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

Two-Dimensional ternary pentagonal BCX (X=P, As, and Sb): promising photocatalyst semiconductors for water splitting with strong piezoelectricity

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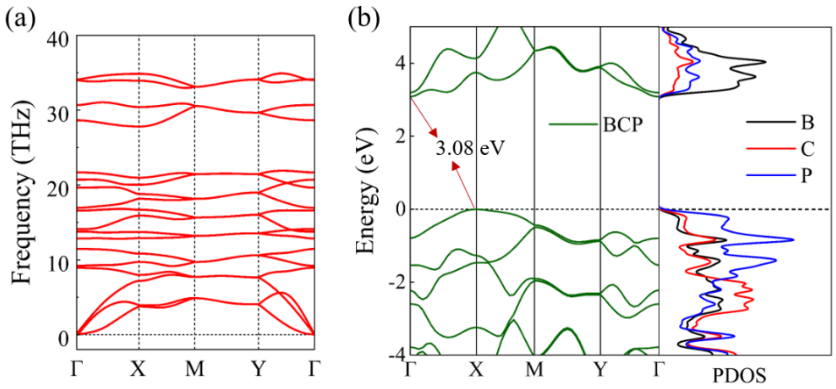

Fig. S1 (a)The phonon spectra, (b) HSE06 band structures and the corresponding partial density of states of BCP monolayer.

Table S1. Elastic constants (C_i, in Nm^{-2}), Young's modulus (E, in Nm^{-2}), and Poisson's ratio (v) of BCX sheets. The reported data for pentagonal BCP are included for comparison.

BCX	C_{11}	C_{12}	C_{22}	C_{66}	E_x	E_y	v_x	v_y
BCP	49.50	63.47	159.68	77.15	24.28	78.31	0.40	1.28
BCAs	50.27	50.11	144.82	62.52	32.93	35.82	0.35	1.00
BCSb	44.28	36.59	114.08	46.16	32.55	36.50	0.32	0.83
BCP[1]	47.49	61.81	153.08	76.04	22.65	73.35	0.40	1.30

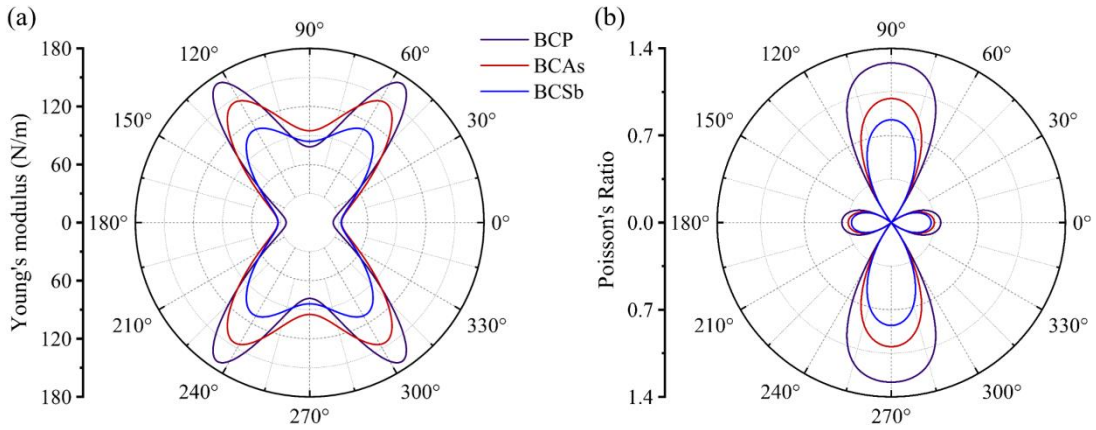

Fig. S2 Orientation−dependent anisotropic characteristics of (a) Young's modulus and (b) Poisson's ratio of BCX monolayers.

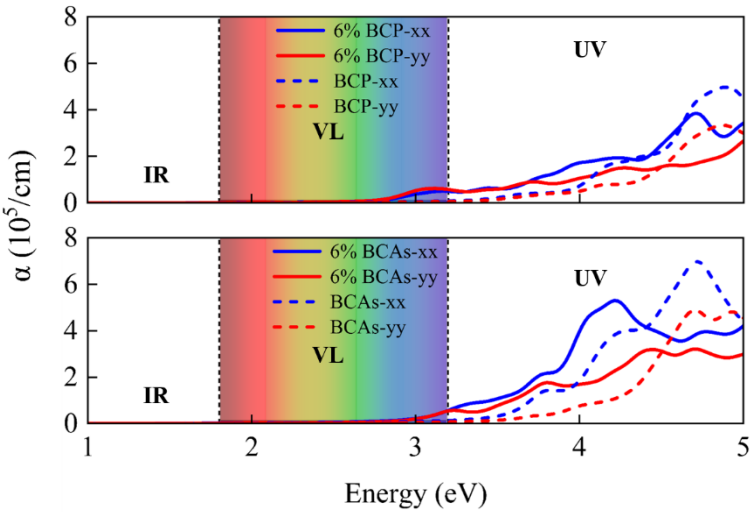

Fig. S3 In−plane optical absorption coefficients of pristine (in dotted line) and 6% strained (in solid line) BCP and BCAs. The energy ranges for the IR (infrared), VL (visible light), and UV (ultraviolet) regions are marked.

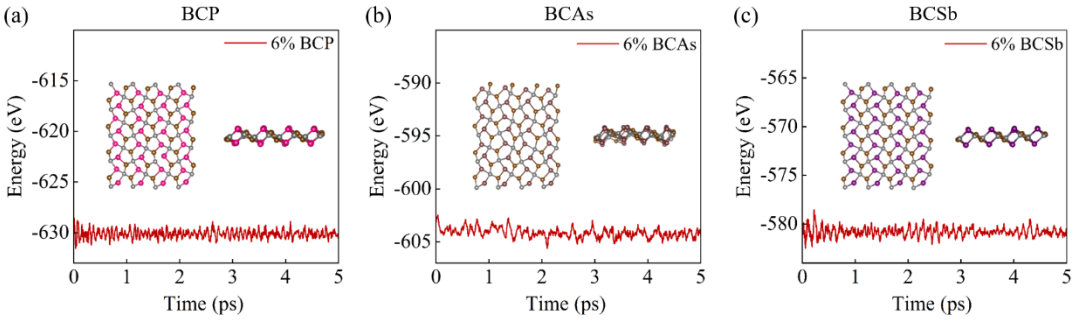

Fig. S4 Energy fluctuations for strained monolayers (a) BCP, (b) BCAs, and (c) BCSb by MD simulations at 300 K. The insets are the snapshots taken from the end of each simulation.

References

1 C. Hou, Y. Shen, W. Sun, Y. Chen, D. Ni and Q. Wang, *J. Mater. Chem. C*, 2022, 10, 10302–10309.