Minimum band gaps of Bi$_2$Te$_3$ and Sb$_2$Te$_3$

The band structures of the four materials in the Bi$_2$Se$_3$ family discussed in the main text are shown in Fig. 1. The band structures have been calculated using VASP [1–4] with the same numerical parameters as those reported in the main text, and including the effects of spin-orbit coupling. Bi$_2$Te$_3$, Bi$_2$Se$_3$, and Sb$_2$Te$_3$ are topological insulators, with the band inversion at the Γ point. Sb$_2$Se$_3$ is a normal insulator at zero pressure.

The minimum gaps of Bi$_2$Se$_3$ and Sb$_2$Se$_3$ occur at the Γ point, but the minimum gaps of Bi$_2$Te$_3$ and Sb$_2$Te$_3$ occur elsewhere in the Brillouin zone. In Bi$_2$Te$_3$, the valence band maximum (VBM) and conduction band minimum (CBM) are located along the high symmetry line from T at \( q = (0.5, 0.5, 0.5) \) to FB at \( q = (0.0, 0.5, 0.5) \). In Sb$_2$Te$_3$, the VBM is located along the high symmetry line from T to FB, and the CBM along the high symmetry line from Γ to T.

In Fig. 2 we show the temperature dependences of the band gaps at the zone center where band inversion occurs, and at the minimum gaps described above, for both Bi$_2$Te$_3$ and Sb$_2$Te$_3$. The results include both thermal expansion and electron-phonon coupling, and have been calculated with the same numerical parameters as described in the main text. In both materials, the temperature dependence of the minimum gaps is weaker than the temperature dependence of the direct gaps. Both thermal expansion and electron-phonon coupling lead to smaller changes in the band gap in absolute terms, but furthermore, in Sb$_2$Te$_3$ thermal expansion acts to enlarge the minimum gap.

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FIG. 1: Static lattice band structures of the Bi$_2$Se$_3$ family of materials calculated within the static lattice approximation, and including spin-orbit coupling.
FIG. 2: Temperature dependence of the Γ-point and minimum band gaps of the Bi$_2$Te$_3$ and Sb$_2$Te$_3$ compounds. Both electron-phonon and thermal expansion contributions have been included.

whereas electron-phonon coupling acts to reduce the minimum gap. These competing effects contribute to the weaker temperature dependence in this material. Overall, the minimum band gaps are enlarged with increasing temperature, and the Γ-point gaps are reduced with increasing temperature.