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Figure S1 (a) Atomic structures of Si_2SSe monolayer from top and side views. The phonon dispersion of (b) SiSe and (c) Si_2SSe monolayers.



Figure S2 (a) Young's modulus and (b) Possion's ratio of SiSe as a function of the inplane angle θ. (c) Young's modulus and (d) Possion's ratio of SiSe as a function of the in-plane angle θ. The areas of negative Poisson's ratio are marked in black.



Figure S3 The tilting degree (Δy) of surface S (Se) atoms for (a) SiS, (b) SiSe, and (c) Si₂SSe monolayers as a function of the uniaxial strain in the x and y direction.



Figure S4 The calculate band structure and partial density of states (PDOS) of (a) SiSe and (b) Si₂SSe monolayers.



Figure S5 (a) Electron and (b) hole effective masses of SiSe monolayer as a function of the in-plane angle θ . (c) Electron and (d) hole effective masses of Si₂SSe monolayer as a function of the in-plane angle θ .