Electronic Supplementary Information

Prediction of 2D group-11 chalcogenides: Insights into novel auxetic M_2X (M = Cu, Ag, Au; X = S, Se, Te) monolayers

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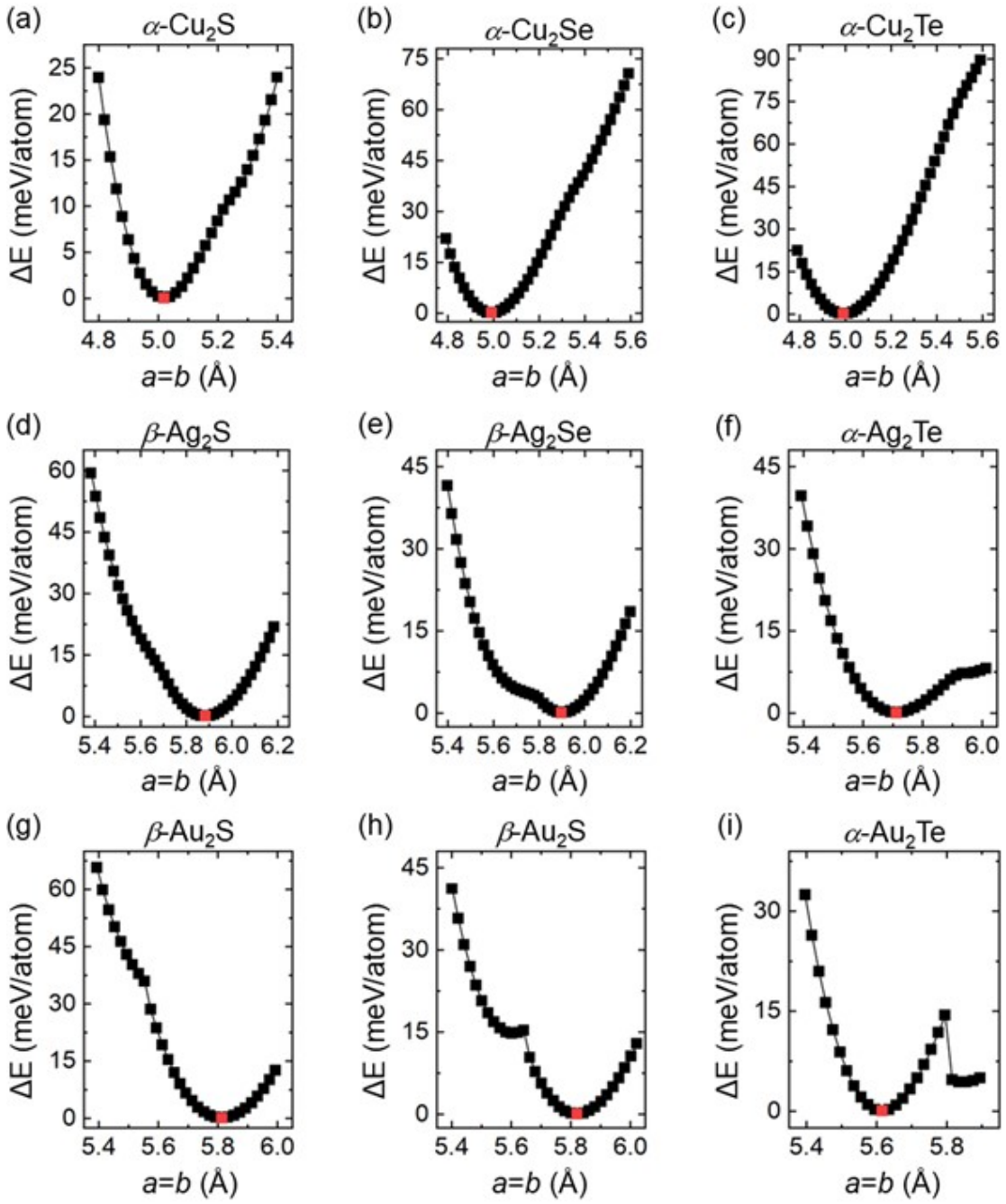

Figure S1. (a)-(i) Relative energies of each M_2X monolayer with different lattice parameters. Red represents the most energetically favorable structure.

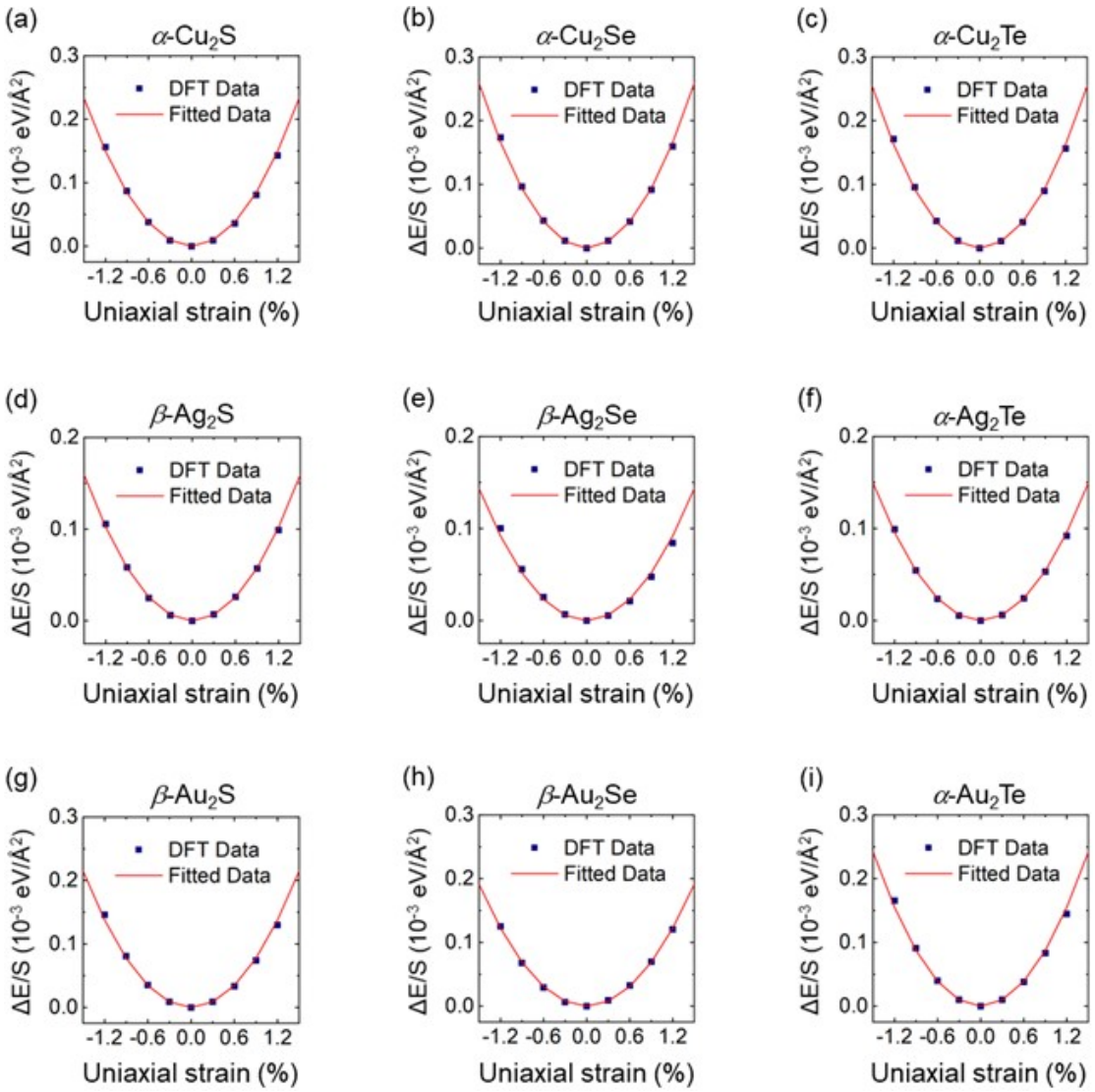

Figure S2. (a)-(i) Strain energies of α-Cu_2S, α-Cu_2Se, α-Cu_2Te, β-Ag_2S, β-Ag_2Se, α-Ag_2Te, β-Au_2S, β-Au_2Se, and α-Au_2Te monolayers with respect to various uniaxial strains along the x direction.

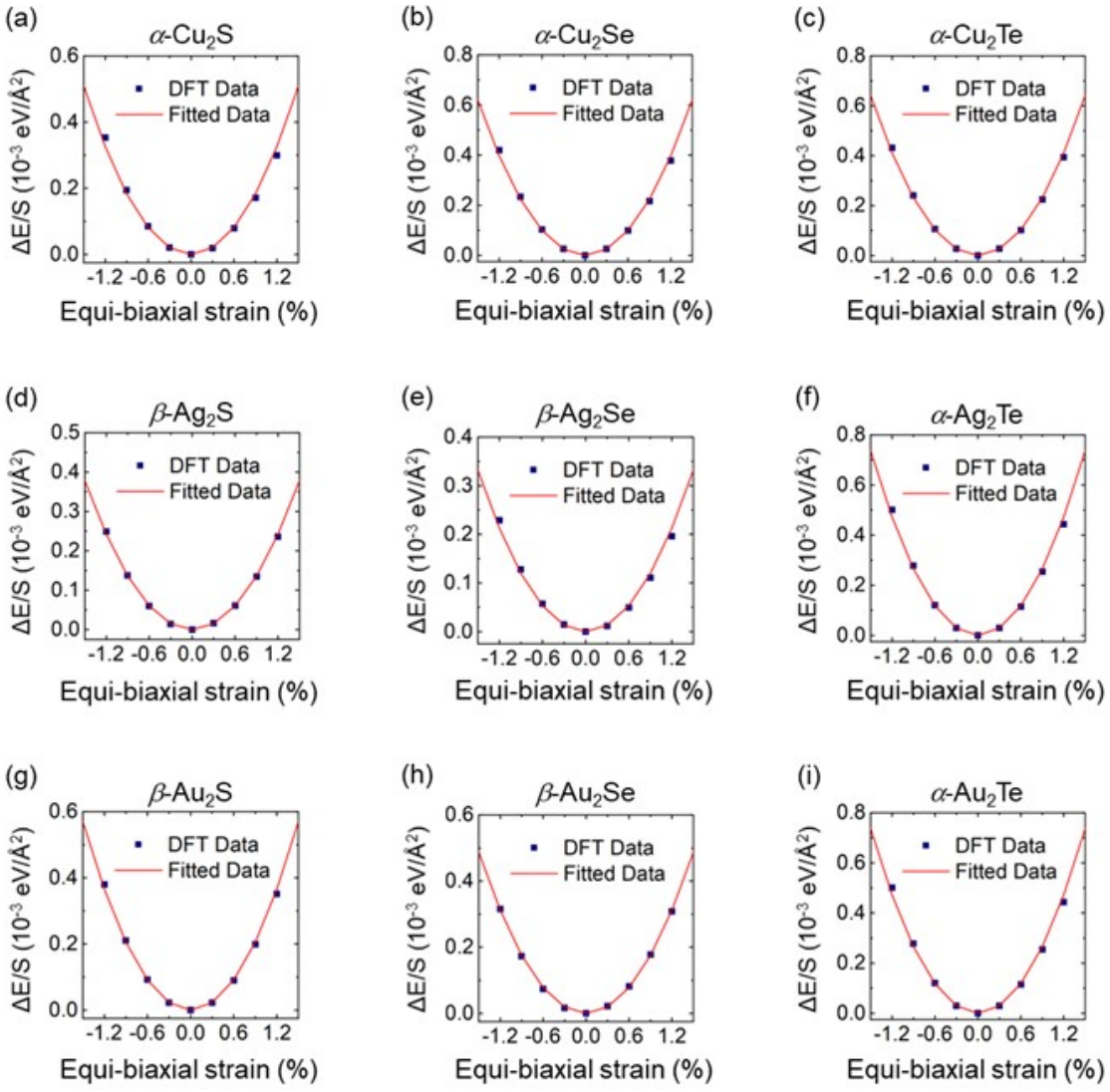

Figure S3. (a)-(i) Strain energies of α-Cu_2S, α-Cu_2Se, α-Cu_2Te, β-Ag_2S, β-Ag_2Se, α-Ag_2Te, β-Au_2S, β-Au_2Se, and α-Au_2Te monolayers with respect to various equi-biaxial strains along the x and y directions.

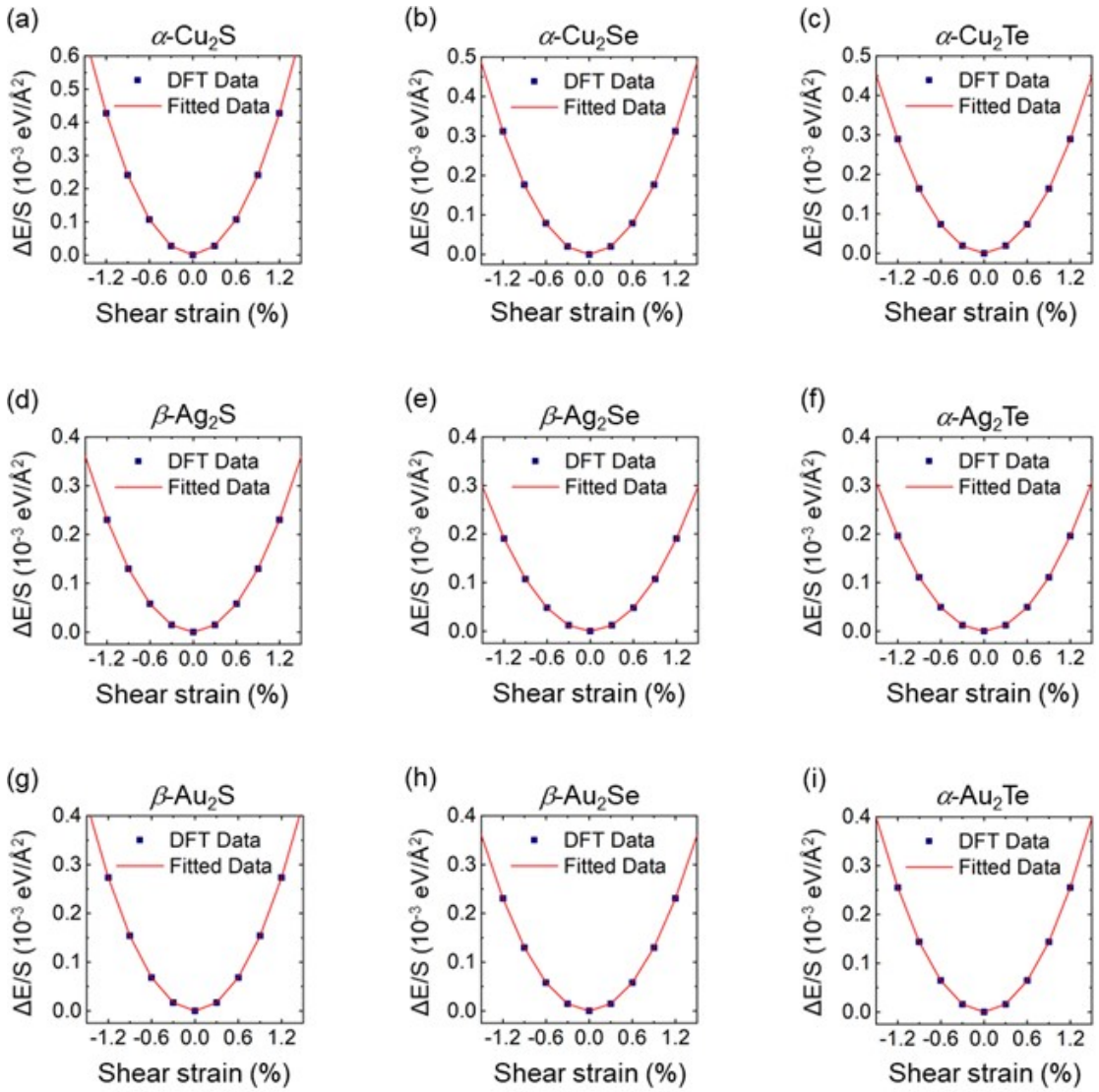

Figure S4. (a)-(i) Strain energies of α-Cu_2S, α-Cu_2Se, α-Cu_2Te, β-Ag_2S, β-Ag_2Se, α-Ag_2Te, β-Au_2S, β-Au_2Se, and α-Au_2Te monolayers with respect to various shear strains along the xy directions.

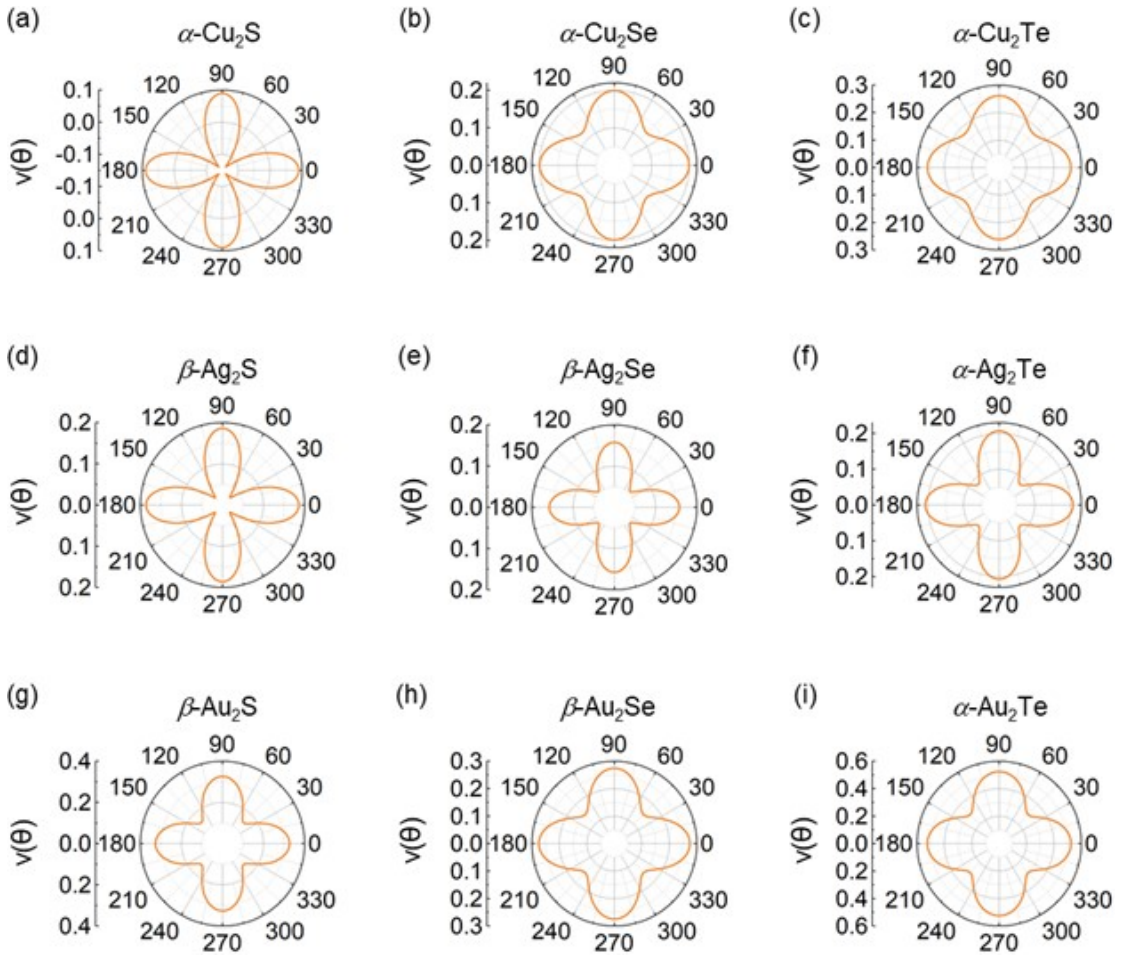

Figure S5. (a)-(i) Calculated orientation-dependent Poisson's ratio ν(θ) of α-Cu_2S, α-Cu_2Se, α-Cu_2Te, β-Ag_2S, β-Ag_2Se, α-Ag_2Te, β-Au_2S, β-Au_2Se, and α-Au_2Te monolayers, respectively.

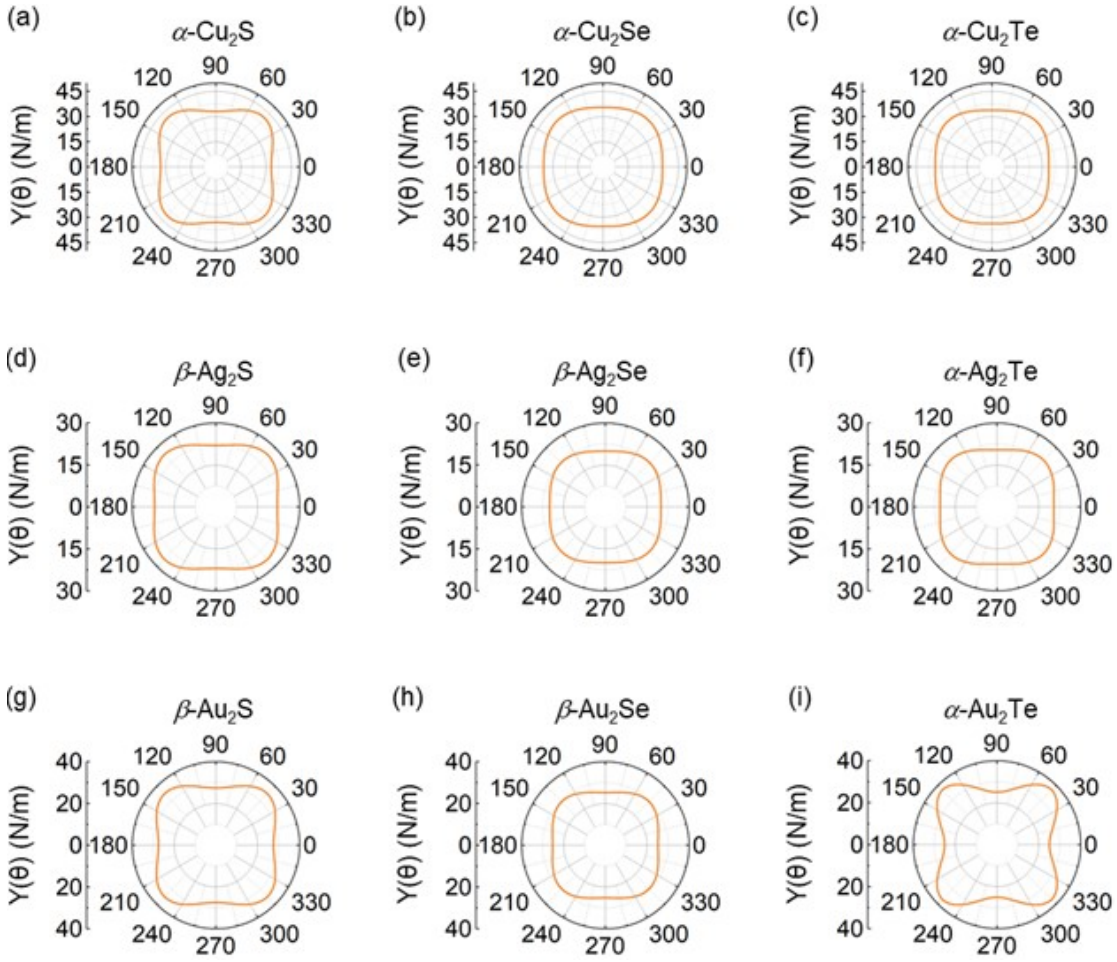

Figure S6. (a)-(i) Calculated orientation-dependent Young's modulus Y(θ) of α-Cu_2S, α-Cu_2Se, α-Cu_2Te, β-Ag_2S, β-Ag_2Se, α-Ag_2Te, β-Au_2S, β-Au_2Se, and α-Au_2Te monolayers, respectively.

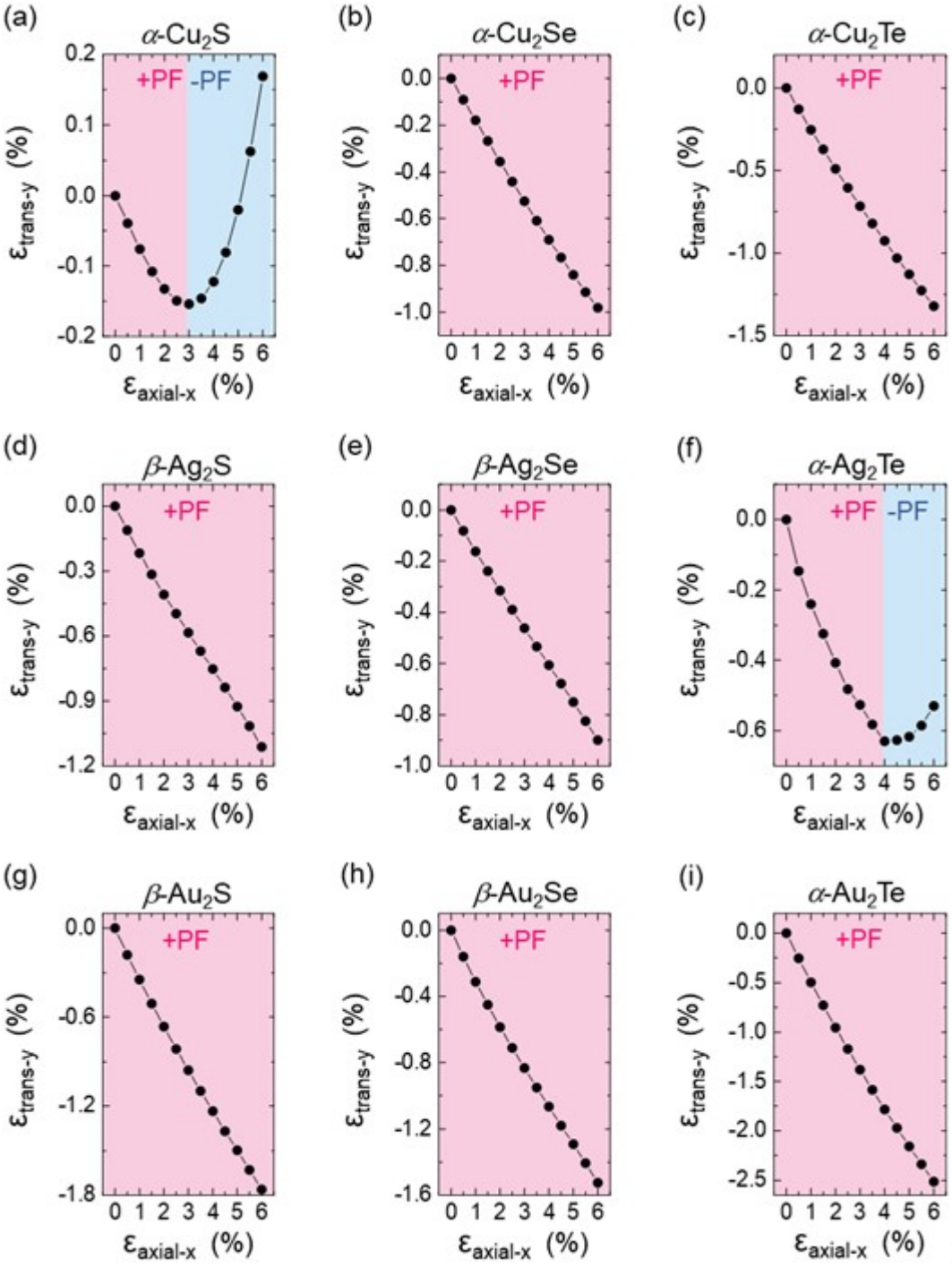

Figure S7. (a)-(i) Variation of transverse strains of α-Cu_2S, α-Cu_2Se, α-Cu_2Te, β-Ag_2S, β-Ag_2Se, α-Ag_2Te, β-Au_2S, β-Au_2Se, and α-Au_2Te monolayers with respect to tensile strains along x direction. The pink and blue shaded regions represent positive Poisson's function (+PF) and negative Poisson's function (−PF), respectively.

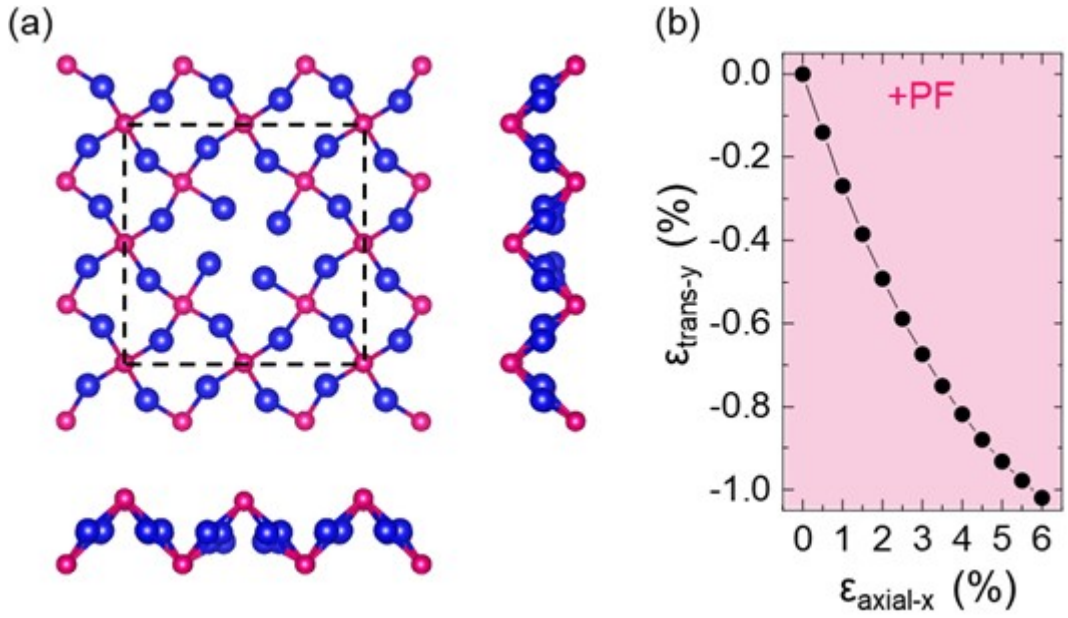

Figure S8. (a) Top and side views of the α-Cu_2S monolayers. (b) The transverse strains of α-Cu_2S monolayers with S vacancy in tensile strains along the x direction. The pink shaded region corresponds to the positive Poisson's function (+PF).

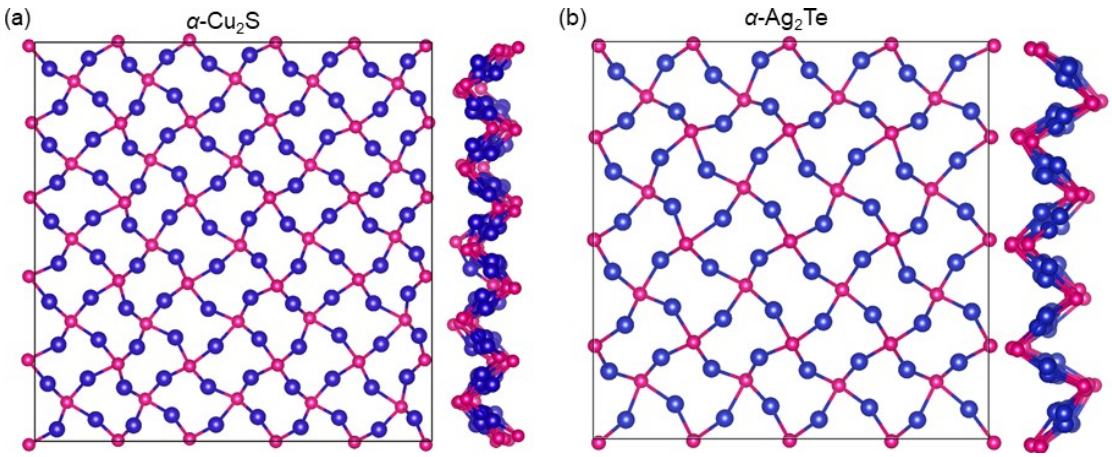

Figure S9. Top and side views of the α-Cu_2S and α-Ag_2Te monolayers taken from ab initio molecular dynamic simulations carried out at 300 K for 2 ps.

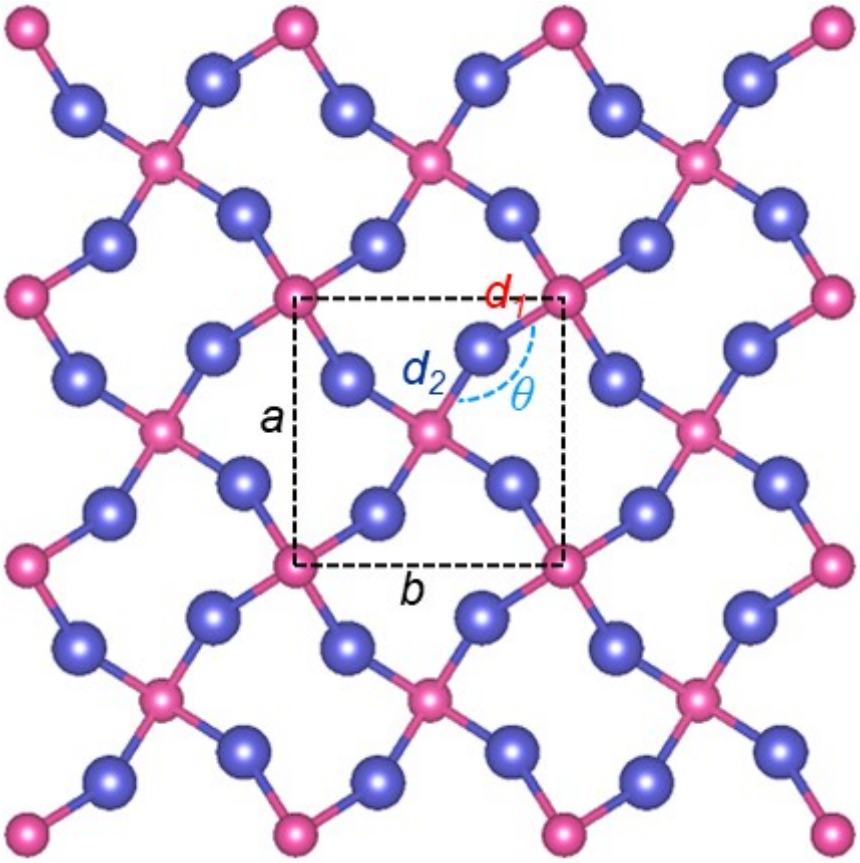

Figure S10. Bond lengths (d_1 and d_2) and bond angle (θ) are indicated by red, dark blue, and light blue, respectively.

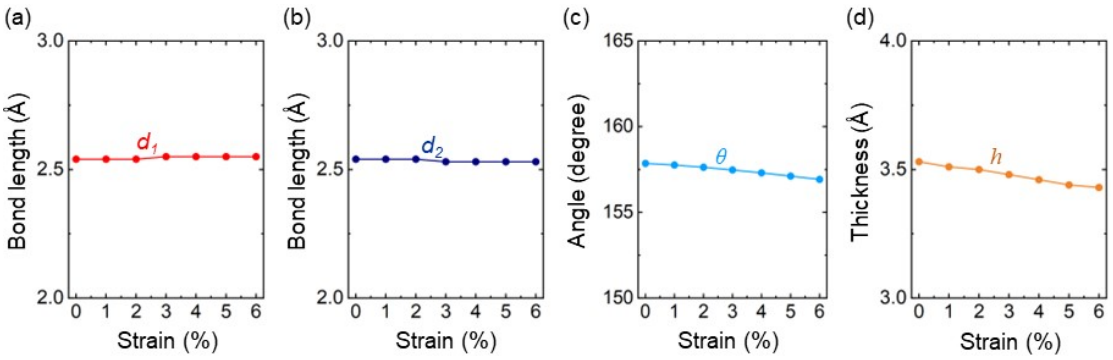

Figure S11. Variation of (a)-(b) bond lengths (d_1 and d_2), (c) bond angle (θ) and (d) thickness (h) of α-Cu_2Te monolayer. Bond lengths (d_1 and d_2) and bond angle (θ) are indicated in Fig. S10.

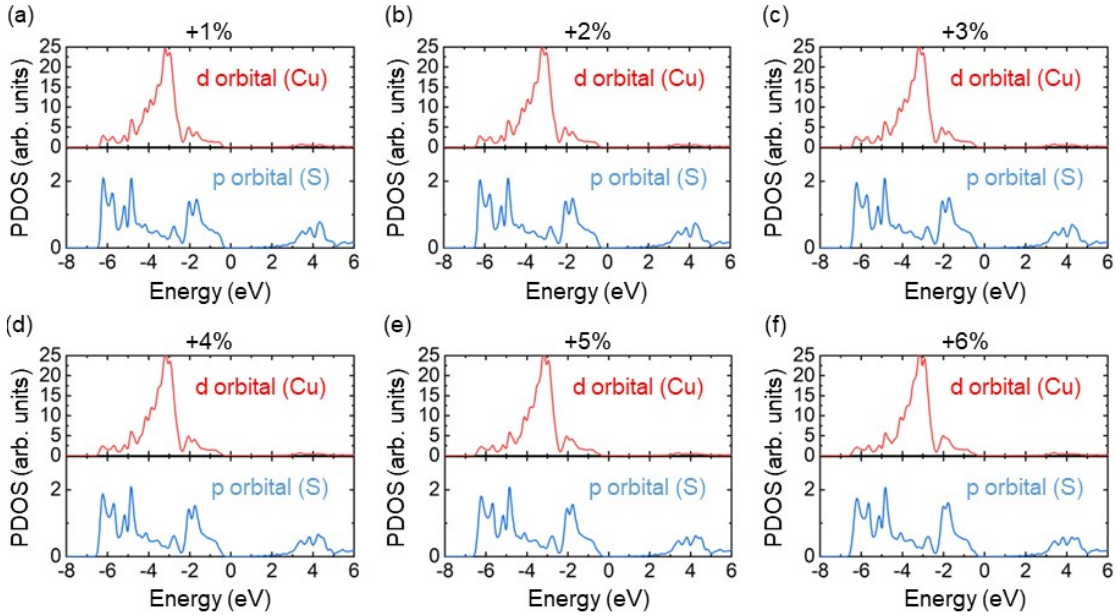

Figure S12. (a)-(f) Projected density of states of α-Cu_2S monolayer with +1%, +2%, +3%, +4%, +5%, and +6% tensile strains, respectively. The d/p orbitals of Cu/S are indicated by red/blue.

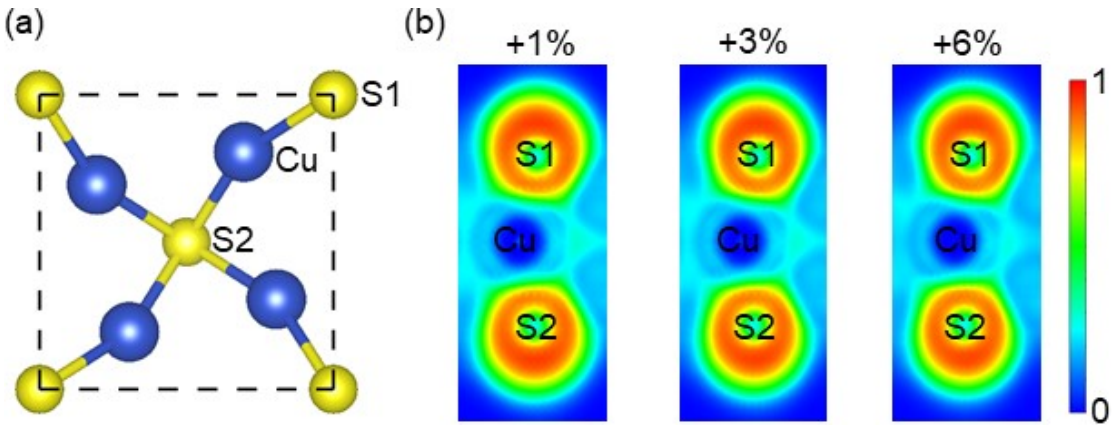

Figure S13. (a)Top view of α-Cu_2S monolayer. (b) Electron localization functions of α-Cu_2S with +1%,+3% and +6% tensile strains, respectively.

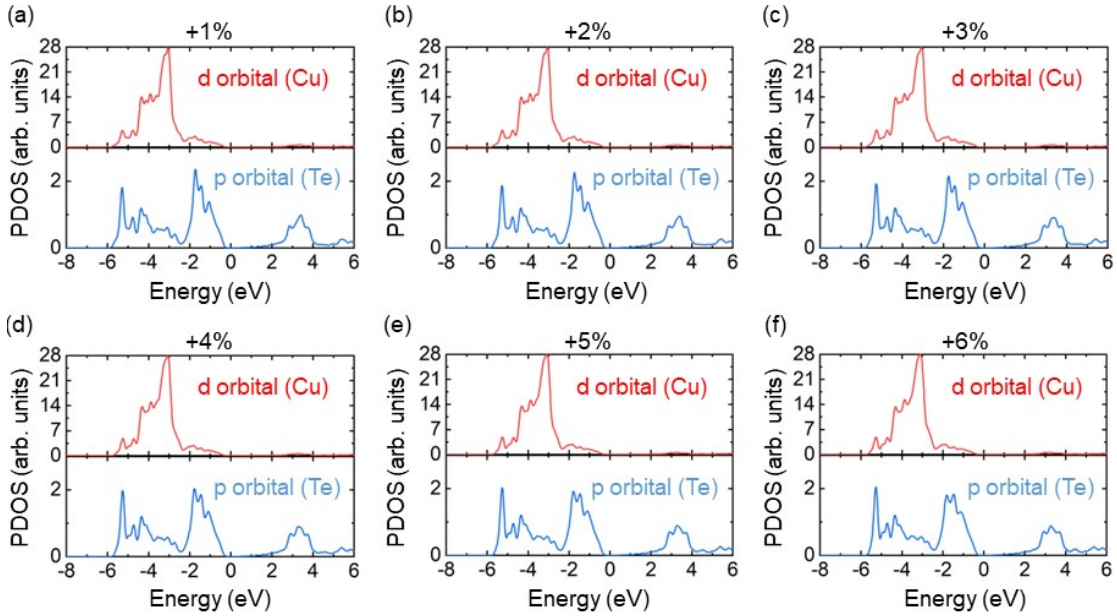

Figure S14. (a)-(f) Projected density of states of α-Cu_2Te monolayer with +1%, +2%, +3%, +4%, +5%, and +6% tensile strains, respectively. The d/p orbitals of Cu/Te are indicated by red/blue.

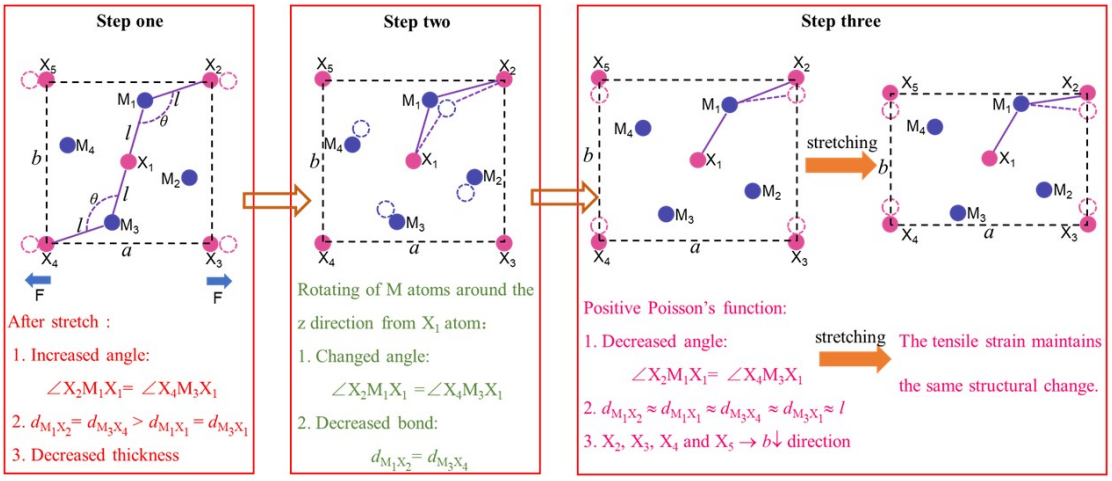

Figure S15. Mechanism of PPF for α-phase monolayers. The solid and dashed M-X bonds are initial and final configurations at each relaxation step, respectively. The dashed circles represent the movements of M and X atoms.

Table S1 Structural parameters (a, b and h) of the α-Cu_2S, α-Cu_2Se, α-Cu_2Te, β-Ag_2S, β-Ag_2Se, α-Ag_2Te, β-Au_2S, β-Au_2Se, and α-Au_2Te monolayers. a (b) and h are the lattice parameters, thickness of α-phase and β-phase monolayers, respectively.

Material	a (Å)	b (Å)	h (Å)
α-Cu_2S	5.02	5.02	2.55
α-Cu_2Se	4.99	4.99	3.00
α-Cu_2Te	4.99	4.99	3.52
β-Ag_2S	5.88	5.88	2.48
β-Ag_2Se	5.90	5.90	2.93
α-Ag_2Te	5.71	5.71	3.54
β-Au_2S	5.81	5.81	2.49
β-Au_2Se	5.82	5.82	2.95
α-Au_2Te	5.62	5.62	3.55

Table S2 Bader analysis of α-Cu_2S monolayer with +1%, +3% and +6% tensile strains, respectively. S1, S2 and Cu atoms correspond to those of Fig. S13 (a).

Strains	S1	S2	Cu
+1%	+0.621*e*	+0.621*e*	-0.312*e*
+3%	+0.628*e*	+0.628*e*	-0.318*e*
+6%	+0.645*e*	+0.645*e*	-0.323*e*