Supplementary Material for "Massive states in topological heterojunctions"

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I. Surface states of a THJ

Since k_z does not commute with position, $[z,k_z]=i$, we simplify the Hamiltonian in Eq. (1) of the main text with the following rotation $|\Psi\rangle = e^{-i\pi\hat{\mathbb{1}}\otimes\hat{\tau}_y/4}|\Psi'\rangle$ to the *chiral* basis (with $\mu=0$)

$$\hat{H}_c = \begin{bmatrix} 0 & v_F k_+ & 0 & \hat{a} \\ v_F k_- & 0 & \hat{a} & 0 \\ 0 & \hat{a}^\dagger & 0 & -v_F k_+ \\ \hat{a}^\dagger & 0 & -v_F k_- & 0 \end{bmatrix}, \tag{1}$$

where we introduce $k_\pm = k_y \pm i k_x$ and the operator $\hat{a} = -[v_F i k_z + \Delta(z)]$. In the following we solve this Hamiltonian for two different potentials $f(z/\ell)$ in $\Delta(z) = \frac{1}{2}(\Delta_2 - \Delta_1)[\delta + f(z/\ell)]$.

a. Domain wall potential

We consider the smooth domain wall $f(z) = \tanh(z/\ell)$ and search for the bound states of the Schrodinger equation. This situation is very similar to that in Ref. [1–3] that we will follow closely. We first perform the change of variable $s = [1-\tanh(z/\ell)]/2$ so that

$$\hat{a} = \frac{2v_F}{\ell} s(1-s)\partial_s - (\bar{\Delta} + \delta\Delta - 2\delta\Delta s), \tag{2}$$

$$\hat{a}^\dagger = -\frac{2v_F}{\ell} s(1-s)\partial_s - (\bar{\Delta} + \delta\Delta - 2\delta\Delta s). \tag{3}$$

We now consider the equations for the squared Hamiltonian in Eq.(1) and decompose the wavefunction into two spinors ϕ_σ, $\sigma=\pm$ so that $\Psi = (\phi_+, \phi_-)$. One finds

$$\left[\frac{1}{2}\left(\{\hat{a}^\dagger,\hat{a}\} + \sigma\left[\hat{a}^\dagger,\hat{a}\right]\right) - (E^2 - v_F^2 k_\parallel^2)\right]\phi_\sigma = 0 \tag{4}$$

$$\implies \left[s(1-s)\partial_s^2 + (1-2s)\partial_s - \left(\frac{\ell}{2v_F}\right)^2\left\{\frac{[\bar{\Delta} + (1-2s)\delta\Delta]^2 - (E^2 - v_F^2 k_\parallel^2)}{s(1-s)} - \sigma\frac{4v_F\delta\Delta}{\ell}\right\}\right]\phi_\sigma = 0. \tag{5}$$

We then perform the following replacement of the wavefunction $\phi_\sigma(s) = s^\alpha(1-s)^\beta u_\sigma(s)$ in order to get rid of the $1/s(1-s)$ singularity and recognize Euler's hypergeometric equation [4]: $s(1-s)\partial_s^2\phi + [c-(1+a+b)s]\,\partial_s\phi - ab\phi = 0$. The parameters α and β fulfill

$$\begin{cases} \alpha^2 = (\ell/2v_F)^2\left[\Delta_1^2 - (E^2 - v_F^2 k_\parallel^2)\right] \\ \beta^2 = (\ell/2v_F)^2\left[\Delta_2^2 - (E^2 - v_F^2 k_\parallel^2)\right] \end{cases}, \tag{6}$$

and in the following we choose the positive roots of those equations. The equation is now

$$\left[s(1-s)\partial_s^2 + [1+2\alpha - 2(1+\alpha+\beta)s]\,\partial_s - \left\{(\alpha+\beta)(\alpha+\beta+1) - \frac{\ell\delta\Delta}{v_F}\left(\sigma + \frac{\ell\delta\Delta}{v_F}\right)\right\}\right]u_\sigma(s) = 0, \tag{7}$$

which corresponds to the Euler hypergeometric differential equation. We now introduce the auxiliary parameters

$$\begin{cases} a_\sigma = 1/2 + \alpha + \beta + \left|1/2 + \sigma\frac{\ell\delta\Delta}{v_F}\right|, \\ b_\sigma = 1/2 + \alpha + \beta - \left|1/2 + \sigma\frac{\ell\delta\Delta}{v_F}\right|, \\ c = 1 + 2\alpha. \end{cases} \tag{8}$$

For each value of σ, there are two solutions to this equation that are described by the hypergeometric functions [4] ${}_2F_1(a,b,c;s) = \sum_{n=0}^\infty \frac{(a)_n(b)_n}{(c)_n} z^n/n!$ with $(x)_n = x(x+1)\cdots(x+n-1)$. The solutions are $u_I(s) = {}_2F_1(a,b,c;s)$ and $u_{II}(s) = s^{1-c}\,{}_2F_1(1+a-c, 1+b-c, 2-c; s)$ but $u_{II}(s)$ does not describe bound states since $\phi_{II}(s\sim 0) = s^\alpha(1-s)^\beta u_{II}(s\sim 0) \sim s^{1+\alpha-c}$ which diverges at $s=0$ ($x=\infty$) since $1+\alpha-c = -\alpha < 0$. On the other hand, while

$\phi_I(s \sim 0) = s^\alpha (1-s)^\beta u_I(s\sim 0) \sim s^\alpha$ goes to zero at $s=0$ ($x=\infty$), one can check its behavior at $s=1$ ($x=-\infty$). We use the following relation from Ref. [4]

$$
\begin{aligned}
{}_2F_1(a,b,c;s) =& \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\ {}_2F_1(a,b,a+b+1-c;1-s) \\
&+ \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}(1-s)^{c-a-b}\ {}_2F_1(c-a,c-b,1+c-a-b;1-s),
\end{aligned}
\tag{9}
$$

and find that for $s\sim 1$ ($x=-\infty$)

$$
\phi_\sigma(s\sim 1) \sim \frac{\Gamma(c)\Gamma(c-a_\sigma-b_\sigma)}{\Gamma(c-a_\sigma)\Gamma(c-b_\sigma)}(1-s)^\beta + \frac{\Gamma(c)\Gamma(a_\sigma+b_\sigma-c)}{\Gamma(a_\sigma)\Gamma(b_\sigma)}(1-s)^{-\beta}
\tag{10}
$$

which should diverge since $\beta>0$ unless $\Gamma(a_\sigma)$ or $\Gamma(b_\sigma)$ diverges. This happens if either a_σ or b_σ is a negative integer and since $a>b$, this should happen on b. Then one has the following quantization, with $n\in\mathbb{N}$,

$$
\sqrt{\Delta_1^2-(E^2-v_F^2k_\parallel^2)} + \sqrt{\Delta_2^2-(E^2-v_F^2k_\parallel^2)} = \left|\frac{2v_F}{\ell}\right| \left[\left|\frac{1}{2}+\sigma\frac{\ell\delta\Delta}{v_F}\right| - (n+\frac{1}{2})\right] \equiv g_\sigma(n),
\tag{11}
$$

and the eigenenergies are thus

$$
E = \pm\sqrt{v_F^2k_\parallel^2 - \frac{1}{4g_\sigma^2(n)}[g_\sigma^2(n)-4\delta\Delta^2][g_\sigma^2(n)-4\bar{\Delta}^2]}.
\tag{12}
$$

Also, as we have shown, the long range behavior of the wavefunctions is described by (i) $\phi_< = (1-s)^\beta = 1/(1+e^{-z/\ell})^\beta$ for $s\sim 1$ ($x\sim-\infty$), and (ii) $\phi_>(s) = s^\alpha = 1/(1+e^{z/\ell})^\alpha$ for $s\sim 0$ ($x\sim\infty$). This implies that $\alpha,\beta>0$ which according to Eq. (6) means that $E^2-(v_Fk_\parallel)^2 < \min(\Delta_1^2,\Delta_2^2)$. Moreover, since α,β also appear in the definition of $b_\sigma=-n$ we find that $\alpha^2-\beta^2 = (\ell/2v_F)^2 4\bar{\Delta}\delta\Delta$ and $\alpha+\beta = g_\sigma(n)\ell/2v_F$.

$$
g_\sigma(n) > 2\sqrt{|\bar{\Delta}\delta\Delta|}.
\tag{13}
$$

Here, we are not interested in the exact form of the wavefunctions, and we will therefore not detail the exact form of the solutions; these technical details can be found in Ref. [1 and 3]. In the main text, we discuss the two limits $\ell \gg v_F/\delta\Delta$ (smooth/thick interface) and $\ell \ll v_F/\delta\Delta$ (abrupt/thin interface). In fact we can consider two situations :

Thick interface, $|\ell| > |v_F/2\delta\Delta|$. In this situation, one can write

$$
g_\sigma(n) = 2\,|\delta\Delta| - \left|\frac{2v_F}{\ell}\right| \left[n + \frac{1-\mathrm{sgn}(\sigma\ell\delta\Delta/v_F)}{2}\right].
\tag{14}
$$

One finds that the two set of states $\sigma=\pm$ are thus related by a family of states with $\phi_+\sim|n\rangle$ and $\phi_-\sim|n+\mathrm{sgn}(\ell\delta\Delta/v_F)\rangle$ as in Landau levels. This implies the existence of a chiral $n=0$ state which has the polarization ϕ_σ with $\sigma=-\mathrm{sgn}(\ell\delta\Delta/v_F)$. For notation simplicity we take $g(n)=g_+(n)=2(|\delta\Delta|-|v_F/\ell|n)$ and from Eq. (13) one finds that $n\in\mathbb{N}$ is such that

$$
n < N_{max.} = \frac{\ell|\delta\Delta|}{|v_F|}\left(1-\sqrt{\left|\frac{\bar{\Delta}}{\delta\Delta}\right|}\right),
\tag{15}
$$

thus one can only find bound states ($N_{max.}\geq 0$) if $|\bar{\Delta}/\delta\Delta|<1$ which corresponds to situations with gap inversion ($\Delta_1\Delta_2<0$).

Thin interface, $|\ell| < |v_F/2\delta\Delta|$. In this situation, one can write

$$
g_\sigma(n) = \left|\frac{2v_F}{\ell}\right| \left[\mathrm{sgn}(\sigma\ell\delta\Delta/v_F)\left|\frac{\ell\delta\Delta}{v_F}\right| - n\right].
\tag{16}
$$

From this expression and from the condition for bound states (13), one finds that

$$
-n > \mathrm{sgn}(\sigma\ell\delta\Delta/v_F)\left|\frac{\ell\delta\Delta}{v_F}\right| + \left|\frac{\ell}{2v_F}\sqrt{\bar{\Delta}\delta\Delta}\right| > \mathrm{sgn}(\sigma\ell\delta\Delta/v_F)\underbrace{\left|\frac{\ell\delta\Delta}{v_F}\right|}_{\in[0,\frac{1}{2}]},
\tag{17}
$$

which has the solution $n = 0$ only for the spinor ϕ_σ with $\sigma = -\text{sgn}(\ell\delta\Delta/v_F)$.

The previous results show that in the smooth interface the bound states have the following spectrum, for $n \in \mathbb{N}$,

$$E = \pm\sqrt{v_F^2 k_\parallel^2 - \frac{1}{f^2(n)}[f^2(n) - \delta\Delta^2][f^2(n) - \bar{\Delta}^2]}, \tag{18}$$

with $f(n) = |\delta\Delta| - |v_F/\ell|n$ and $n < N_{max.} = \frac{\ell|\delta\Delta|}{|v_F|}\left(1 - \sqrt{\left|\frac{\bar{\Delta}}{\delta\Delta}\right|}\right)$. More explicitly one can write

$$E = \pm\sqrt{v_F^2 k_\parallel^2 + 2n(1 - \bar{\Delta}^2/\delta\Delta^2)\left|\frac{v_F\delta\Delta}{\ell}\right| \frac{\left(1 - \left|\frac{v_F}{2\ell\delta\Delta}\right|n\right)\left(1 + \frac{|v_F/\ell|}{\Delta_1}n\right)\left(1 - \frac{|v_F/\ell|}{\Delta_2}n\right)}{\left(1 - \left|\frac{v_F}{\ell\delta\Delta}\right|n\right)^2}} \tag{19}$$

$$\approx \pm\sqrt{v_F^2 k_\parallel^2 + 2n(1 - \bar{\Delta}^2/\delta\Delta^2)\left|\frac{v_F\delta\Delta}{\ell}\right|} + o\left(\frac{v_F}{\ell}\right) \tag{20}$$

which correspond to the limit of a large interface, $\ell \gg v_F/\delta\Delta$.

b. Surface states for the linearized potential

In order to obtain more physical insight in the nature of the MSS, let us now focus on the limit of a linearized interface $\ell \gg \xi$, for which the length ℓ_n in Eq. (3) of the main text of the lower energy states ($n \ll N$) yields $\ell_n \approx \ell_S/\sqrt{2n}$ with $\ell_S = \sqrt{\ell\xi/(1-\delta^2)}$. The values for ℓ_S [5] and N [6] strongly depend on the underlying interface potential. The spectrum (19) is then identical to Landau bands of the Dirac equation in a uniform magnetic field with a magnetic length ℓ_S (20). The relation to Landau levels can be made explicit by linearizing the gap function $\Delta(z)$ around the interface with $f(z/\ell) = v_F z/\ell_S^2$ in (1). Choosing $z = 0$ as the position where $\Delta(z)$ changes sign, we write

$$\Delta(z) \simeq \text{sgn}(\Delta_2 - \Delta_1) v_F z/\ell_S^2, \tag{21}$$

as in Ref. 7. The operators $\hat{c} = \ell_S\hat{a}/\sqrt{2}v_F, \hat{c}^\dagger = \ell_S\hat{a}^\dagger/\sqrt{2}v_F$ act as ladder operators, $\left[\hat{c}, \hat{c}^\dagger\right] = \text{sgn}(\Delta_2 - \Delta_1)$. Following the procedure for Landau bands [8], in the case $\Delta_2 > 0 > \Delta_1$ [9], we write the eigenstates in the form $\Psi_n = [\alpha_{1,n}|n-1\rangle, \alpha_{2,n}|n-1\rangle, \alpha_{3,n}|n\rangle, \alpha_{4,n}|n\rangle]$. The eigenstates $|n\rangle$ of the number operator $\hat{n} = \hat{c}^\dagger\hat{c}$ are the usual harmonic-oscillator wavefunctions, in terms of the Hermite polynomials $H_n(z)$,

$$\psi_n(z) \propto H_n(z/\ell_S)e^{-z^2/4\ell_S^2}, \tag{22}$$

centered at the interface (around $z = 0$) with a typical localization length

$$\sqrt{2n}\ell_S \simeq \sqrt{2n}\ell_n \simeq \sqrt{2n\ell\xi/(1-\delta^2)} \tag{23}$$

due to their Gaussian factor. Notice that the expression of the localization length coincides with that [Eq. (3)] of the main text in the limit of a smooth interface, for $\ell \gg \xi$.

The spectrum and eigenstates for $n \geq 1$ are obtained by diagonalizing the Hamiltonian

$$\hat{H}_{c,n} = v_F \begin{bmatrix} 0 & k_+ & 0 & \frac{\sqrt{2n}}{\ell_S} \\ k_- & 0 & \frac{\sqrt{2n}}{\ell_S} & 0 \\ 0 & \frac{\sqrt{2n}}{\ell_S} & 0 & -k_- \\ \frac{\sqrt{2n}}{\ell_S} & 0 & -k_+ & 0 \end{bmatrix}. \tag{24}$$

Moreover, the $n = 0$ state is special in that it is chiral with $\Psi_0 = [0, 0, \alpha|0\rangle, \beta|0\rangle]$ and the Hamiltonian acting on the (α, β) coefficients is $\hat{H}_{c,0} = v_F(k_y\hat{\sigma}_x - k_x\hat{\sigma}_y) \otimes \hat{P}_{\text{sgn}(\Delta_2-\Delta_1)}$ where $\hat{P}_\sigma = [\hat{\tau}_z - \sigma\hat{\mathbb{1}}]/2$ is a projection operator on the chiral $|\sigma\rangle = |\pm\rangle$-states.

II. Surface states in an electric field

a. Lorentz boost

We assume a z-dependent chemical potential $\mu(z) = \frac{1}{2}(\mu_2 - \mu_1)f(z/\ell)$ in Eq. (1) which has the same profile $f(z/\ell)$ than the gap $\Delta(z)$ with $f(\pm\infty) = \pm 1$. Performing a Lorentz boost [10, 11] on Eq. (1) with $\mu(z)$, one finds $|\tilde{\Psi}\rangle = \mathcal{N}e^{-\eta\hat{\mathbb{1}}\otimes\hat{\tau}_z/2}|\Psi\rangle$ in the new frame of reference. The Schrödinger equation then becomes $\hat{H}'_c|\tilde{\Psi}\rangle = \varepsilon|\tilde{\Psi}\rangle$ for $\tanh(\eta) \equiv \beta = -(\mu_2 - \mu_1)/(\Delta_2 - \Delta_1) \in [-1, 1]$, with

$$\hat{H}'_c = -\frac{1}{2}(\mu_2 - \mu_1)\delta\hat{\mathbb{1}} + \hat{H}_c(v'_F, \xi', \delta', \ell) \tag{25}$$

and $\hat{H}_c$ defined in Eq. (1) with $v'_F = \sqrt{1-\beta^2}v_F$, $\xi' = \xi/\sqrt{1-\beta^2}$ and

$$\delta' = \frac{1}{1-\beta^2}\left[\delta + \frac{\varepsilon(\mu_2 - \mu_1)/2}{(v_F/\xi)^2}\right]. \tag{26}$$

The surface states spectrum with and without a chemical potential drop are thus related by renormalized v_F, ξ and δ, and by a shift in the spectrum of $\mu_S = -\frac{1}{2}(\mu_2 - \mu_1)\delta$. This shift is used in ARPES measurements [12, 13] for estimating the electrostatic band bending within the hypothesis $\delta = 1$.

b. Case of a linearized potential

Much intuition can be also gained by considering a linearized interface $\ell \gg \xi$ (*i.e.* a uniform electric field) corresponding to a spectrum

$$\varepsilon_{n,\pm} = -\frac{1}{2}(\mu_2 - \mu_1)\delta \pm v'_F\sqrt{k_\parallel^2 + 2(1-\beta^2)^{1/2}n/\ell_S^2}, \tag{27}$$

where $\ell_S = \sqrt{\ell\xi}$ is independent of δ [10]. We recover the flattening of surface states band dispersion with $v'_F = \sqrt{1-\beta^2}v_F$ [7, 14–16], the reduction of the band gap of the MSS with $(v_F/\ell_n)' = (1-\beta^2)^{3/4}v_F/\ell_n$ [10, 17–19] and, moreover we identify the surface chemical-potential as $\mu_S = -\frac{1}{2}(\mu_2 - \mu_1)\delta$, which corresponds to the value of $\mu_S = \mu(z_0)$ at the position z_0 where gap vanishes, $\Delta(z_0) = 0$. This surface chemical potential μ_S naturally depends on the gap asymmetry ($\delta \neq 0$) : the surface states are restricted within the smallest band gap on each side of the THJ, corresponding to a chemical potential drop smaller than the critical voltage $|\mu_2 - \mu_1| < eV_c$.

Note that the chemical doping of the pn-junction is μ_c. In the case $|\Delta_1| < |\Delta_2|$, with the convention of opposite chemical potentials in each bulk semiconductor, its value depends on $\mu_2 - \mu_1$: (*i*) for $\mu_2 - \mu_1 < -(\Delta_2 + \Delta_1)$, $\mu_{c,1} = \frac{1}{2}(\Delta_2 + \Delta_1)$, (*ii*) for $-(\Delta_2 + \Delta_1) < \mu_2 - \mu_1 < \Delta_2 + \Delta_1$, $\mu_{c,2} = -\frac{1}{2}(\mu_2 - \mu_1)$ and, (*iii*) for $\mu_2 - \mu_1 > \Delta_2 + \Delta_1$, $\mu_{c,3} = -\frac{1}{2}(\Delta_2 + \Delta_1)$. The surface doping is $\mu_{c,s} = \mu_c - \mu_S$ and with our model $|\mu_{c,s}| < |\delta\Delta_1|$.

III. Stability of the chiral surface state

The gapless surface state ($n = 0$) does not depend on $\Delta(z)$ nor on the interface width ℓ. The chiral eigensolutions $\Psi_+ = (\phi_{1,+}, \phi_{2,+}, 0, 0)$ and $\Psi_- = (0, 0, \phi_{1,-}, \phi_{2,-})$ to the Hamiltonian (1) correspond to the $n = 0$ surface state, with a spectrum $\varepsilon_\pm = \pm v_F|\mathbf{k}_\parallel|$. Within the Aharonov-Casher argument [20, 21], only Ψ_+ or Ψ_- is a bounded solution, as demonstrated in Refs. [14, 22, 23]. Indeed, the component $\phi_{i,s}$ ($i =\uparrow\downarrow$; $s = \pm$) is a solution of

$$[v_F\partial_z + s\Delta(z)]\,\phi_{i,s} = 0, \tag{28}$$

for which the long-range behavior is (i) $\phi_{i,s} \sim e^{-s\lambda_1 z}$ with $\lambda_1 = \Delta_1/v_F$ for $z < 0$ and (ii) $\phi_{i,s} \sim e^{-s\lambda_2 z}$ with $\lambda_2 = \Delta_2/v_F$ for $z > 0$. In the case of an infinite-sized sample, these solutions decay only if $s\lambda_2 > 0 > s\lambda_1$ which corresponds to $s = \mathrm{sgn}(\Delta_2 - \Delta_1)$ and $\Delta_1\Delta_2 < 0$. Thus, the $n = 0$ mode exists as soon as there is band inversion and its chirality is given by $\mathrm{sgn}(\Delta_2 - \Delta_1)$.

IV. Interpretation of ARPES data in terms of a topological heterojunction

For Bi_2Se_3, one finds $v_F = 2.3$ eV Å [24] to $v_F = 3 \ldots 5$ eV Å [25] and $2\Delta = 350$ meV [26], and thus $\xi \approx v_F/\Delta = 6.5 \ldots 23$ Å. In an oxidizing atmosphere, an oxide layer forms and we estimate the size of the interface as its depth $\ell \approx 1 \ldots 2$ nm [27]. We thus expect $N \approx \ell/\xi = 1 \ldots 3$ MSS, as observed in [12, 13]. Moreover, we thus find $\ell_S = \sqrt{\ell\xi} \approx 8 \ldots 20$Å and thus an order of magnitude for the MSS band gaps $\Delta_{MSS} \approx v_F/\ell_S = 100 \ldots 600$ meV which is in reasonable agreement with the results found in [12, 13].

From [12], we can extract the following band gaps: (i) $\Delta_{+,n=1} \approx 330$ meV and $\Delta_{+,n=2} \approx 450$ meV for the electron-like MSS and (ii) $\Delta_{-,n=1} \approx -330$ meV and $\Delta_{-,n=2} \approx -400$ meV for the hole-like MSS. The ratios of the $n = 1$ and $n = 2$ MSS band gaps from the Dirac point are expected to be $\sqrt{2} \approx 1.4$, within the linear-gap approximation, and here we find $\Delta_{+,2}/\Delta_{+,1} \approx 1.36$ and $\Delta_{-,2}/\Delta_{-,1} \approx 1.2$. We read these bands gaps from the extremal surface potential in [12] which we identify as $V_s = \pm 200$ meV by setting $V_s = 0$ as the potential were the MSS are the furthest to the Dirac point. In our theory we expect the *same* band gaps for the electron-like and the hole-like MSS for opposite band bending since all quantities depend on $\beta^2 \sim V_s^2$. The fact that the experimentally observed gaps are roughly the same is a strong indication of the topological origin of the surface states, in agreement with our theoretical model, and indicates the absence of relevant band bending.

The breakdown voltage for a THJ involving Bi_2Se_3 is $eV_c > 2\Delta = 350$meV. We thus expect that $\beta = V/V_c$ introduced in the main text is $\beta < \beta_{max} = V_s/V_c = 0.56$. Thus, the renormalisation in [12] of the Fermi velocity is at most $v_F'/v_F = \sqrt{1-\beta^2} = 0.82$ and that of the band gap is at most $\Delta'/\Delta = (1-\beta^2)^{3/4} = 0.75$. It is hard to tell from figures in [12, 13] if these quantities are indeed renormalized within the reading precision.

These points show that a quantitative analysis of the ARPES measurements on oxidized Bi_2Se_3 may provide insights in the band inversion surface states and help identify the breakdown voltage.

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