Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Two-Dimensional Stanane: Strain-Tunable Electronic Structure, High Carrier Mobility, and Pronounced Light Adsorption

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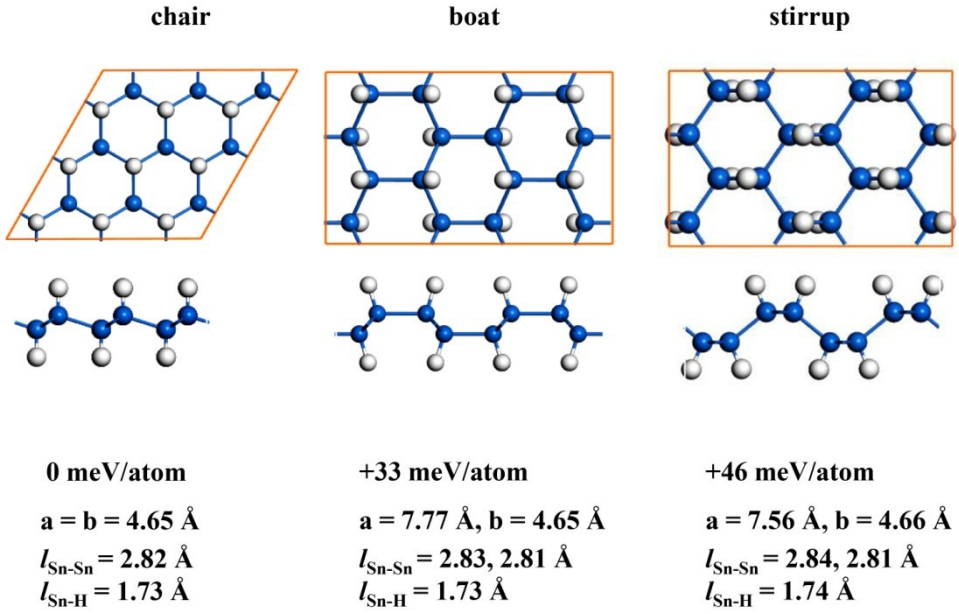

Fig. S1 The top and side views of chair, boat, and stirrup forms of stanane monolayer with relative cohesive energies. The respective cell parameters (*a*, *b*), lengths of Sn-Sn (l_{Sn-Sn}) and Sn-H (l_{Sn-H}) bonds are also given.

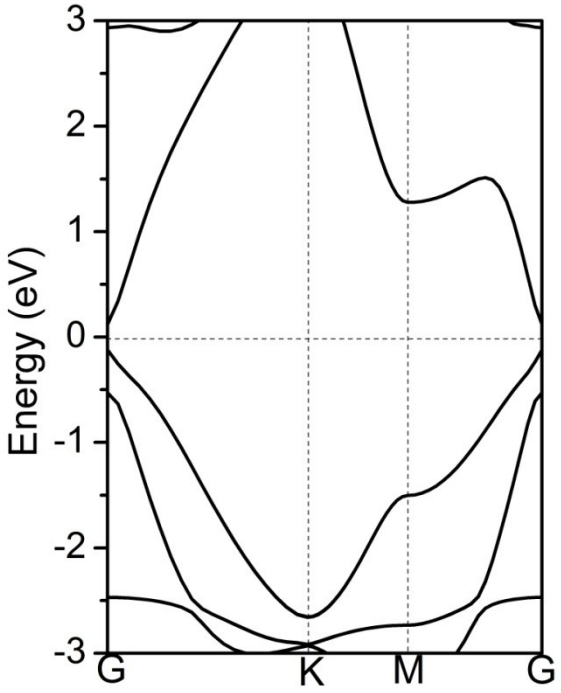

Fig. S2 Band structure of stanane computed at PBE+SOC level.

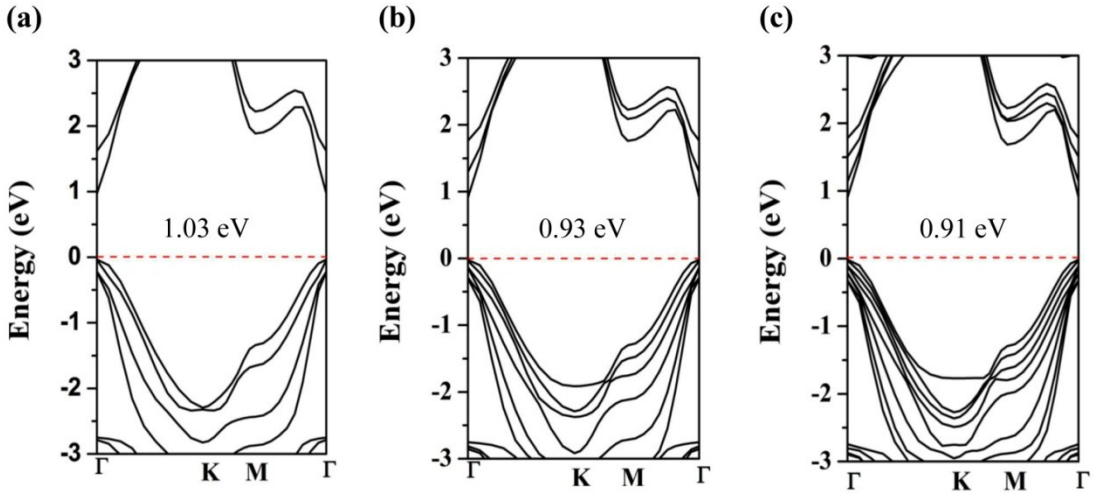

Fig. S3 Band structures of stanane (a) bilayer, (b) trilayer, and (c) four-layer computed at HSE06 level.

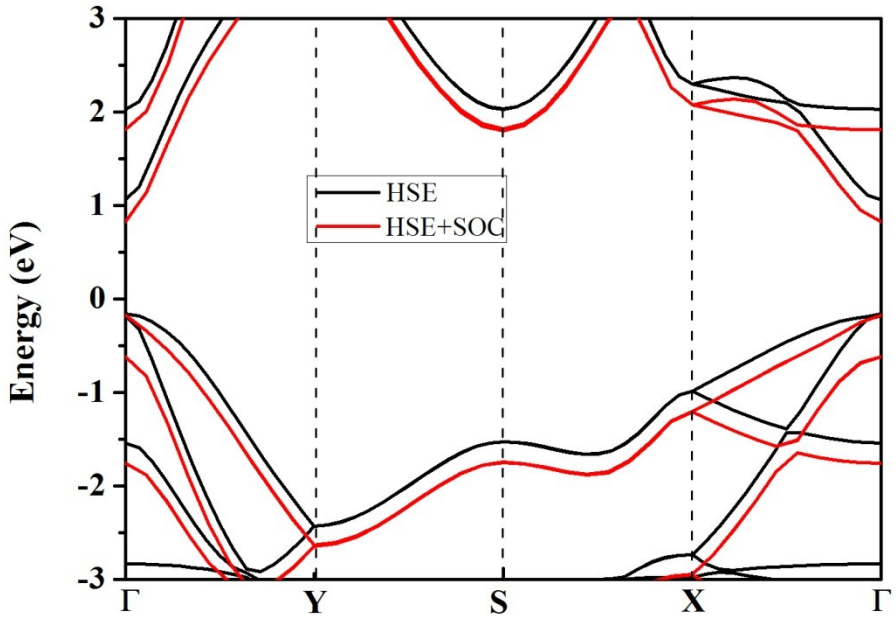

Fig. S4 Band structure of stanane monolayer in the rectangle supercell.

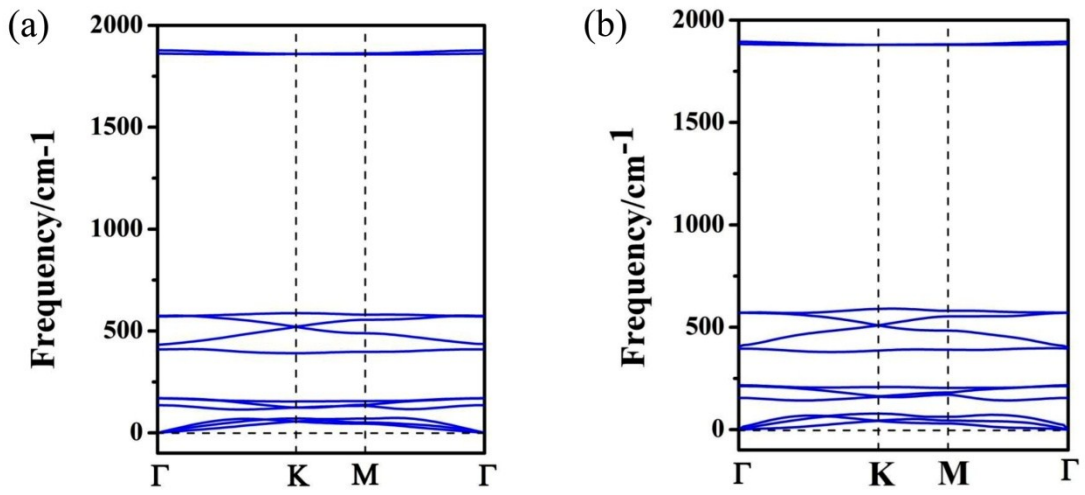

Fig. S5 Phonon band structures of stanane with (a) 5% tensile strain and (b) 3% compress strain.

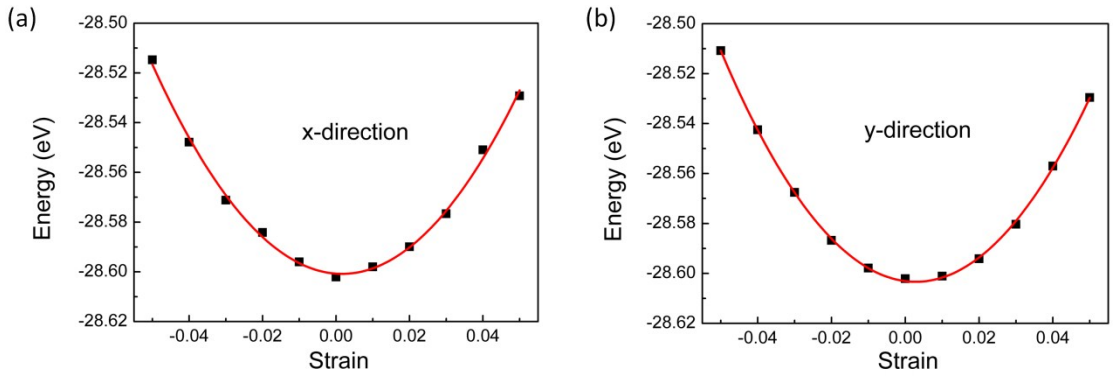

Fig. S6 Total energy-strain relationship of stanane along *x* (a) and *y* (b) directions. Δl refers to the dilation along *x* or *y*, while l_0 refers to the lattice constant of *a* or *b* at equilibrium geometry.

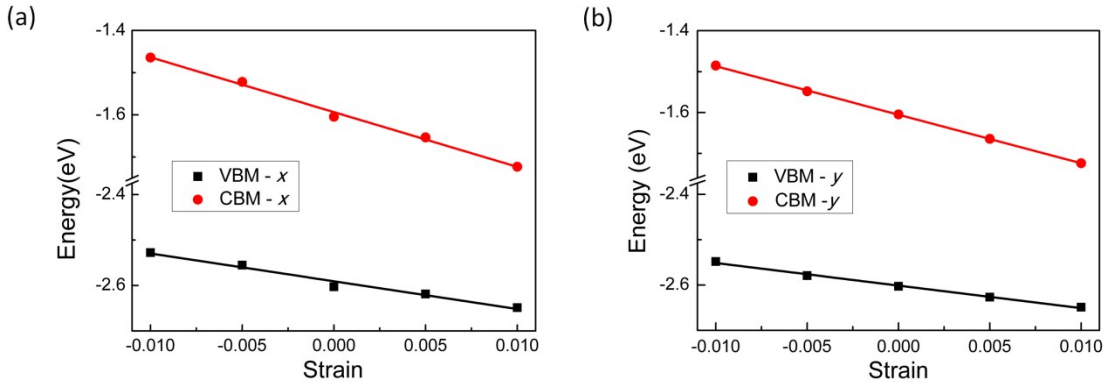

Fig. S7 Shifts of CBM and VBM under uniaxial strain along *x* and *y* directions for stanane.