Supplementary Information for:

Two- and one-dimensional quantum spin Hall states in stanene-functionalized GaSnTe and InSnTe compounds

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S1. Transformation matrix for the edge calculations

To simulate different types of edges we construct periodic 3D slab-like supercells for 1SL and 2SL thin films based on the unit (1×1) model with rectangle shape [1]. The initial trigonal unit cell is defined in the basis as follows:

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$$R_1 = \begin{pmatrix} a/2 & 0 & 0 \\ a/2 & \sqrt{3}a/2 & 0 \\ 0 & 0 & c \end{pmatrix},$$

where *a* and *c* are the unit cell parameters of the trigonal cell. The modified (1×1) unit cell for the edge electronic structure calculations is defined in this basis as:

$$R_2 = \begin{pmatrix} a & 0 & 0 \\ 0 & \sqrt{3}\,a & 0 \\ 0 & 0 & c \end{pmatrix}$$

These two cells are connected by the transformation:

$$T = R_2 R_1^{-1},$$

Where the transformation matrix is:

$$T = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

S2. DAFH analysis

Table S1. Set of DAFH orbitals for 3*d*4*s*4*p* valence state of Ga atom in GaSnTe. Only orbitals with occupation number larger than 0.1 are considered.

DAFH orbital type	Association state	Number of DAFH orbitals	Occupation number	Orbital norm, localized within Ga basin, %	Orbital norm, localized within neighbouring basins, %
d-like	3*d*	5	2.00	100	-
s-like	4*s*	1	1.26	63	17 (Sn) 5 (Te) 5 (Te) 5 (Te)
p-like	4*p*	3	0.40	21	56 (Te) 10 (Sn)

Table S2. Set of DAFH orbitals for 4*d*5*s*5*p* valence state of Sn atom in GaSnTe. Only orbitals with occupation number larger than 0.1 are considered.

DAFH orbital type	Association state	Number of DAFH orbitals	Occupation number	Orbital norm, localized within Sn basin, %	Orbital norm, localized within neighbouring basins, %
d-like	4*d*	5	2.00	100	-
s-like	5*s*	1	1.51	76	7 (Ga) 5 (Sn) 5 (Sn) 5 (Sn)
p-like	5*p*	3	0.75	38	33 (Sn) 9 (Ga) 3 (Sn) 3 (Sn)

[1]Sukky Jun, Phys. Rev. B 78, 073405 (2008)