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Supplementary Materials for

Experimental evidence of hourglass fermion in the candidate nonsymmorphic topological insulator KHgSb

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This PDF file includes:

Crystal structure of KHgSb determined from powder XRD data

To determine the crystal structure of KHgSb, we have performed XRD measurements at room temperature on KHgSb powder obtained by grinding the single crystals (fig. S1). Because the KHgSb samples are very sensitive to air, we sank the powder in oil. The broad peak in the low-angle range comes from the oil.

The previous calculations [*22*, *24*] have investigated the topological nature of the double-layered structure with space group $P6_3/mmc$ (SG 194) and single-layered structure with space group $P\text{-}6m2$ (SG 187). We refine the powder XRD data to these two structures in fig. S1, A and B, respectively. Except for the peaks from the Sb flux, all the diffraction peaks are indexed with SG 194. In contrast, the peaks corresponding to the (*hkl*) reflections with l = odd in SG 194 cannot be indexed with SG 187. For instance, the peak at 23.1°, indicated by red arrow in fig. S1, is indexed with the (101) reflection in SG 194 while there is no corresponding reflection peak for SG 187. The refinements unambiguously exclude the single-layered structure.

In addition to SG 194 assumed in the theory paper [*22*], there are another two possible space groups $P6_3mc$ (SG 186) and $P\text{-}3m1$ (SG 164) when taking into account the occupation of atoms in one unit cell of a double-layered structure. As compared with SG 194, the crystal structures in SG 186 and SG 164 are distorted.

In SG 164, the HgSb layers alternately displace with an equal distance towards +z and –z directions. This causes two different intervals between the adjacent HgSb layers. One should observe the (00l) diffractions with l = odd in the single crystal XRD data on the (001) plane for SG 164. Since such diffractions are not observed in Fig. 1F, SG 164 can be excluded.

In SG 186, the HgSb layers are buckled, in which the Hg and Sb atoms displace towards +z and –z directions, respectively. The intensity ratios of the diffraction peaks are slightly different between SG 194 and SG 186. It is hard to distinguish between them based on the XRD data. The displacement of atoms in SG 186 causes very minor effects on the

electronic structure. It is crucial that the nonsymmorphic glide symmetry $\overline{M}_x$ is still preserved in SG 186, which protects the hourglass-shaped band dispersion. The calculated Wilson loop confirms that it belongs to the same nontrivial topology as in SG 194.

Based on the analysis of the XRD data, we determine that KHgSb has a nonsymmorphic double-layered structure with SG 194 or SG 186. Both of them preserve the nonsymmorphic glide symmetry $\overline{M}_x$, which defines the same nontrivial topology. For clarity, our discussion is limited to SG 194, which has been assumed in the theory paper [*22*]. Detailed calculations of the nontrivial topology and related electronic structure of SG 186 will be presented elsewhere.

The refined lattice parameters in SG 194 are $a = b = 4.7752(2)$ Å, $c = 10.2074(7)$ Å, $\alpha = \beta = 90°$, $\gamma = 120°$. The atomic positions of K, Hg, and Sb are (0, 0, 0), (1/3, 2/3, 3/4), and (1/3, 2/3, 1/4), respectively. They are very close to those reported previously [*29*] and used in our calculations (see Materials and Methods).

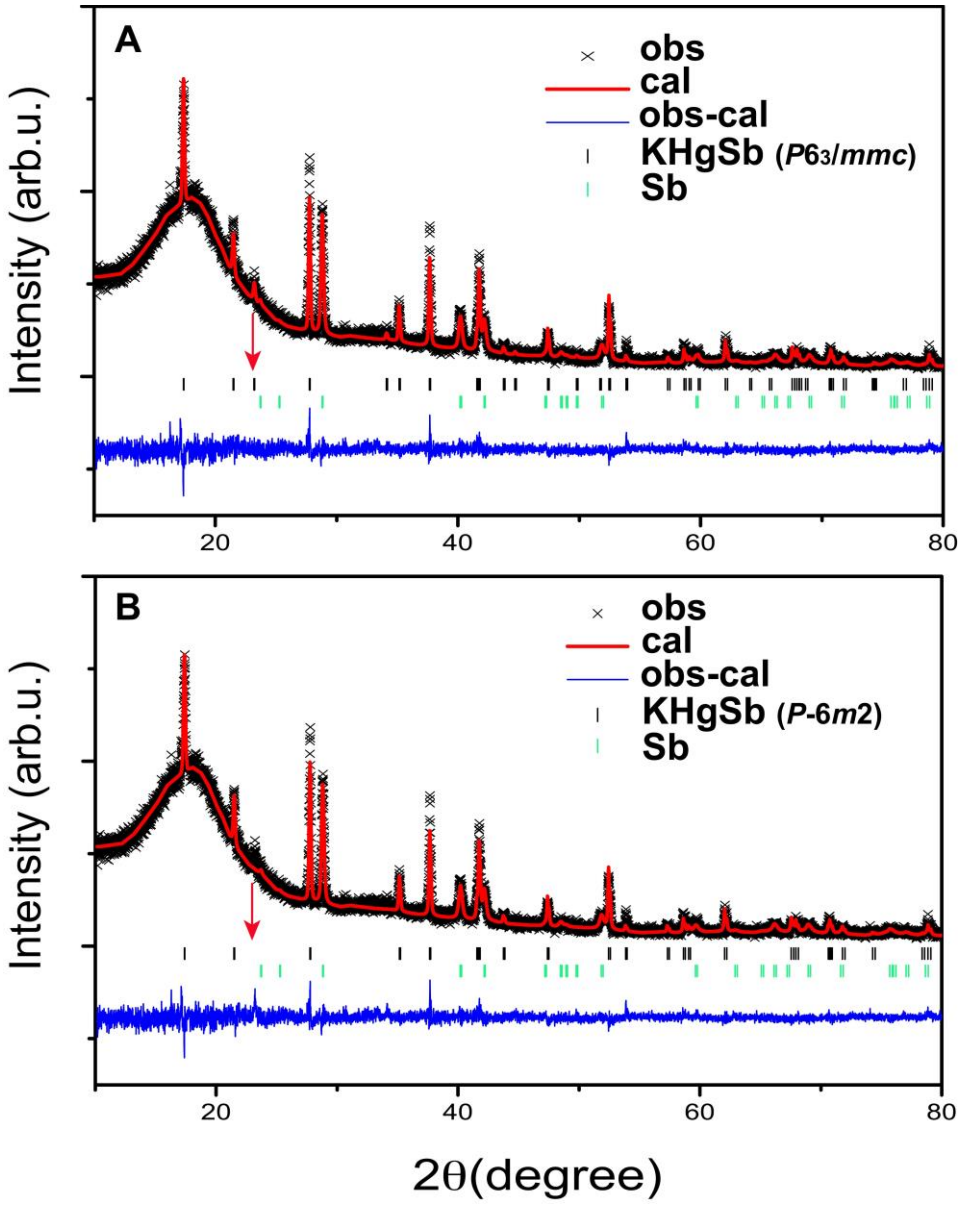

fig. S1. Refinements of powder XRD data of KHgSb. (**A**) Refinement to the double-layered structure (*P*6$_3$/*mmc* #194). (**B**) Refinement to the single-layered structure (*P*-6*m*2 #187). The observed (obs) and calculated (cal) patterns and the difference between them (obs-cal) are plotted. The vertical bars show the Bragg peak positions. The red arrow indicates the peak at 23.1°, which is indexed with the (101) reflection in *P*6$_3$/*mmc* while there is no corresponding reflection peak for *P*-6*m*2.

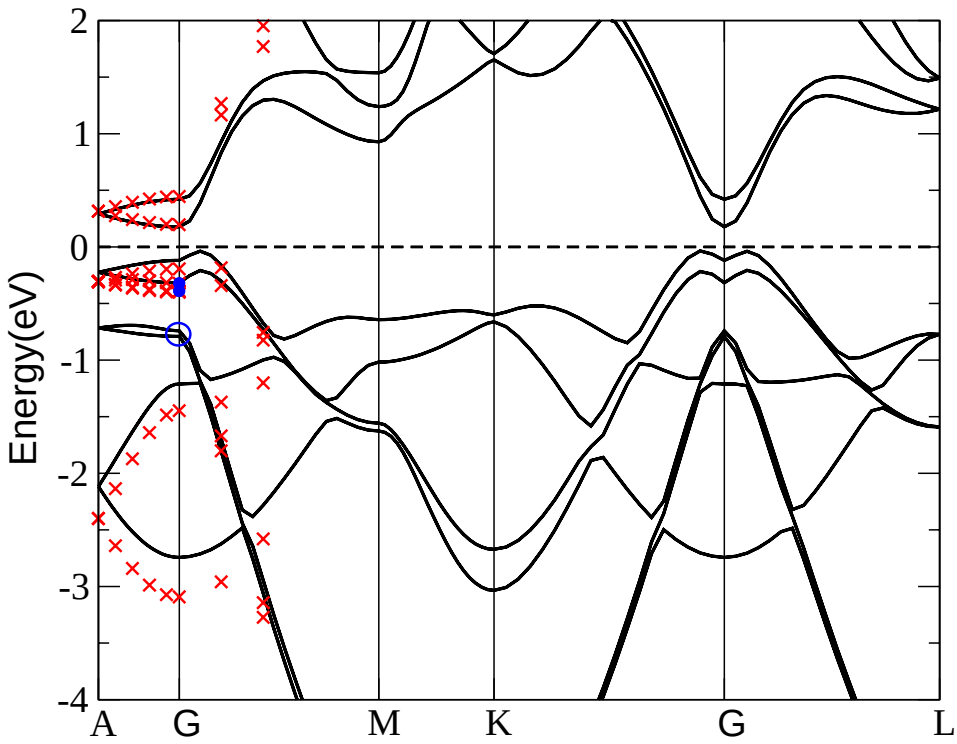

fig. S2. Band inversion confirmed by HSE06. The GGA band structure shows the inverted Hg *s* orbital is about 0.75 eV below E_F, as indicated by a blue circle. Considering the underestimation of the band gap by GGA calculations, we further confirm the band inversion by the calculations using hybrid functional HSE06 [*30*], indicated by red crossings. The HSE06 data show that the Hg *s* orbital (blue dots) is a little higher than in the GGA data but still below the band gap.