

Supporting Information for

Strong anisotropy nodal lines in TiBe family

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I. BAND STRUCTURE OF OTHER TIBE FAMILY MATERIALS

We calculate the band structures of other TiBe family materials and present in Fig.S1, similar nodal lines semimetal character can be found for all these compounds around Fermi level.

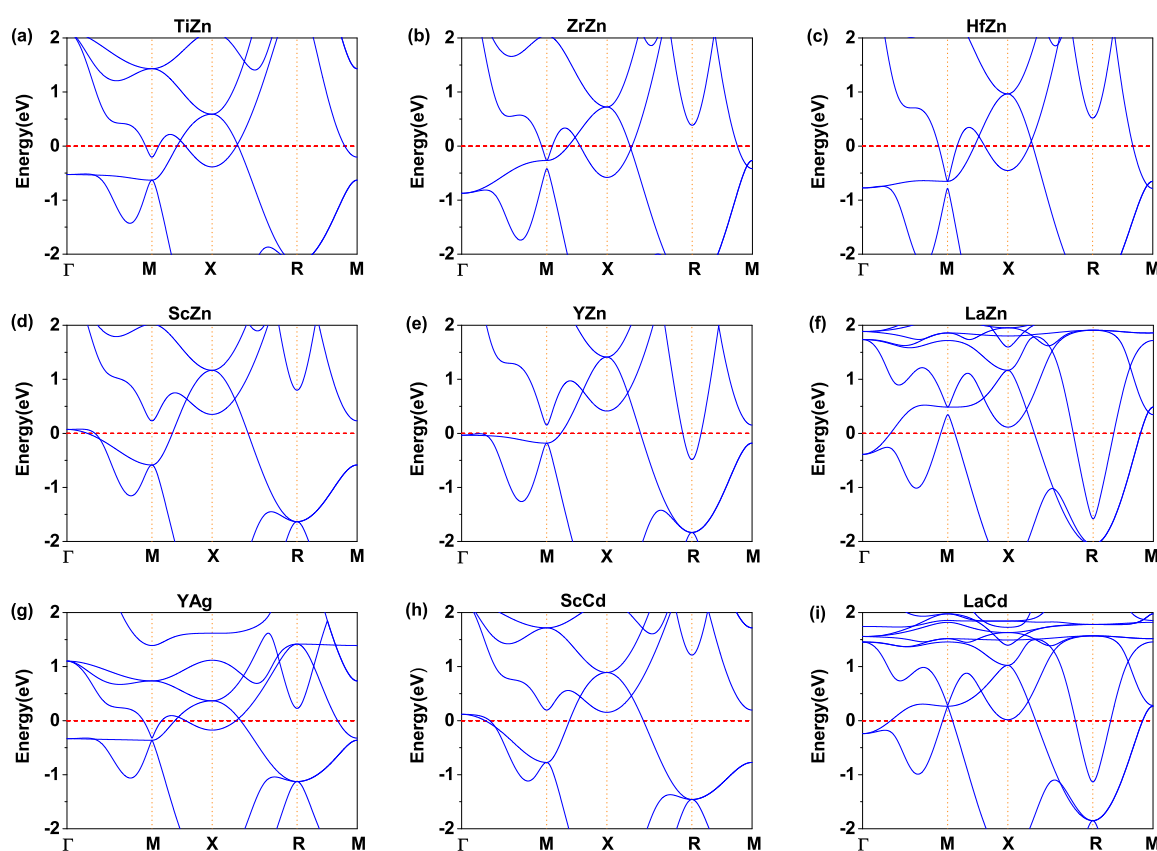


Figure S1: (color online)(a) Band structures of other materials of TiBe family (a) TiZn, (b) ZrZn, (c) HfZn, (d) ScZn, (e) YZn, (f) LaZn (g) YAg, (h) ScCd, (i) LaCd. Similar bands features as TiBe can be observed around Fermi level.

II. TIBE'S BAND STRUCTURE WITH HSE06 FUNCTION

The 3D bands in the planes of (a) $k_z = 0.95 \pi/a$ and (b) $k_z = 1.05 \pi/a$ (a is the value of crystal constant) are plotted in Fig.S2. We found the band gap has been opened between the two bands around Fermi level in these two planes.

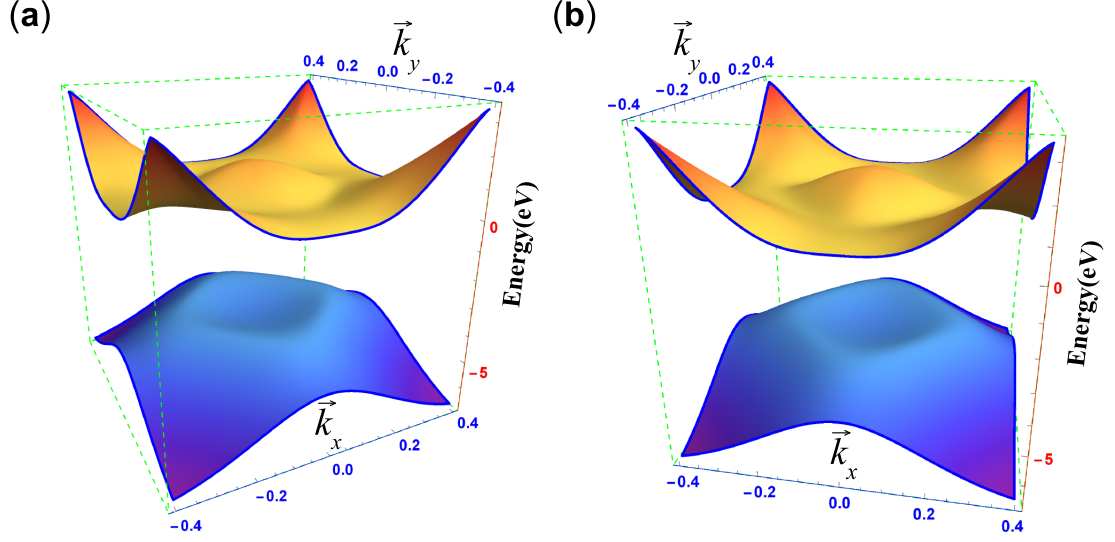


Figure S2: (color online) 3D bands in the planes of (a) $k_z = 0.95 \pi/a$ and (b) $k_z = 1.05 \pi/a$.

III. 3D ENERGY BAND DISPERSION OF LOW-ENERGY K·P MODEL

3D energy bands of the low-energy k·p model is shown in Fig.S3, the nodal line is formed with the crossing line of the orange surface $E_1(\mathbf{k})$ and blue surface $E_2(\mathbf{k})$.

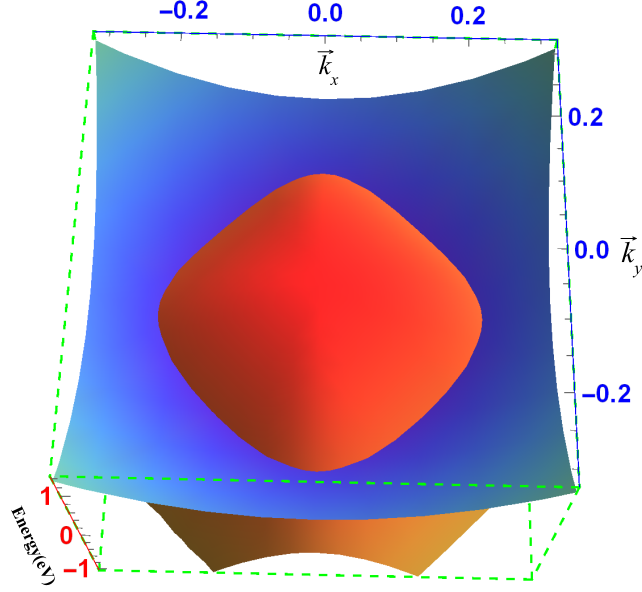


Figure S3: (color online) 3D energy bands of the low-energy k·p model as a function of k_x and k_y .

IV. TIBe'S BAND STRUCTURE WITH HSE06 FUNCTION

We plot the TiBe's band structure with HSE06 hybrid function in Fig.S4. We found no obvious changes have been happened comparing the results of PBE.

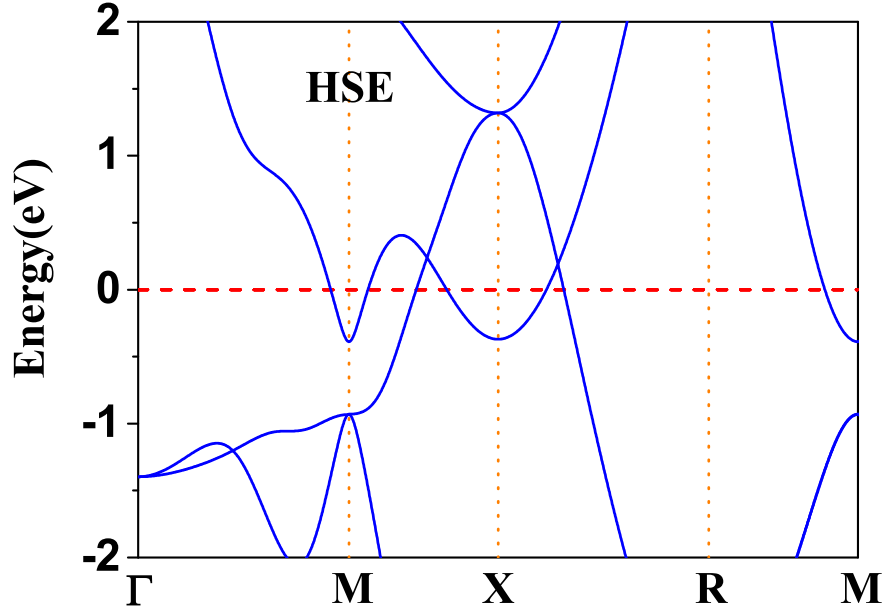


Figure S4: (color online)(a)TiBe's band structure with the help of HSE06 hybrid function.

V. TIBE BAND STRUCTURE WITH SPIN-ORBITAL COUPLING(SOC)

Band structure of TiBe with SOC as show in Fig.S5(a)-(c). (b) and (c) denote the enlarged band structure around green and red circles in (a), the energy gap only 21.6 meV and 13.2 meV for C_1 and C_2 in main manuscript, respectively. We also plot the energy difference distribution for the two bands around Fermi level in Fig.S5(d). We found no energy band crossing point exist around X points when considering SOC.

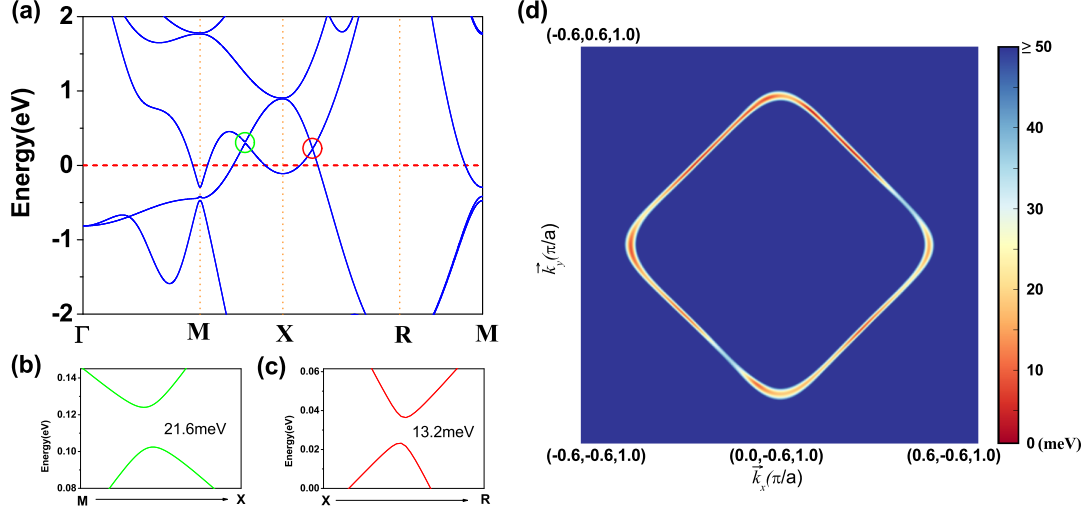


Figure S5: color online)(a) Band structure of TiBe along high symmetry lines with SOC. (b) and (c) denote the enlarged band structure surround by green and red circles in (a). (d) The energy difference distribution for the two bands around Fermi level in the plane of $k_z = \pi/a$.

Table S1: Parity product of occupied states at the TRIM points. The Z_2 indices are (1;111).

TRIM point	R	Γ	$M (\times 3)$	$X (\times 3)$
Parity product	+	-	-	-

VI. TABLE OF THE PARITIES PRODUCT FOR TIME-REVERSAL INVARIANT POINTS.

The parities product of the occupied states at eight time-reversal invariant momenta (TRIM) point are shown in Tab.S1. According to topological index calculations of inversion symmetry materials, The Z_2 indices are (1;111), the first index is 1 and it indicates TiBe is a strong three dimensional topological insulator if disregard the metallization around M points¹.

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¹ L. Fu and C. L. Kane, Phys. Rev. B **76**, 045302 (2007).