. Joubert, Phys. Rev. B 59, 1758 (1999).

37. V. I. Anisimov, J. Zaanen, and O. K. Andersen, Phys. Rev. B 44, 943 (1991).

38. A. I. Liechtenstein, V. I. Anisimov, and J. Zaanen, Phys. Rev. B 52, R5467 (1995).

39. S. J. Youn, Journal of Magnetics 10, 71 (2005).

40. P. Amiri, S. J. Hashemifar, and H. Akbarzadeh, Phys. Rev. B 83, 165424 (2011).

41. C.-X. Liu, X.-L. Qi, H. Zhang, X. Dai, Z. Fang, and S.-C. Zhang, Phys. Rev. B 82, 045122 (2010).

Appendix A: In-plane magnetization

As a comparison, we also calculated the bandstructure of Bi$_2$Se$_3$/MnSe superlattice with Mn spins along the in-plane [100] direction. The bandstructure along $k_y$ ($\Gamma$-K) direction with projection of the bands to the Bi and Se atoms of the top and bottom surfaces is shown in fig. 5(a). Similar to the case of [001] spin orientation shown in Fig. 2, the Dirac-cone states are located about 0.4 eV below the bulk gap of Bi$_2$Se$_3$. One prominent feature is that the Dirac-cone states of the top and bottom surfaces are shifted to opposite directions along $k_y$ axis. For a Fermi energy above the Dirac cone, the Fermi surfaces from the top and bottom surfaces of Bi$_2$Se$_3$ will shift to opposite directions in the momentum space. Fig. 5(b) illustrates the opposite shift of the two Fermi surfaces along $k_y$ direction, and the corresponding spin directions.

By fitting the effective model (11) with an in-plane exchange field, we have extracted the exchange coupling $M$ and inter-edge interaction $t$. For the 4-13 superlattice structure with in-plane magnetization, we obtain $M = 9$ meV, and $t = 19$ meV. The value of $t$ mostly depends on the thickness of MnSe and Bi$_2$Se$_3$ slabs, so $t$ in the case of in-plane magnetization is similar to the value for perpendicular magnetization. However the exchange coupling is quite anisotropic, and it is much smaller in the case of in-plane magnetization compared to the perpendicular one.

Appendix B: Sb$_2$Te$_3$/MnTe interface

Other materials in our study include the Sb$_2$Te$_3$/MnTe heterostructure. The calculated bandstructure of the 4-13 superlattice with projection of the bands to the Sb and Te atoms at the top and bottom surfaces is shown in fig. 6(a). In contrast to the Bi$_2$Se$_3$/MnSe heterostructure, there is complicated hybridization of bulk and surface states in the Sb$_2$Te$_3$/MnTe heterostructure, and the Dirac-cone feature cannot be easily identified.

We project the bands separately to the Sb$_2$Te$_3$ slab and the MnTe slab in the superlattice, as shown in fig. 6(b). Although the bulk band gap of MnTe at $\Gamma$ point is much larger than Sb$_2$Te$_3$, the bulk band gap of Sb$_2$Te$_3$ is located close in energy to the top of valence band of MnTe, and the Dirac surface states overlap in energy with the valence band of MnTe. Therefore it is less likely to realize a fully gapped system in Sb$_2$Te$_3$/MnTe heterostructure.

Appendix C: Bi$_2$Se$_3$/MnTe interface

We have also studied the Bi$_2$Se$_3$/MnTe heterostructure with supercell composed of 4 QLs of Bi$_2$Se$_3$ and 7 layers of MnTe. The calculated bandstructure with projection of the bands to the Bi and Se atoms at the top and bottom
surfaces is shown in fig. 7. Similar to the Sb$_2$Te$_3$/MnTe heterostructure, the surface states and bulk states in the Bi$_2$Se$_3$/MnTe heterostructure are also strongly hybridized, and the Dirac-cone feature can not be easily identified.

FIG. 5: (Color online) (a) Bandstructure of the Bi$_2$Se$_3$/MnSe superlattice along $k_y$ ($\Gamma$-K) direction. The red and blue symbols show the projection of the wavefunctions to the Bi and Se atoms at the top and bottom surfaces. (b) a schematic showing the Fermi surfaces of $n$-doped surface states at the two surfaces of Bi$_2$Se$_3$. The Fermi energy is taken at the dashed line in (a). The calculation is performed for superlattice structure composed of 4 QLs of Bi$_2$Se$_3$ and 13 layers of MnSe, with Mn spins along [100] direction.

FIG. 6: (Color online) Bandstructure of the Sb$_2$Te$_3$/MnTe superlattice. The two panels show the projection of the wavefunctions to the Sb and Te atoms at the top (red symbols) and bottom (blue symbols) surfaces (a), and that to the two materials Sb$_2$Te$_3$ and MnTe (b). The calculation is done for the superlattice structure composed of 4 QLs of Sb$_2$Te$_3$ and 13 layers of MnTe, with Mn spins along [001] direction.
FIG. 7: (Color online) Bandstructure of the Bi$_2$Se$_3$/MnTe superlattice, showing the projection of the wavefunctions to the Bi and Se atoms at the top (red symbols) and bottom (blue symbols) surfaces. The calculation is done for the superlattice structure composed of 4 QLs of Bi$_2$Se$_3$ and 7 layers of MnTe, with Mn spins along [001] direction.