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Supplementary Information for

Topology on a new facet of bismuth

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Supporting Information Text

1. Mirror Chern Number ($n_{\mathcal{M}}$)

To determine the topological phase belonging to Bi, the mirror Chern number $n_{\mathcal{M}}$ of the three mirror planes in Bi is calculated. The $n_{\mathcal{M}}$ is defined as,

$$n_{\mathcal{M}} = (\mathcal{C}_+ - \mathcal{C}_-)/2,$$

where $\mathcal{C}_\pm$ is the mirror Chern number of each subspace $\{\pm\}$ carrying opposite mirror eigenvalues im ($m = \pm$) and is calculated as

$$\begin{aligned} \mathcal{C}_\pm &= \int \frac{d\boldsymbol{k}}{(2\pi)} \Omega_\pm, \\ \Omega_\pm(\boldsymbol{k}) &= \sum_{n<E_f} \sum_{n\neq m} 2\,\mathrm{Im}\, \frac{\langle \psi^\pm_{n\boldsymbol{k}} | v_x | \psi^\pm_{m\boldsymbol{k}} \rangle \langle \psi^\pm_{m\boldsymbol{k}} | v_y | \psi^\pm_{n\boldsymbol{k}} \rangle}{(E_{m\boldsymbol{k}} - E_{n\boldsymbol{k}})^2}. \end{aligned}$$

The integration is carried in the 2D $\boldsymbol{k}$ space where states ($\psi_{n\boldsymbol{k}}$) are invariant with respect to the mirror symmetry $\mathcal{M}$. In the above equation, $E_{m\boldsymbol{k}}$ is the eigenenergy of band m, and $v_{x,y}$ is the velocity operator. Our calculation shows that $n_{\mathcal{M}} = 0$ in Bi.

2. Wannier Charge Center (WCC)

The Wannier charge center (WCC) has been shown to be an useful way to analyze whether the surface states are protected by the bulk topology (1–7). Essentially, WCC is the position of the Wannier state in the unit cell and has been widely used in the modern theory of polarization for calculating bulk polarization (8–11). The WCC can be calculated by solving the eigenvalue of position operator $P\hat{x}P = Pe^{-i\delta k_x \hat{x}}P$ projected on the Bloch states (1, 12), where P is the projection operator. By adopting the periodic gauge,

$$|u_{\boldsymbol{k}+\boldsymbol{G}}\rangle = e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}|u_{\boldsymbol{k}}\rangle, \qquad [1]$$

where $|u_{\boldsymbol{k}}\rangle$ is the periodic part of the Bloch wavefunction at $\boldsymbol{k}$, and $\boldsymbol{G}$ is the reciprocal vector, the eigenvalue ($\bar{x}$) of $P\hat{x}P$ has been shown to being equal to the non-Abelian Berry phase of $\langle u_{\boldsymbol{k}_\perp+G_x}|u_{\boldsymbol{k}_\perp}\rangle$ (1) in the parallel transport,

$$\bar{x} = -\frac{1}{2\pi}\mathrm{Im}\,\log(\langle u_{\boldsymbol{k}_\perp+G_x}| \prod_{k_x=\delta k_x}^{G_x-\delta k_x} P(k_x)|u_{\boldsymbol{k}_\perp}\rangle) \qquad [2]$$

where $\boldsymbol{k}_\perp$ is the k vector normal to k_x and $P(k_x) = |u_{\boldsymbol{k}_\perp+k_x}\rangle\langle u_{\boldsymbol{k}_\perp+k_x}|$.

We then applied eq. 2 to calculate the WCC of the surface Brillouin zone (SBZ) of Bi ($1\bar{1}0$) and (111) surfaces. For the ($1\bar{1}0$) surface, where $[1\bar{1}0]\,\|\,\hat{x}$, the SBZ ($\boldsymbol{k}_\perp$) is spanned on the $k_y - k_z$ plane. The calculated WCCs ($\bar{x}$) along high symmetry $\boldsymbol{k}_\perp$ path is shown in Figure. S1(a), where the high symmetry k points are expressed in the unit of $(\frac{2\pi}{b}, \frac{2\pi}{c})$. Two dominant WCC sheets (A and B indicated in Figure. S1(a)) are found in a unit cell, and are well separated along the high symmetry $\boldsymbol{k}_\perp$ paths. However, this can not rule out the $C_{2[1\bar{1}0]}$ protected TCI phase, since the $C_{2[1\bar{1}0]}$ protected surface states on ($1\bar{1}0$) can locate at a generic $\boldsymbol{k}_\perp$. By scanning the full SBZ, we found the connection between WCC sheet A and B (see Figure. 2(g)(h) in the main text) and confirm the $C_{2[1\bar{1}0]}$ protected topology.

We also studied the WCCs on the (111) surface, and the result is shown in Figure. S1(b-d). On the (111) surface, where $[111]\|\,\hat{z}$, the SBZ ($\boldsymbol{k}_\perp$) is spanned by k_x and k_y. The results show that the WCC sheets are fully disconnected. Moreover, the calculated WCCs at the unit cell boundary, $\bar{z} = 1$ (Figure. S1(b)), almost reproduces the property of surface states calculated in a semi-infinite (111) surface (see Figure. 4(d)). This result reconfirms that $n_{\mathcal{M}} = 0$.

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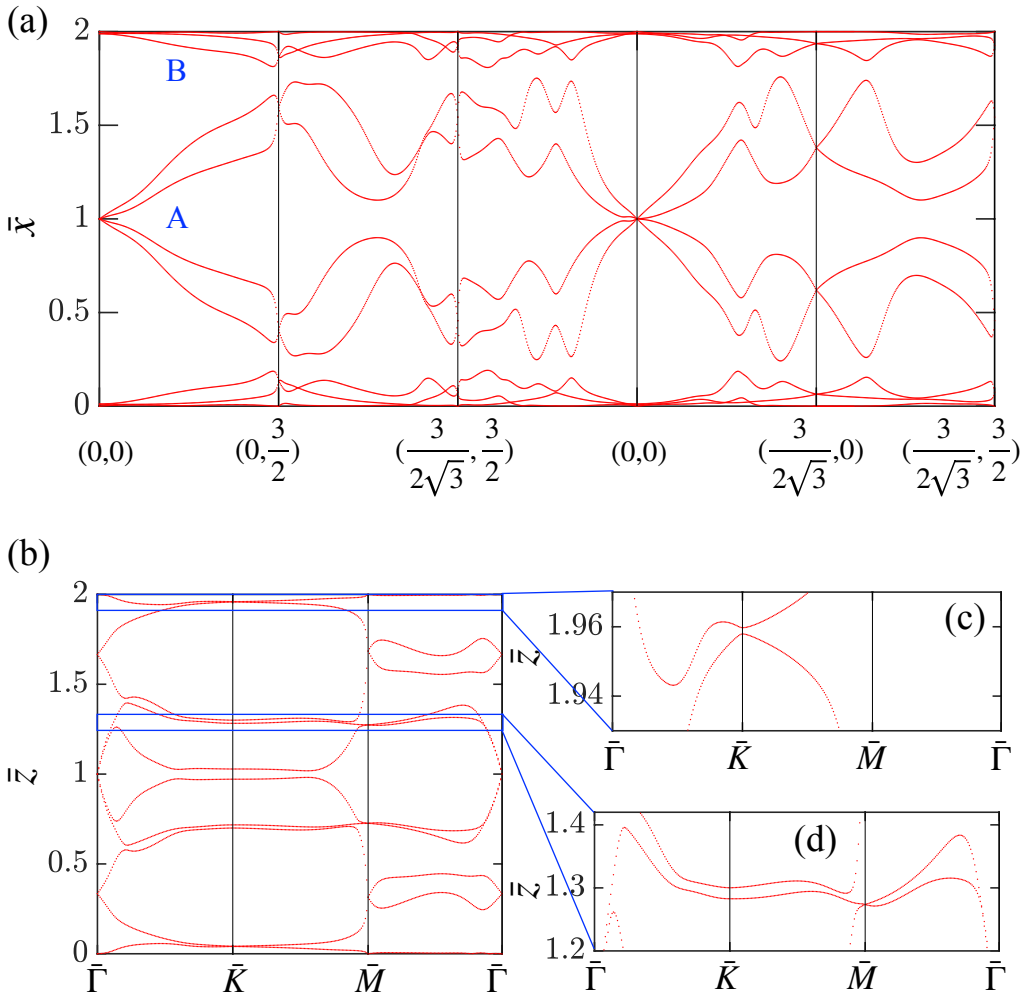

Fig. S1. (a) WCCs of $\bar{x}(k_y, k_z)$ on $(1\bar{1}0)$ surface along high symmetry k paths. (b) WCCs of $\bar{z}(k_x, k_y)$ on (111) surface along the k paths with the k points indicated in the main text. (c,d) The zoomed-in WCCs of (b) show the fully disconnected characteristic of WCC sheets.

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