Supplemental Material for "Temperature effects in the band structure of topological insulators"

Bartomeu Monserrat[1,2,*] and David Vanderbilt[1]

[1] *Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-8019, USA*
[2] *TCM Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom*

(Dated: September 22, 2016)

Minimum band gaps of Bi_2Te_3 and Sb_2Te_3

The band structures of the four materials in the Bi_2Se_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_3Te_3, Bi_2Se_3, and Sb_2Te_3 are topological insulators, with the band inversion at the Γ point. Sb_2Se_3 is a normal insulator at zero pressure.

The minimum gaps of Bi_2Se_3 and Sb_2Se_3 occur at the Γ point, but the minimum gaps of Bi_2Te_3 and Sb_2Te_3 occur elsewhere in the Brillouin zone. In Bi_2Te_3, the valence band maximum (VBM) and conduction band minimum (CBM) are located along the high symmetry line from T at $\mathbf{q} = (0.5, 0.5, 0.5)$ to FB at $\mathbf{q} = (0.0, 0.5, 0.5)$. In Sb_2Te_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_2Te_3 and Sb_2Te_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_2Te_3 thermal expansion acts to enlarge the minimum gap

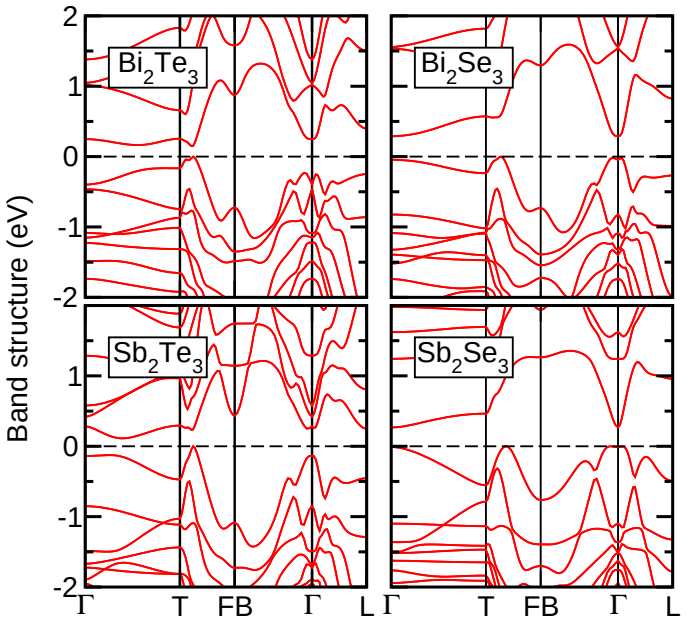

FIG. 1: Static lattice band structures of the Bi_2Se_3 family of materials calculated within the static lattice approximation, and including spin-orbit coupling.

*Electronic address: monserrat@physics.rutgers.edu

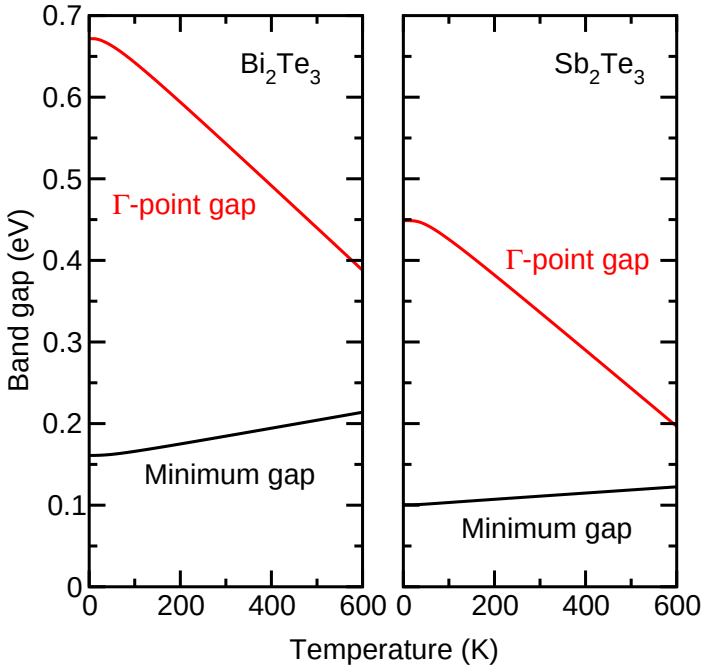

FIG. 2: Temperature dependence of the Γ-point and minimum band gaps of the Bi_2Te_3 and Sb_2Te_3 compounds. Both electron-phonon and thermal expansion contributions have been included.

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.

[1] G. Kresse and J. Hafner, Phys. Rev. B **47**, 558 (1993).
[2] G. Kresse and J. Hafner, Phys. Rev. B **49**, 14251 (1994).
[3] G. Kresse and J. Furthmüller, Comput. Mater. Sci. **6**, 15 (1996).
[4] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).