Electronic Supplementary Information for The penta-X_2C family: flexible, auxetic, promising two dimensional photocatalysts with high carrier mobility for water splitting

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Mechanical properties of Penta-X_2C family

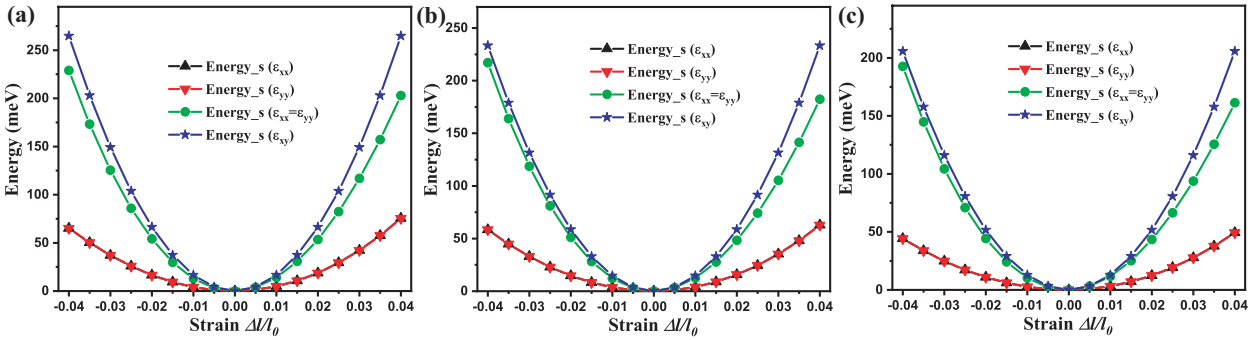

Fig.S1 Strain energy of (a) Penta-P_2C (b) Penta-As_2C (c) Penta-Sb_2C under uniaxial, shear and biaxial in-plane strain, respectively. Note that the uniaxial strain curve is calculated via fixing the lateral lattice constant.

As shown in Fig.S1, the strain energy as a function of ε in the range of -4%$< \varepsilon <$ 4% with an increment of 0.5% are calculated to obtain the elastic stiffness constants.

For the tetragonal symmetry of penta-X_2C (X=P, As, Sb) family, the strain ε parallel to the θ (θ is the angle respect to a direction) direction $\varepsilon_{\parallel}$ and the strain ε perpendicular to the θ direction $\varepsilon_{\perp}$ induced by the unit stress $\sigma(\theta)$ can be expressed as [1, 2]

$$\varepsilon_{\parallel} = \frac{C_{11}\sin^4\theta + C_{22}\cos^4\theta - 2C_{12}\sin^2\theta\cos^2\theta}{C_{11}C_{22} - C_{12}^2} + \frac{\sin^2\theta\cos^2\theta}{C_{66}}$$

$$\varepsilon_{\perp} = \frac{(C_{11} + C_{22})\sin^2\theta\cos^2\theta - C_{12}(\sin^4\theta + \cos^4\theta)}{C_{11}C_{22} - C_{12}^2} - \frac{\sin^2\theta\cos^2\theta}{C_{66}}$$

, respectively.

Thus, the orientation dependent Young's modulus (Y(θ)) and Poisson's ratio ($\nu(\theta)$) can be obtained via the following equations:

$$Y(\theta) = \frac{\sigma}{\varepsilon_{\parallel}} = \frac{C_{11}C_{22} - C_{12}^2}{C_{11}\sin^4\theta + C_{22}\cos^4\theta + (\frac{C_{11}C_{22} - C_{12}^2}{C_{66}} - 2C_{12})\sin^2\theta\cos^2\theta} \quad \text{(S1)}$$

$$\nu(\theta) = -\frac{\varepsilon_{\perp}}{\varepsilon_{\parallel}} = \frac{C_{12}(\sin^4\theta + \cos^4\theta) - (C_{11} + C_{22} - \frac{C_{11}C_{22} - C_{12}^2}{C_{66}})\sin^2\theta\cos^2\theta}{C_{11}\sin^4\theta + C_{22}\cos^4\theta + (\frac{C_{11}C_{22} - C_{12}^2}{C_{66}} - 2C_{12})\sin^2\theta\cos^2\theta} \quad \text{(S2)}$$

, respectively.

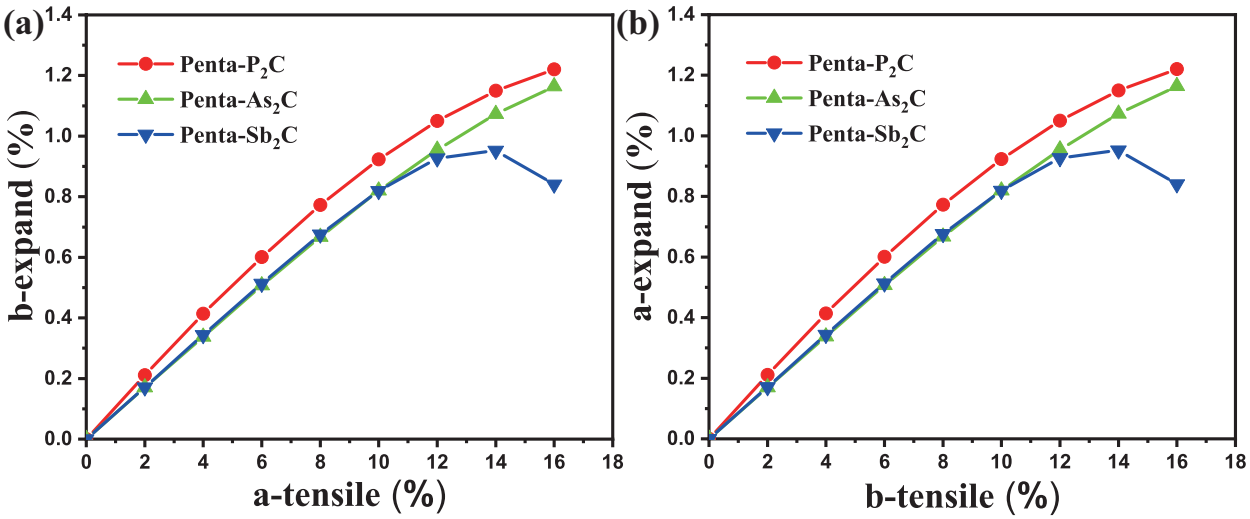

Fig.S2 Lattice constant expansion ratio versus tensile ratio tested by tensile strain (a) along the ***a*** direction and (b) along the ***b*** direction Penta-P_2C, Penta-As_2C, and Pena-Sb_2C, respectively.

The orbital-projected band structures and density of states for Penta-X_2C family

The elastic constant and deformation potential constant of Penta-X_2C family

[1] H. Wang, X. Li, P. Li, and J. Yang, Nanoscale **9**, 850 (2017).

[2] V. Wang and W. Geng, Journal of Physical Chemistry C **121**, 10224 (2017).

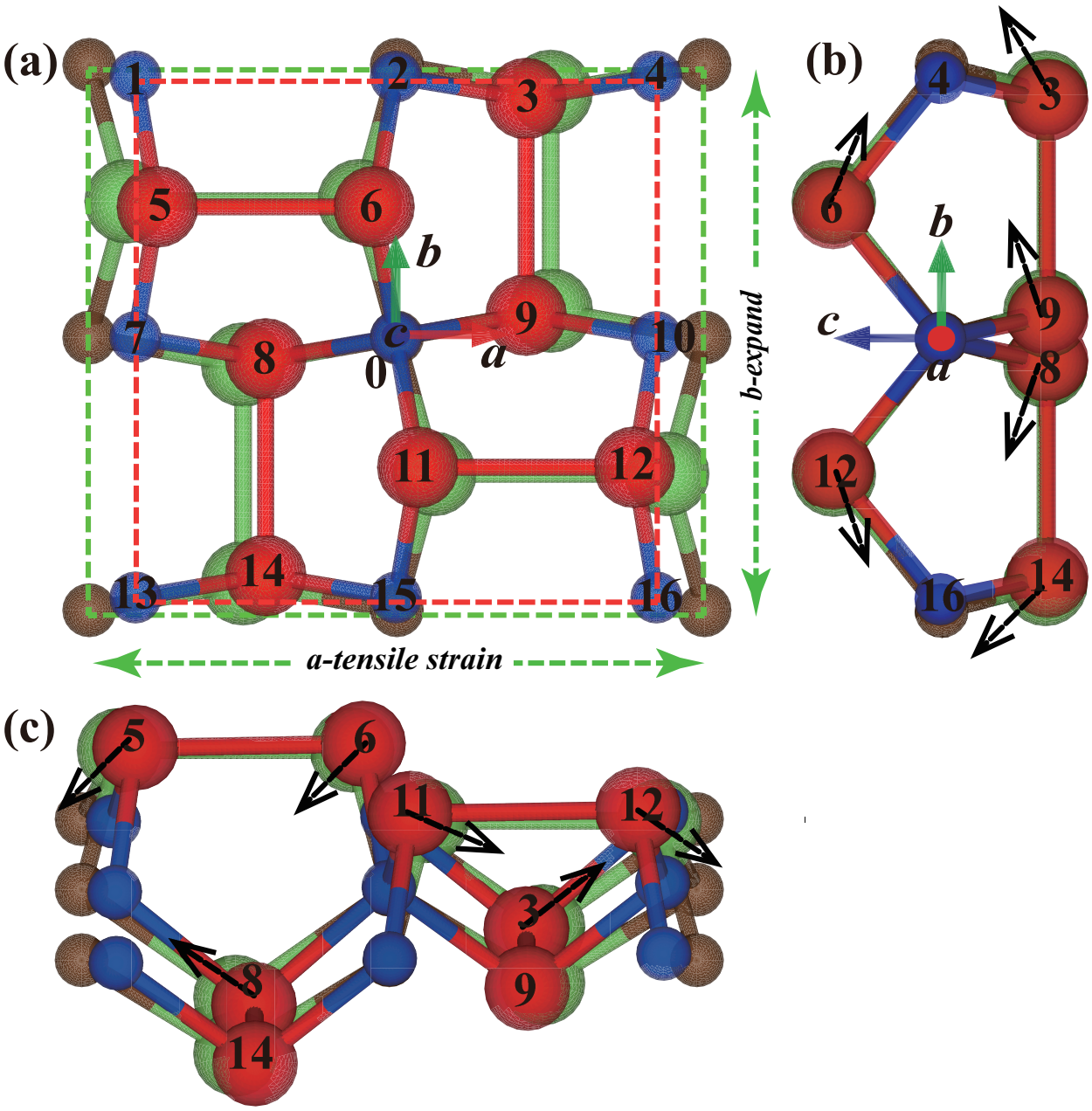

Fig.S3 Illustration for Penta-X_2C family stretched along the ***a*** direction (marked in green dash line) compared with the initial unitcell (marked in red dash line). The Atoms are moved in the direction of the attached arrows.

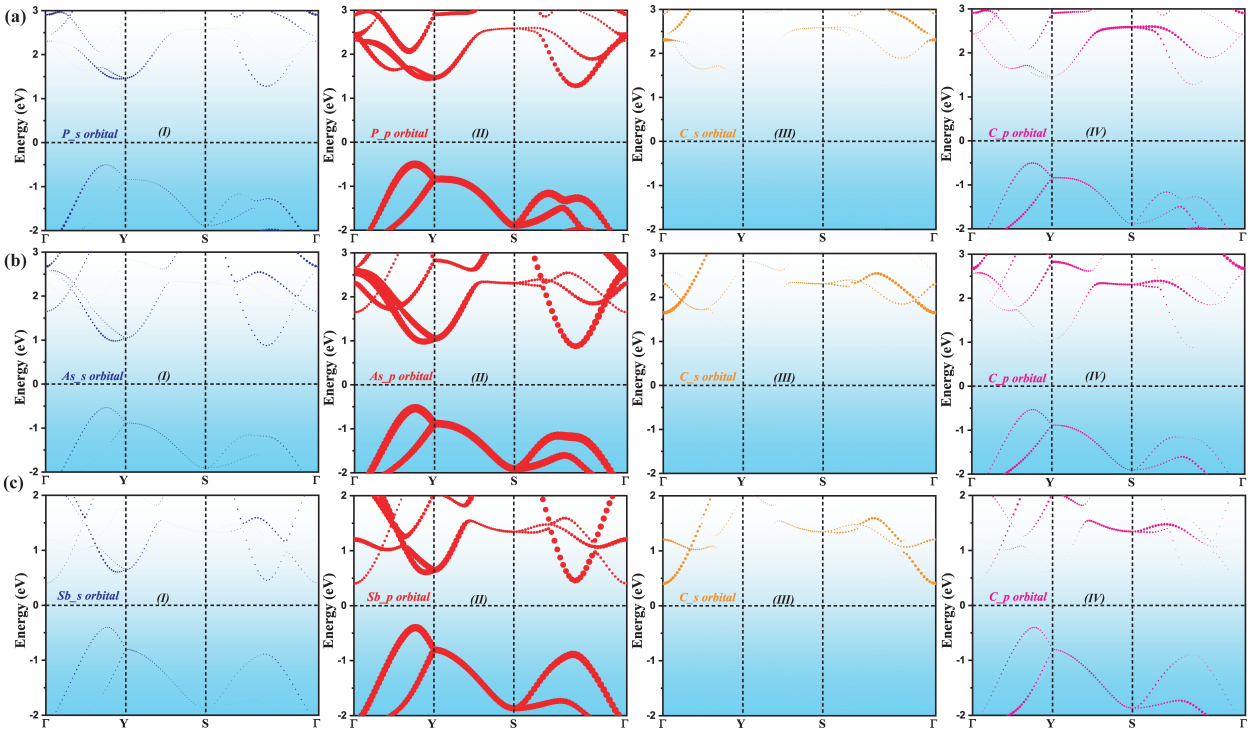

Fig.S4 The orbital-projected band structures of (a) Penta-P_2C (b) Penta-As_2C (c) Penta-Sb_2C, respectively.

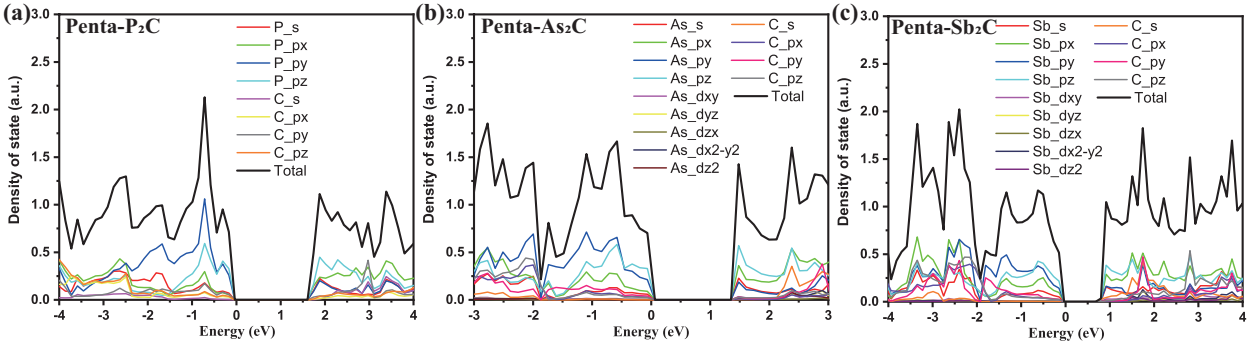

Fig.S5 (a)(b) (c) Projected electronic density of states of Penta-X_2C (X = P, As, Sb), respectively.

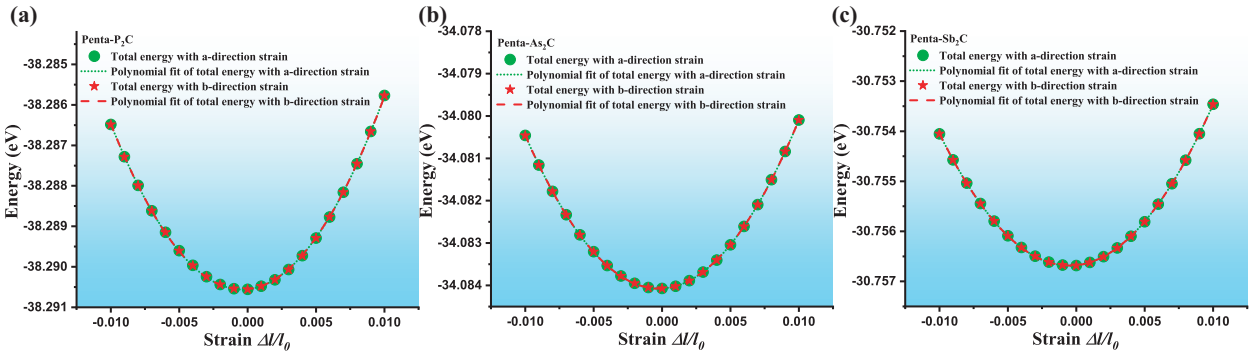

Fig.S6 The polynomial fitting total energy for elastic constant of (a) Penta-P_2C (b) Penta-As_2C (c) Penta-Sb_2C, respectively.

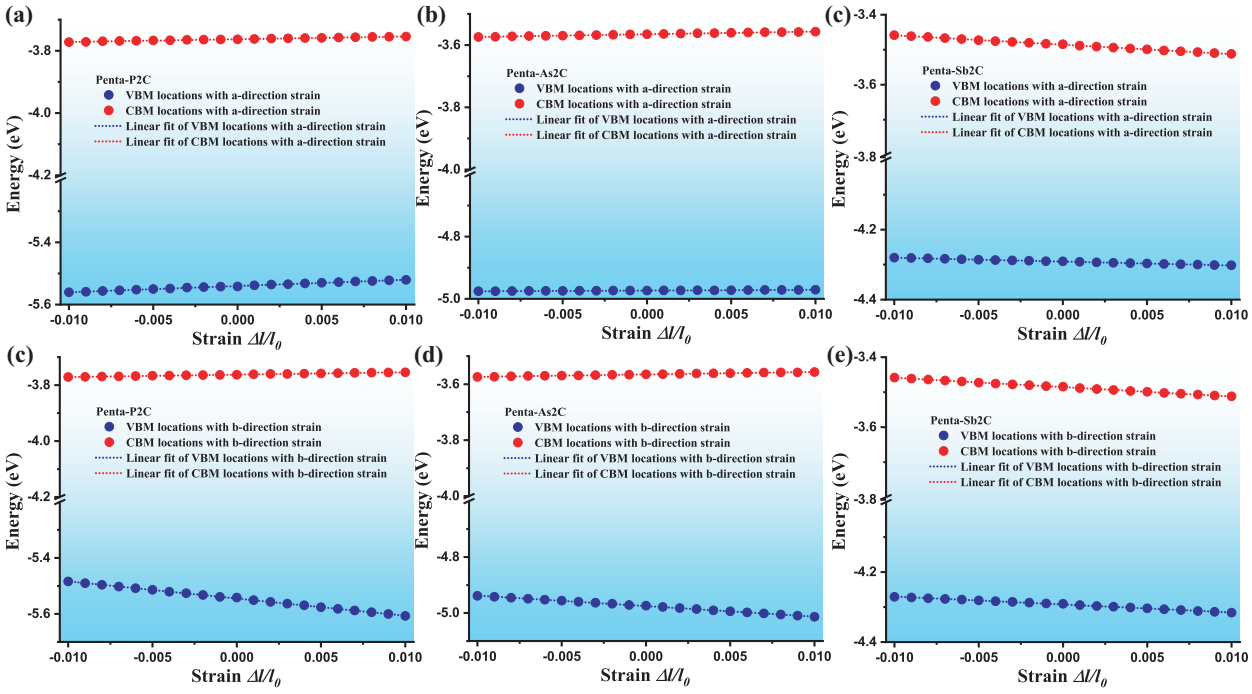

Fig.S7 The linear fitting of VBM and CBM locations of (a) (c) Penta-P_2C (b)(d) Penta-As_2C (c)(e) Penta-Sb_2C corresponding to the applied strain along $\boldsymbol{a}$ and $\boldsymbol{b}$ direction, respectively.