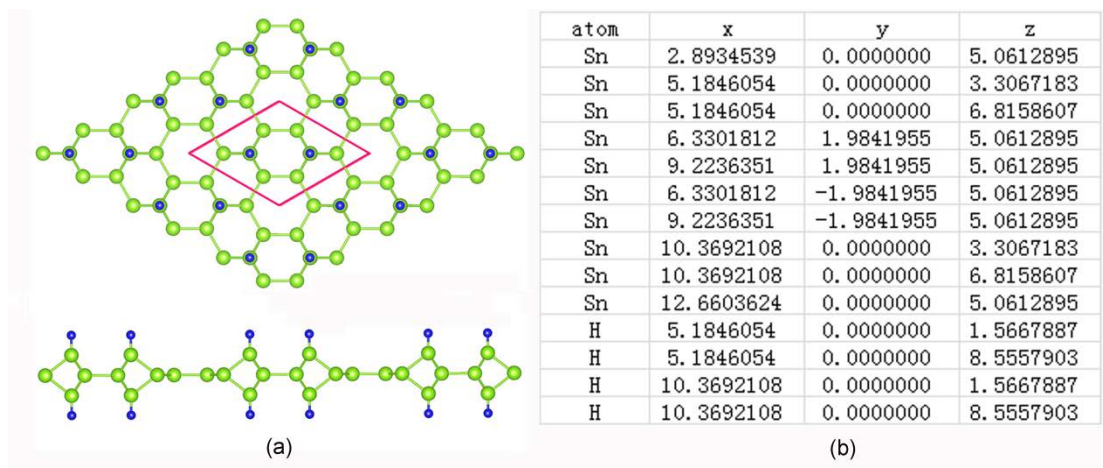Supplementary Information for

Dumbbell Stanane: A large-gap quantum spin Hall insulator

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atom	x	y	z
Sn	2.8934539	0.0000000	5.0612895
Sn	5.1846054	0.0000000	3.3067183
Sn	5.1846054	0.0000000	6.8158607
Sn	6.3301812	1.9841955	5.0612895
Sn	9.2236351	1.9841955	5.0612895
Sn	6.3301812	-1.9841955	5.0612895
Sn	9.2236351	-1.9841955	5.0612895
Sn	10.3692108	0.0000000	3.3067183
Sn	10.3692108	0.0000000	6.8158607
Sn	12.6603624	0.0000000	5.0612895
H	5.1846054	0.0000000	1.5667887
H	5.1846054	0.0000000	8.5557903
H	10.3692108	0.0000000	1.5667887
H	10.3692108	0.0000000	8.5557903

(a)   (b)

Figure S1. (a) Top (up panel) and side (down panel) views of a 3×3 supercell of DB stanane. The green atoms are Sn, and the blue atoms are H. The rhombus in red lines indicates a unit cell. (b)The atomic coordinates (in angstroms) in a unit cell of DB stanane. The data of the two base vectors have been presented in the text.
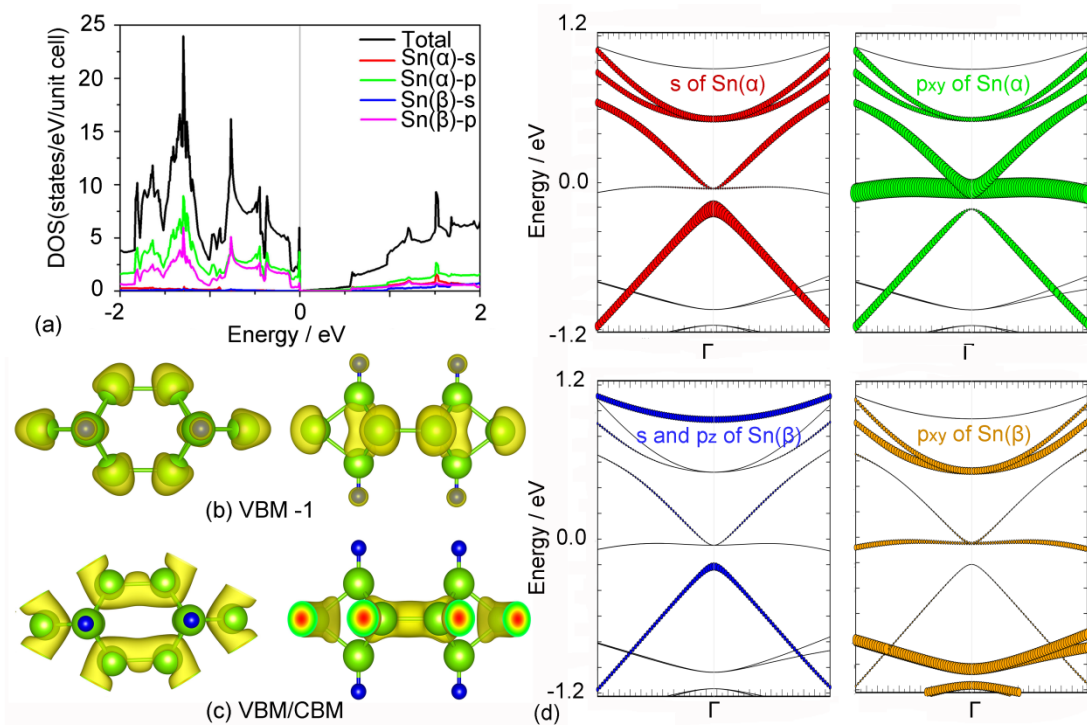
Figure S2. (a) Orbital-resolved electron density states of DB stanane without considering SOC. The DOS data were obtained by integrating the whole BZ. (b) and (c) are the isosurfaces of the electron wavefunctions of VBM-1 and VBM at Γ point. The isosurfaces of the CBM at the Γ point atom resemble those of VBM and thus are not presented. (d) The orbital-resolved electronic band structures in the vicinity of Fermi level obtained from DFT calculations without considering SOC. Contributions of different atomic orbitals are represented by the dots in different colors and sizes. Large dot means higher contribution while smaller one indicates lower contribution. The smooth lines represent zero contributions. S-orbital of Sn(α) atoms (red dots), s- and p_z-orbitals of Sn(β) (blue dots), p_{xy}-orbitals of Sn(α) atoms (green dots) and p_{xy}-orbitals of Sn(β) (brown dots).
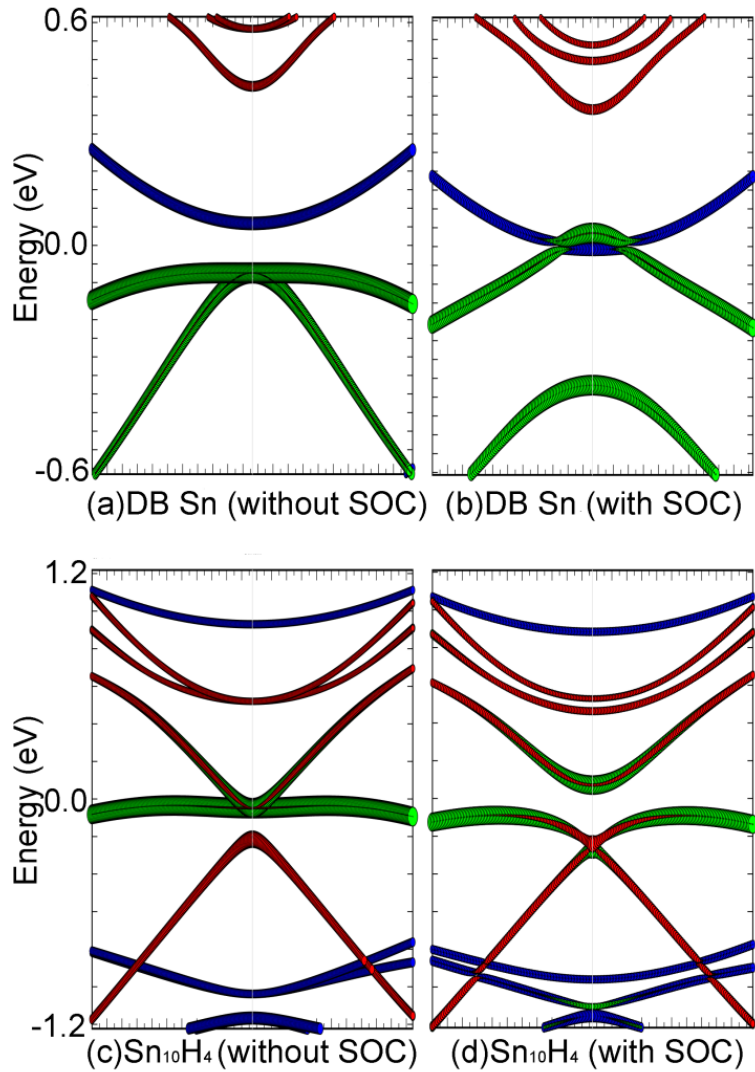
Figure S3. Comparison between the orbital-resolved band structures of DB stanene and DB stanane in the vicinity of the Γ point obtained from DFT calculations without (left panel) and with (right panel) SOC. The dots in different colors and sizes indicate the contribution of different atomic orbitals. S-orbital of Sn(α) atom (red). p_{xy}-orbital of Sn(α) (green), p_z-orbital of Sn(α) (blue). The p_z-p_{xy} band inversion takes place in the pristine DB stanene owning to SOC while it is s-p_{xy} band inversion in DB stanane.