Supplementary Material: Flat Band and Z_2 Topology of Kagome Metal $CsTi_3Bi_5$

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1 Materials and Methods

1.1 Sample growth and characterization

$CsTi_3Bi_5$ single crystals were synthesized by the self-flux method. The mixture with a mole ratio of Cs : Ti : Bi = 1 : 1 : 10 was loaded into an alumina crucible and then sealed in a quartz tube. The tube was heated to 1273 K for 12 hours and kept for 12 hours. Then it was slowly cooled down to 873 K in 150 hours. After that, the tube was taken into a centrifuge to separate the single crystal from the excess flux. Hexagonal $CsTi_3Bi_5$ single crystals with a typical size of 1-3 mm were obtained.

1.2 Transport, heat capacity, and magnetic measurements

Due to its air sensitivity, the measurements on $CsTi_3Bi_5$ were carried out in air-free conditions. The X-ray diffraction (XRD) pattern in Fig. 1(c) was collected by Rigaku Smartlab-9 kW diffractometer with Cu Kα radiation at room temperature. The crystallographic parameters were determined by the single-crystal XRD device (Bruker) collected at 100 K using graphite-monochromatic Mo Kα radiation (λ = 0.71073 A). Magnetization measurements were performed by Magnetic Property Measurement System (MPMS3, Quantum Design). Heat capacity and resistivity measurements were performed by Physical Property Measurement System (PPMS, Quantum Design). A standard four-probe method with a probe current of 1 mA was applied for resistivity measurement.

1.3 ARPES measurement

ARPES measurements were performed at the BL03U beamline of the Shanghai Synchrotron Radiation Facility (SSRF) and beamline 13U of the National Synchrotron Radiation Laboratory (NSRL). The energy resolution was set at 15 meV for Fermi surface mapping and 7.5 meV for band structure measurements. The angular resolution was set at 0.1°. Samples were cleaved *in situ* under ultra-high vacuum conditions with pressure better than 5×10^{-11} mbar and temperatures below 20 K.

1.4 First-principles calculations

The first-principles calculations were performed based on the density functional theory (DFT) using the projector augmented wave (PAW) method[1,2] implemented in the Vienna ab initio simulation package (VASP)[3,4] to obtain the electronic structures. The generalized gradient approximation (GGA) with the exchange-correlation functional of Perdew, Burke and Ernzerhof (PBE) for the exchange-correlation functional[5] was adopted. The kinetic energy cutoff was set to 550 eV for the plane wave bases. The BZ was sampled by Γ-centered Monkhorst-Pack method[6] with a 12 × 12 × 6 k-mesh for the 3D periodic boundary conditions in the self-consistent process. The maximally localized Wannier functions (MLWFs) were extracted from the DFT calculations via the Wannier90 package[7]. Surface Green's function calculations were calculated using the Sancho 1985 algorithm[8] as implemented in the WannierTools package[9]. The irreducible representations were obtained by using the IRVSP program[10].

2. High pressure resistivity

Fig. S1(a) depicts electric transport measurements under different pressures (p) from 1.3 GPa

to 46.9 GPa. When p < 3.2 GPa, $CsTi_3Bi_5$ keeps the normal metallic behavior down to 1.6 K. When p = 3.2 GPa, the resistivity curves have an abrupt drop at low temperature, implying a possible pressure-induced superconductivity. By taking the temperature whose resistance is 90% of normal metallic state value as the superconducting onset temperature T_c, we find that T_c is about 3.6 K under the pressure p = 3.2 GPa, and reaches a maximum of 5.6 K when p = 5.5 GPa. With further increasing pressure, T_c decreases slowly, until the drop of the resistivity is almost undetectable when p > 29.4 GPa. Fig. S1(b) is the low-temperature resistivity under different external magnetic fields at pressure p = 23.3 GPa. With an increasing magnetic field, the drops of resistance are gradually suppressed, consistent with the evolution of superconductivity under a magnetic field. However, the non-zero resistivity state and weak drop of the resistance reflect the small inclusion of a superconducting impurity phase, implying that the signal of the superconductivity is likely caused by the Bi impurities.

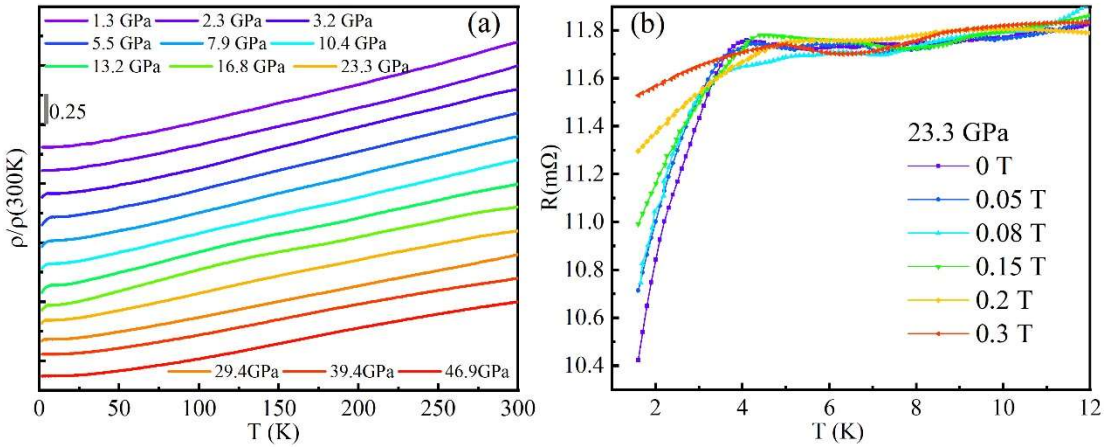

Fig. S1. Resistivity variation with pressure in $CsTi_3Bi_5$. (a) Normalized resistivity ρ/ρ(300 K) under various pressures with temperature ranging from 1.6 K to 300 K. (c) Resistance of 23.3 GPa under different magnetic fields.

3 ARPES and DFT results

To further investigate its detailed electronic structure, the band structures along the high-symmetry direction by combining ARPES measurements and DFT calculated results are demonstrated in Figure S2. Both ARPES spectra along $\Gamma - K - M$ $(\Gamma - M)$ and $A - H - L$ $(A - L)$ paths show very similar features.

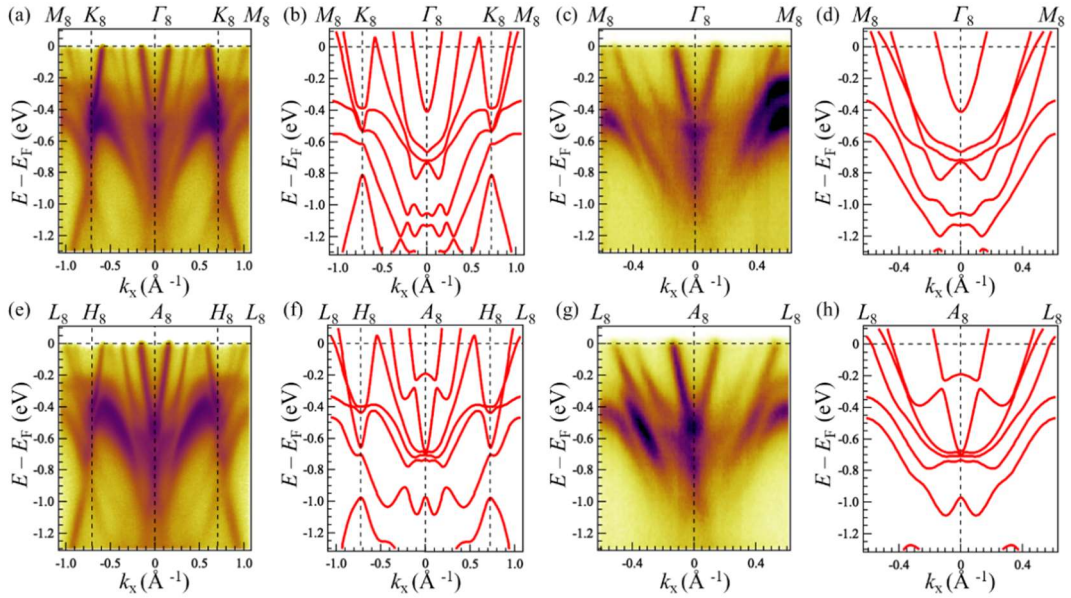

Fig. S2. Detailed band structure of $CsTi_3Bi_5$ at $k_z = 0$ and $k_z = \pi$ plane. (a) ARPES spectra taken along the $M - K - \Gamma - K - M$ direction. (b) DFT calculated band structure along the $M - K - \Gamma - K - M$ direction. (c-d) Same as (a-b) but along the $M - \Gamma - M$ direction. (e-f) Same as (a-b) but along the $L - H - A - H - L$ direction. (g-h) Same as (a-b) but along the $L - A - L$ direction. Note that the calculated E_F is shifted upward $0.1\ eV$ to match the experiment.

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