Supplemental Material for "Spin-Orbit Coupling Determined Topological Phase: Topological Insulator and Quadratic Dirac Semimetals"

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A. Surface Band Structure for the Triple Degeneracy

To illustrate the topology of triple degenerate point in Y_3XC (X=Ga, Tl), we plot the surface spectrum on (001) surface. Obviously, there exists surfaces states starting from the triple degenerate point (see in Fig. S1).

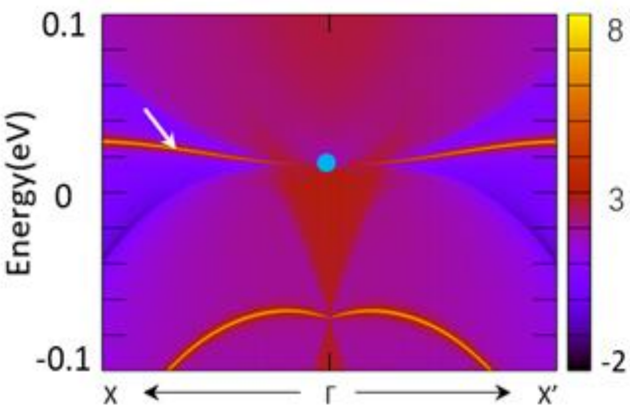

Fig.S1 Surface spectrum for the triple degenerate in Y_3GaC on (001) surface. The white arrow points to the surface states, cyan dot marks the triple degenerate point.

B. Topological Phase Transition Induced by a Zeeman Field

In this SM, we use the model to study topological phase transition under a Zeenman field. We have mentioned that the effective model we have derived Eq. (2) is based on states of $j = 3/2$, then the Zeeman field can be written in the form of

$$\mathcal{H}_{\mathrm{Z}} = -\boldsymbol{B} \cdot \boldsymbol{J},$$

with $\mathbf{J}$ as the vector of the $\mathrm{J} = 3/2$ spin matrices.

Under a Zeeman field, the time reversal symmetry is broken, the quadratic Dirac point is expected to be transformed into pairs of Weyl points. To demonstrate it, we apply a Zeeman field along high symmetric path, namely, [100] direction.

In this case, $\mathcal{H}_{\mathrm{Z}} = -MJ_x$, the total Hamiltonian takes the form of $\mathcal{H} = \mathcal{H}_{\mathrm{soc}} + \mathcal{H}_Z$. We first search band crossings along k_x axis, then two pairs (W1, W2) of Weyl points are expected to appear. For concreteness, the eigenenergies for $\mathcal{H}$ along $\mathrm{k_x}$ are given by

$$E_{1,2} = -\alpha k_x^2 \pm \frac{B}{2}, \qquad E_{3,4} = \alpha k_x^2 \pm \frac{3B}{2}.$$

Accordingly, if $\alpha > 0$, $E_{1,2}$ will cross with E_4 at $K_1 = \left(\pm\sqrt{\frac{\mathrm{B}}{\alpha}}, 0{,}0\right), K_2 = \left(\pm\sqrt{\frac{\mathrm{B}}{2\alpha}}, 0{,}0\right)$, respectively. Taking suitable parameters, we present the energy spectrum under a Zeeman field around the quadratic Dirac point in Fig.S1.

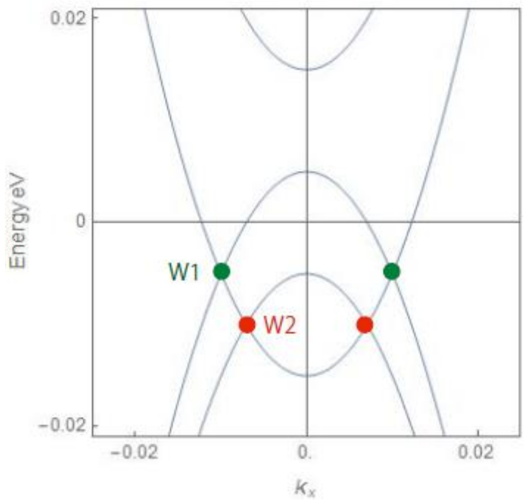

Fig.S2 Band structure under a Zeeman field along [100] direction. In the calculation, we take $\mathrm{M} = 0, \mathrm{B} = 10\ \mathrm{meV}, \alpha = 10\ \mathrm{eV \cdot Å}, \gamma = 17\ \mathrm{eV \cdot Å}$.

Effective Hamiltonian for Weyl Points

For the first pair of Weyl points which locate at $K_1 = \left(\pm\sqrt{\frac{B}{\alpha}}, 0,0\right)$, one can derive the degenerate eigenstates at these two points, specifically,

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(-1,0,0,1)^T,\ \ |\psi_2\rangle = \frac{1}{\sqrt{2}}(0,-1,1,0)^T.$$

Then the effective Hamiltonian around K_1 is given by

$$\mathcal{H}_1 = \begin{pmatrix} \langle\psi_1|\mathcal{H}_{soc}|\psi_1\rangle & \langle\psi_1|\mathcal{H}_{soc}|\psi_2\rangle \\ \langle\psi_2|\mathcal{H}_{soc}|\psi_1\rangle & \langle\psi_2|\mathcal{H}_{soc}|\psi_2\rangle \end{pmatrix}.$$

Then we expand the model at K_1, after a unitary transformation, we have the Hamiltonian takes the form as

$$\mathcal{H}_1(\boldsymbol{q}) = v_x q_x \sigma_z + [(\gamma_+ q_-^2 + \gamma_- q_+^2)\sigma_+ + h.c.],$$

with $\gamma_\pm = \frac{1}{8}\left(\sqrt{3}\alpha \pm \gamma\right), q_\pm = q_y \pm i q_z, \sigma_\pm = \sigma_x \pm i\sigma_y$. The chirality of the Weyl point is determined by $\mathrm{sgn}\ \ (|\gamma_+| - |\gamma_-|) = \pm 2$.

The effective Hamiltonian expanded from K_2=$\left(\pm\sqrt{\frac{B}{2\alpha}}, 0,0\right)$ can be derived in the same way. Here, the degenerate states take the form of

$$\psi_3 = \frac{1}{2\sqrt{2}}\left(-2,-\sqrt{3},0,1\right)^T, \qquad \psi_4 = \frac{1}{2\sqrt{2}}\left(0,1,2,\sqrt{3}\right)^T.$$

Such that the effective Hamiltonian for the band crossing around K_2 is given by

$$\mathcal{H}_2 = \begin{pmatrix} \langle\psi_3|\mathcal{H}_{soc}|\psi_3\rangle & \langle\psi_3|\mathcal{H}_{soc}|\psi_4\rangle \\ \langle\psi_4|\mathcal{H}_{soc}|\psi_3\rangle & \langle\psi_4|\mathcal{H}_{soc}|\psi_4\rangle \end{pmatrix}.$$

To derive the main feature at K_2, we also expand it at this point, thus

$$\mathcal{H}_2(\boldsymbol{q}) = v_x q_x \sigma_z + v_y q_y \sigma_y - v_z q_z \sigma_x.$$

Here, $v_y = v_z = \gamma\sqrt{\frac{M}{\alpha}}$, $v_x = 2\sqrt{M\alpha}$. This model is a typical single Weyl point.