Supplementary Information for

Topologization of β-antimonene on Bi$_2$Se$_3$ via proximity effects

K. Holtgrewe[1], S. K. Mahatha[2,3 ✉], P. M. Sheverdyaeva[2], P. Moras[2], R. Flammini[4], S. Colonna[4], F. Ronci[4], M. Papagno[5], A. Barla[2], L. Petaccia[6], Z. S. Aliev[7], M. B. Babanly[8], E. V. Chulkov[9,10, 11,12], S. Sanna[1], C. Hogan[4] and C. Carbone[2]

[1]Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

[2]Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, 34149 Trieste, Italy

[3]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, D-22607 Hamburg, Germany

[4]Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Via del Fosso del Cavaliere 100, 00133 Roma, Italy

[5]Dipartimento di Fisica, Università della Calabria, Via P. Bucci, 87036 Arcavacata di Rende (CS), Italy

[6]Elettra Sincrotrone Trieste, Strada Statale 14 km 163.5, 34149 Trieste, Italy

[7]Azerbaijan State Oil and Industry University, AZ1010 Baku, Azerbaijan

[8]Institute Catalysis and Inorganic Chemistry, Azerbaijan National Academy of Science, AZ1143 Baku, Azerbaijan

[9]Centro de Física de Materiales, CFM-MPC, Centro Mixto CSIC-UPV/EHU, Apdo. 1072, 20080 San Sebastián/Donostia, Basque Country, Spain

[10]Donostia International Physics Center (DIPC), P. de Manuel Lardizabal 4, 20018 San Sebastián, Basque Country, Spain

[11]Saint Petersburg State University, 198504 Saint Petersburg, Russia

[12]Institute of Strength Physics and Materials Science, Russian Academy of Sciences, 634021 Tomsk, Russia

✉email: sanjoymahatha@gmail.com

This Supplementary Information contains (1) Band structure of free standing 1BL and 2BL antimonene and parity analysis., (2) Full spin texture of β-antimonene/Bi_2Se_3 hetero-structures.

1. Topological invariants in free-standing β-antimonene

According to Fu and Kane, the topological Z_2 invariant can be computed from the parity of valence bands at the TRIM (time reversal invariant momentum) points in centrosymmetric materials:

$$(-1)^\nu = \prod_{i=1}^{TRIM} \delta_i \quad \text{where} \quad \delta_i = \prod_{m=1}^{N} \xi_{2m}^i$$

Here ξ is the parity eigenvalue and N is the number of occupied bands. Computed parities are reported in Table S1. Since $\nu = 0$ for both systems, free-standing 1 BL and 2 BL β-antimonene are classed as conventional insulators (CI).

1 BL β-antimonene	Parity eigenvalues	Parity product
$\delta(\Gamma)$	$+ - + + + ; - - -$	$-$
$3\delta(M)$	$- + + - - ; + - +$	$-$

2 BL β-antimonene	Parity eigenvalues	Parity product
$\delta(\Gamma)$	$+ - + - + + + - - - ; + + +$	$-$
$3\delta(M)$	$- + - + + - - - + + ; - + +$	$-$

Table S1. Parity eigenvalues of free-standing β-antimonene. Semi-colons separate occupied from unoccupied states.
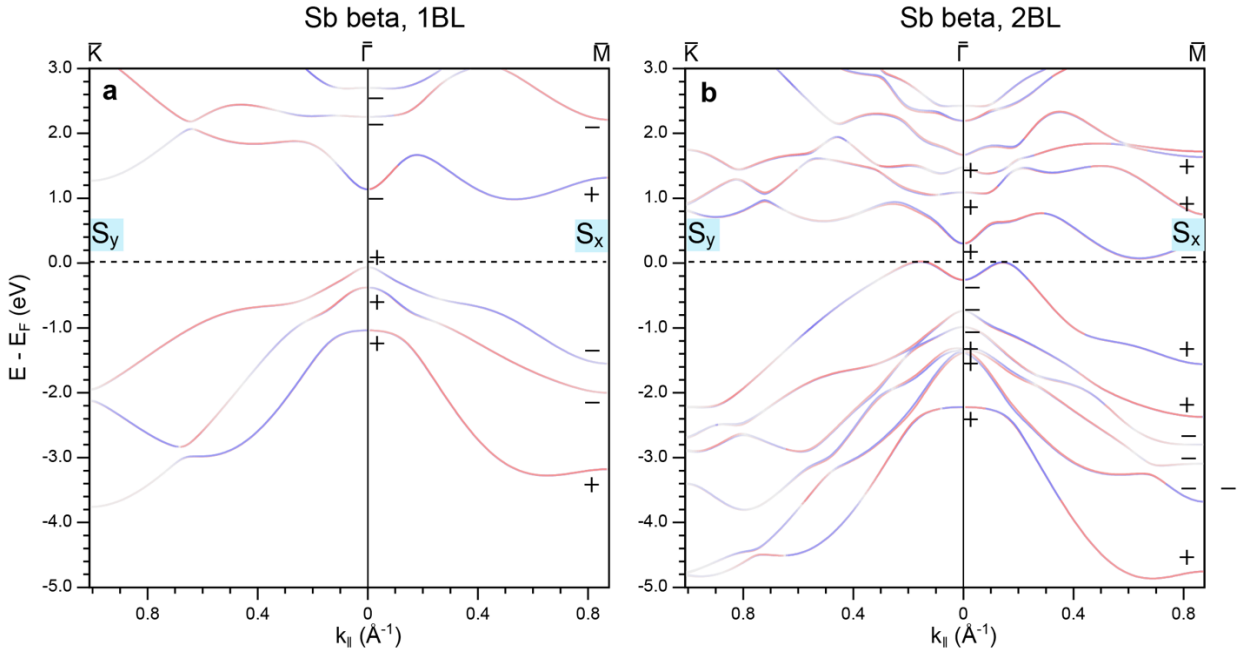

Figure S2. Band structure of free-standing a 1 BL and **b** 2 BL β-antimonene. All bands are doubly degenerate in spin. Spin texture of one band is indicated.

2. Spin texture of β-antimonene/Bi₂Se₃ hetero-structures

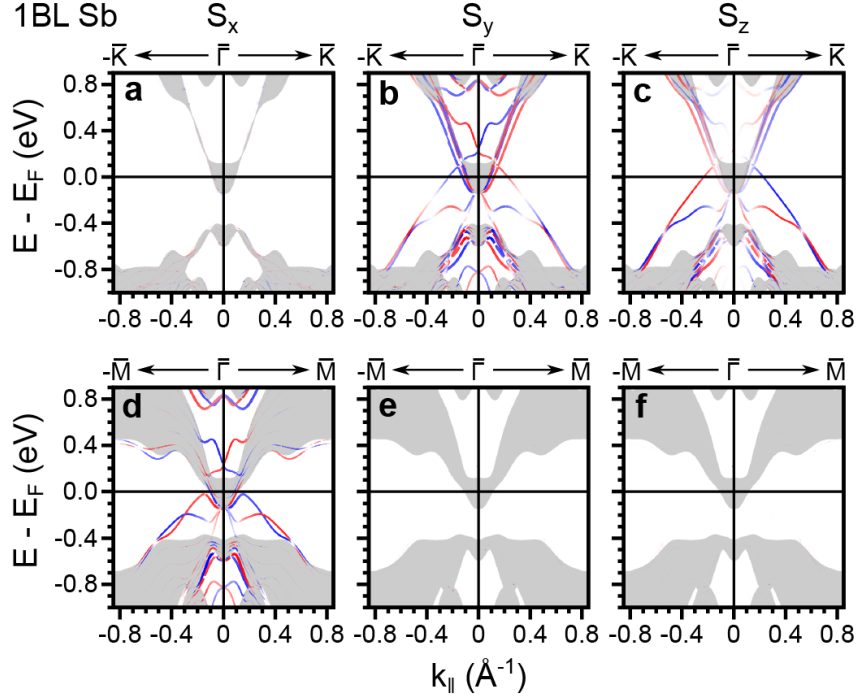Figures S3 and S4 demonstrate the chiral spin texture for 1 BL and 2 BL β-antimonene on Bi₂Se₃.

Figure S3. **Computed spin textures of 1 BL β-antimonene on Bi₂Se₃. a,d** S_x, **b,e** S_y and **c,f** S_z component along the $\overline{K}$-$\overline{\Gamma}$-$\overline{K}$ (top row) and $\overline{M}$-$\overline{\Gamma}$-$\overline{M}$ (bottom row) directions. Spin up and spin down channels are represented in blue and red, respectively.
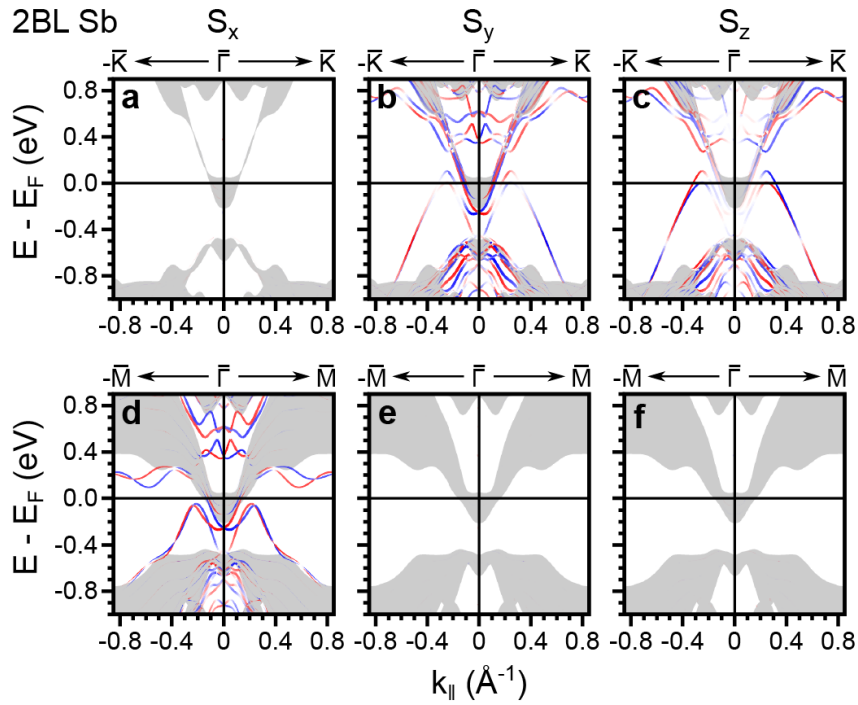

Figure S4. **Computed spin textures of 2 BL β-antimonene on Bi₂Se₃. a,d** S_x, **b,e** S_y and **c,f** S_z component along the $\overline{K}$-$\overline{\Gamma}$-$\overline{K}$ (top row) and $\overline{M}$-$\overline{\Gamma}$-$\overline{M}$ (bottom row) directions. Spin up and spin down channels are represented in blue and red, respectively.