Symmetry-enforced chiral hinge states and surface quantum anomalous Hall effect in the magnetic axion insulator Bi$_{2-x}$Sm$_x$Se$_3$

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Supplementary Materials for
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THIS PDF FILE INCLUDES:

- Appendices: A to C.
- Figures: S1 to S4.
APPENDIX

Appendix A: Layer construction of the axion insulator protected by inversion symmetry

It is known that many topological crystalline states can be adiabatically deformed into a stacking of decoupled layers, called the “layer construction” of the corresponding topological crystalline states [1]. Axion insulator protected by inversion symmetry can also be layer constructed. Consider a lattice having a vector along $z$–axis of unit length. The inversion center is put at the origin, and due to the lattice translation, $\mathbf{r} = (0, 0, n/2)$ are also inversion centers, where $n$ is an integer. The real-space construction of the axion insulator has Chern insulators with inversion center is put at the origin, and due to the lattice translation, $\mathbf{r}_n$ inversion symmetry can also be layer constructed. Consider a lattice having a vector along $z$-axis of unit length. The inversion center is put at the origin, and due to the lattice translation, $\mathbf{r}_n = (0, 0, n/2)$ are also inversion centers, where $n$ is an integer. The real-space construction of the axion insulator has Chern insulators with inversion.

$\Psi$ to denote the state having $C = +1$ at $z = n$ and $C = -1$ at $z = n + 1/2$. Starting from $\Psi$, we create at $z = n + 1/4$ and $z = n - 1/4$ a pair of Chern insulators out of vacuum, with Chern numbers $\pm 1$ respectively. Then we move the $C = 1$ layers ($C = -1$ layers) at $z = n + 1/4$ upward (downward), and $C = +1$ layers ($C = -1$ layers) at $z = n - 1/4$ downward (upward). When the Chern insulators move the distance of 1/4, two $C = -1$ layers meet with the original $C = +1$ layers at $z = n$ and two $C = +1$ layers meet with the original $C = -1$ layers at $z = n + 1/2$, making after annihilation the $\Psi'$ state. Since the entire process does not break inversion or closing the gap, we have $\Psi \sim \Psi'$.

Appendix B: Effects of Surface Reconstruction

In the above calculations, we have not considered the effects of surface reconstructions. However, it is always an important issue for the detection of the chiral hinge states in realistic materials. To study the surface reconstruction in Sm doped Bi$_2$Se$_3$ by first principle calculations with the full charge density self consistency is computationally too demanding and is not of the scope of this paper. In the present study, we will mimic the effects of surface reconstruction by changing the surface potentials in our tight binding model and test how robust the hinge states is against the strength of such surface reconstruction potentials. Two types of the surface reconstruction potentials have been considered here. The first type is the $3 \times 1$ surface modulation along the $\mathbf{a}$ and $\mathbf{b}$ direction on (100) and (010) surfaces respectively. The thickness of modulation is as thick as one unit cell. For convenience, we define the strength of the modulating on-site energy on atom Bi and Se as $\Delta E_{\text{Bi}} = -\Delta E_{\text{Se}} = \delta E$. The corresponding spectral functions for $\delta E = 100$ meV, 75 meV, 50 meV, 0 meV, -50 meV, -100 meV are shown in Fig. S3(a-f), respectively. Compared with the results without surface reconstruction shown in Fig. S3d, an additional trivial hinge mode in the gap of surface states can be introduced by such a surface reconstruction potential. With the changing of $\delta E$ from 100 meV to -100 meV, this trivial hinge mode moves across the surface gap but the two chiral hinge modes keep almost unchanged, which show the robustness of the chiral hinge modes.

The second type of surface reconstruction considered here is the weakening of the surface bonds, where we reduce the hopping integral between the first and the inner layers by some given ratio and test again the robustness of the chiral hinge states. The corresponding spectral functions for the weakening ratio $w = 1.0$, 0.7 and 0.0 are plotted in Fig. S3d, Fig. S3g and Fig. S3h, respectively. Comparing with the normal state as shown in Fig. S3d, a 30% (1-0.7) percent weakening could bring in an evident changes to the spectral functions. However, the nontrivial hinge modes in the gap only change a little. When $w = 0$, the outmost layer is completely peeled off and the behaviour of the chiral hinge states should be fully restored, as shown in Fig. S3h.

Appendix C: Comparison between GGA+SOC and Wannier+SOC Band structures

The tight-binding Hamiltonian of pure Bi$_2$Se$_3$ crystal is constructed by the maximally-localized spinor Wannier functions, where the spin-orbit coupling (SOC) is fully considered ab-initially. The obtained Wannier+SOC Hamiltonian is in good agreement with the first-principle calculation by the generalized gradient approximation (GGA) plus spin-orbit coupling, as shown by the band structures plotted in Fig. S4.
REFERENCES

FIG. S1. The orbital-resolved density of states of SmBi$_{23}$Se$_{36}$ calculated by LDA method.
FIG. S2. The bi-semi-infinite open boundary geometry mentioned in the main text to calculate the hinge states. The geometry is divided into three parts, interface layer, upper layers (ULs, divided into PLs which are positively labelled as $R_i$) and lower layers (LLs, divided into PLs which are negatively labelled as $R_i$). Hamiltonian of each PL and interface layer as well as hopping matrix among them are given in this figure.
FIG. S3. The effects of surface reconstructions to the projected spectral functions on the interface layer. a-f are for the surface potential modulation and d,g,h are for the surface bonds weakening and termination effects. The shifts of on-site energy are $\delta E=100$ meV, 75 meV, 50 meV, 0 meV, -50 meV, -100 meV for a, b, c, d, e, f, respectively. The weakening ratios are $w=1.0, 0.7, 0.0$ in d, g, h, respectively.
FIG. S4. The band structure of Bi$_2$Se$_3$ calculated by GGA+SOC (red solid line) and Wannier+SOC method (green dashed line).