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SUPPLEMENTARY INFORMATION

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[Supplementary Information] **A large-gap topological insulator matrix with a single surface Dirac cone**

Y. Xia, D. Qian, D. Hsieh, L. Wray, A. Pal, H. Lin, A. Bansil, D. Grauer, Y. S. Hor, R. J. Cava and M. Z. Hasan

Topic: Confirming the calculated valence and surface band structure by comparison with experimental ARPES data over a wider energy range

The calculated valence band dispersion is in good correspondence while making a comparison with the experimental data taken in both the $\overline{\Gamma} - \overline{M}$ and $\overline{\Gamma} - \overline{K}$ directions (Fig. S1). The first and twelfth quintuple blocks are taken as the surfaces of the slab. The fraction of electron charge residing in the atomic spheres of these two surface blocks are presented by the color of the bands. Bright lines indicate bands located inside the bulk sample. These bands should overlap with a bulk energy band at a particular k_z value, after projected onto the 2D surface BZ. The calculation agrees with data after shifting the E_F of the calculated result to 200 meV above the bottom of the lowest conduction band. Doping the semiconductor matrix with electrons allows one to study the connectivity of the surface and bulk states at all energies between the valence and conduction bands, thereby determining the unique and specific class of topological order of the parent materials [7].

In the measured spectra, the strongest quasiparticle signals are typically observed near normal electron emission, at around 1.5-2.0 eV. This band corresponds to a pure surface band lying outside the bulk projection of states. Strong quasiparticle signals near

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$\overline{\Gamma}$ are of surface origin, based on their direct correspondence with the band calculation. Our energy dependent study of the bands suggests insignificant k_z dependence of these states, confirming the 2D (surface) nature of the bands.

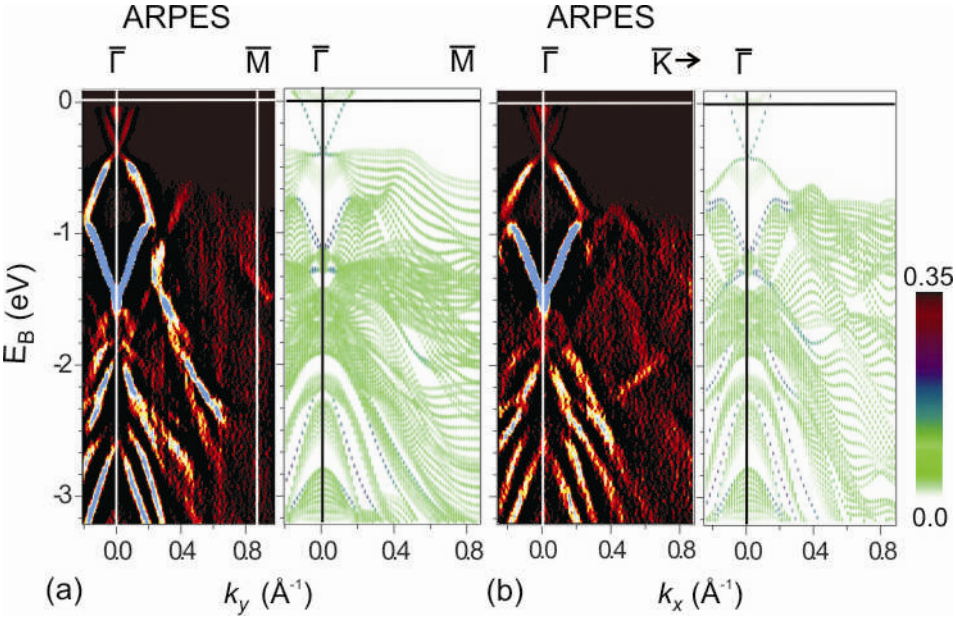

Fig S1: Experimental band dispersions are compared with theoretical calculations. The band second-derivative images and first-principles calculation results along $\overline{\Gamma} - \overline{M}$ (**a**) and $\overline{\Gamma} - \overline{K}$ directions (**b**) are presented. The color of the calculated bands represents the fraction of electronic charge residing in the surface layers. A rigid shift of E_F is included to match the lowest energy excitations in the ARPES data with calculations, a consequence of the system being somewhat electron-doped. The strongest signals are observed from the surface states.

We would like to note that the calculated bandwidth is smaller than the measured values. A better agreement requires a renormalization of the theoretical results by a self-energy $\Sigma(\vec{k},E) = \Sigma'(\vec{k},E) + i\Sigma''(\vec{k},E)$. A similar adjustment of *ab initio* results to match

experimental band data was used for graphite. It is believed that the underestimation of quasiparticle bandwidths by LDA is due to its failure to account for many body effects in describing the excited final states. Approximating $\Sigma'(\vec{k}, E)$ by a linear function stretches the band dispersion [31]. For Bi_2Se_3, an approximately 30% stretch is required to match the lowest energy excitations to theory.

[31] Heske, C. *et al*. Band widening in graphite. *Phys. Rev. B* **59**, 4680 (1999).