Electronic Supplementary Information for

High out-of-plane negative Poisson's ratios and strong light harvesting in two-dimensional SiS_2 and its derivatives

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1 Calculation Method

For monolayer SiS_2, four independent elastic constants (C_{11},C_{12},C_{22} and C_{66}), which can be obtained via energy–strain approach or stress–strain approach. Once the independent elastic constants are obtained, the direction-dependent Young's modulus and Poisson's ratio can be calculated via following equations:

$$E(\theta) = \frac{d_4}{cos^4\theta + d_2 cos^2\theta sin^2\theta + d_3 sin^4\theta} \tag{S1}$$

$$\nu(\theta) = \frac{d_0 cos^4\theta - d_1 cos^2\theta sin^2\theta + d_0 sin^4\theta}{cos^4\theta + d_2 cos^2\theta sin^2\theta + d_3 sin^4\theta} \tag{S2}$$

where, $d_0 = \frac{C_{12}}{C_{22}}$, $d_1 = \frac{C_{11}}{C_{22}} + 1 - \frac{C_{11}C_{22}-C_{12}^2}{C_{22}C_{66}}$, $d_2 = -(2\frac{C_{12}}{C_{22}} - \frac{C_{11}C_{22}-C_{12}^2}{C_{22}C_{66}})$, $d_3 = \frac{C_{11}}{C_{22}}$ and $d_4 = \frac{C_{11}C_{22}-C_{12}^2}{C_{22}}$.

2 Properties of MX_2

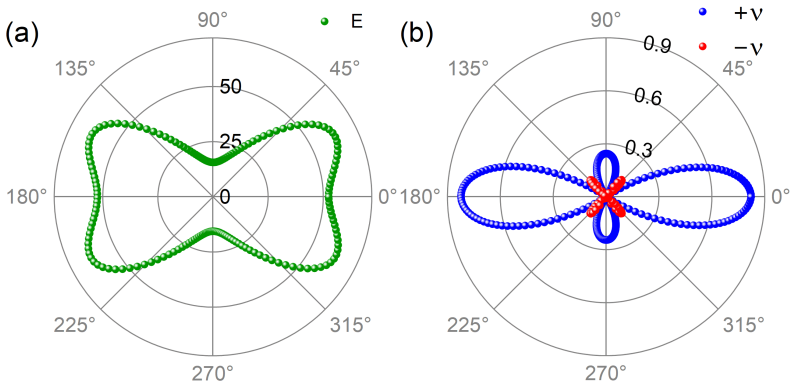

Figure S1: (a) The polar plot of Young's modulus (GPa) and Poisson's ratio (b) of bulk SiS_2 in the xy plane.

Table S1: The lattice parameters(Å), maximum Young's Modulus E_{max}(GPa), in-plane Poisson's ratio(ν_i) and HSE level Bandgap E_g(eV) of SiS_2 with different layer numbers.

Layer	a	b	E_{max}	ν_i	E_g
Monolayer	5.93	8.09	96.95	-0.12	4.50
Bilayer	5.93	8.12	99.50	-0.14	4.45
Trilayer	5.92	8.15	63.71	-0.13	4.38
Bulk	5.93	8.09	63.84	-0.13	4.15

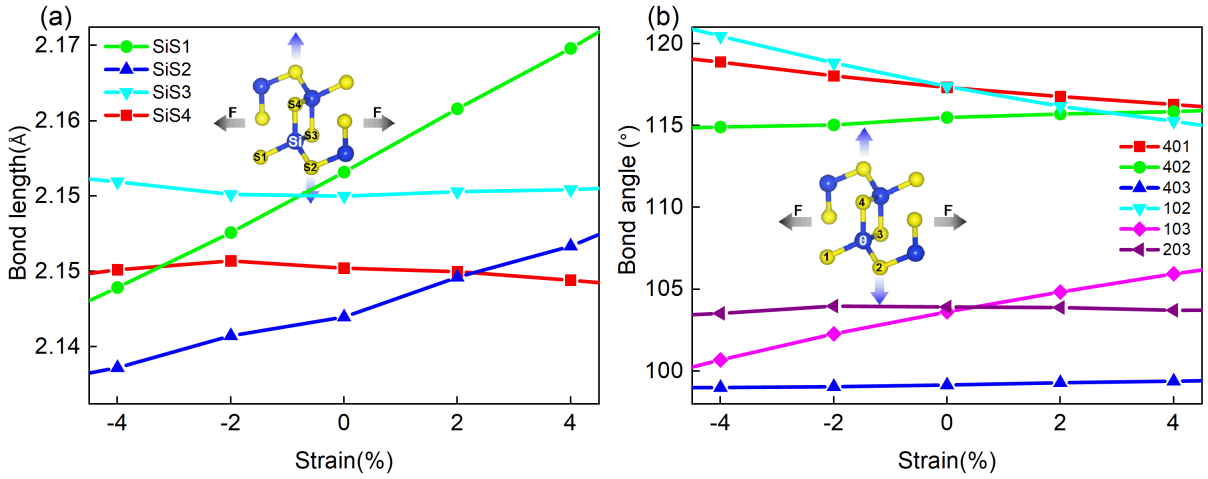

Figure S2: The variation of bond lengths (a) and bond angles (b) with strain within the linear elastic range. From the graphs of bond length and bond angle changes, it is evident that under external stress, the bond lengths of Si-S1, Si-S2, and Si-S4 increase with the increase in strain, while the bond length of Si-S3 decreases with increasing strain. Simultaneously, bond angle 102 decreases with increasing strain, while bond angle 304 remains almost constant with strain. This overall effect results in an increase in the distance between the upper and lower atomic layers, leading to an out-of-plane negative Poisson's ratio.

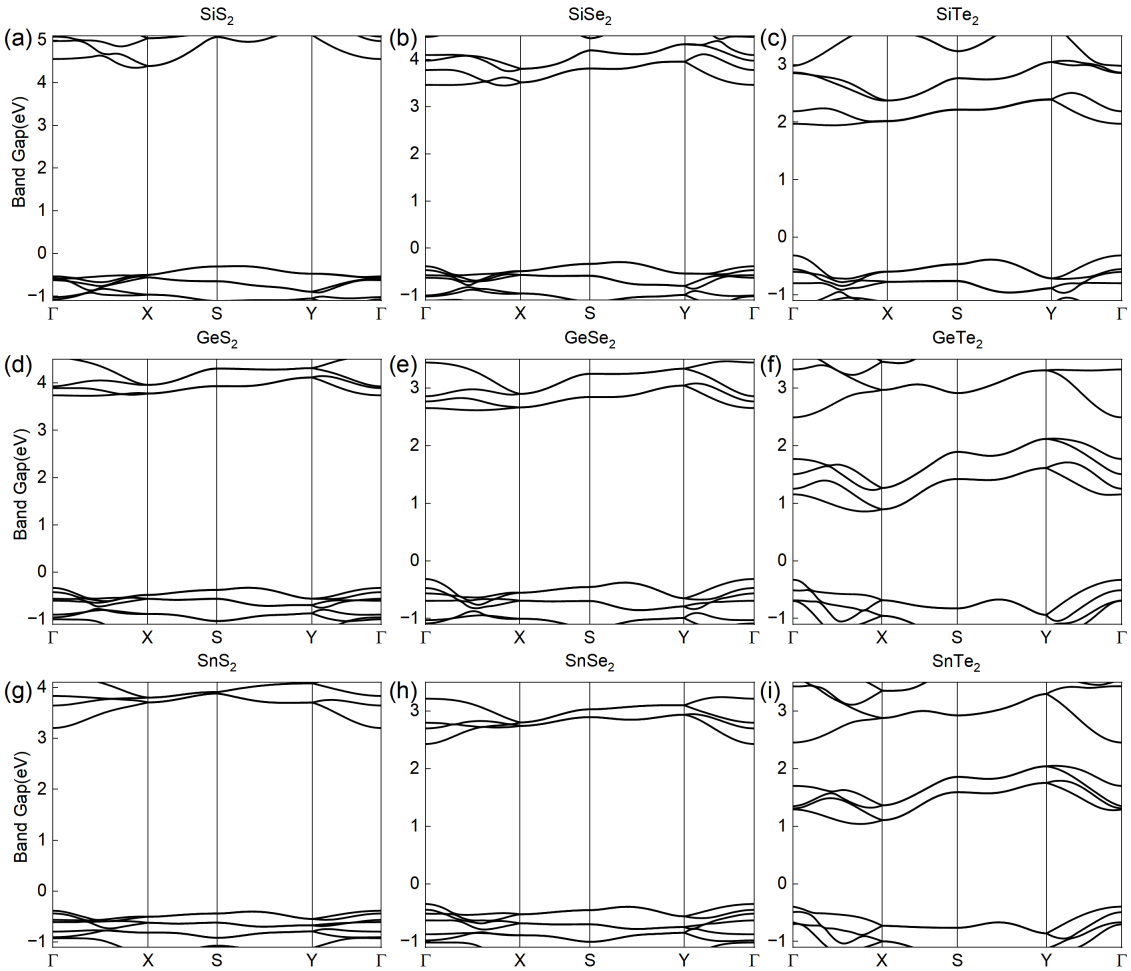

Figure S3: (a-f) The HSE level band structures of MX_2(M = Si,Ge,Sn and X = S,Te), respectively.

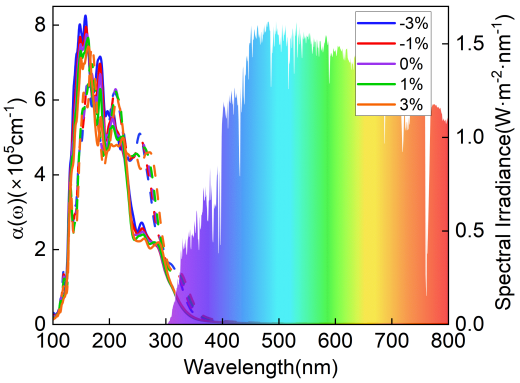

Figure S4: The optical absorption of SiS_2 in the xy direction under strain. The solid line represents the y-direction, while the dashed line represents the x-direction.

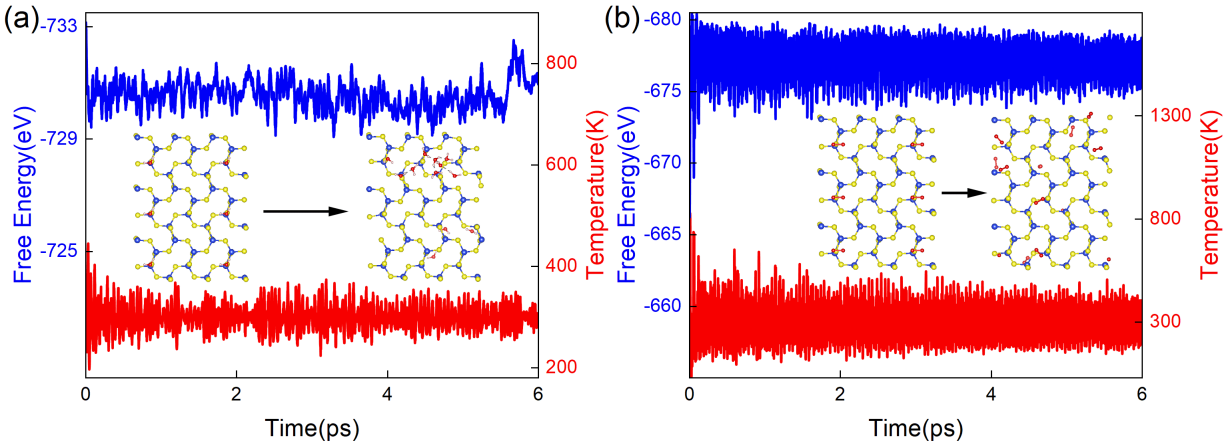

Figure S5: (a) and (b) represent the molecular dynamics simulations of SiS_2 at 300K under the influence of H_2O and O_2 molecules, respectively.