Electronic Supplementary Information for The penta-X$_2$C family: flexible, auxetic, promising two dimensional photocatalysts with high carrier mobility for water splitting

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Mechanical properties of Penta-X$_2$C family

Fig. S1 Strain energy of (a) Penta-P$_2$C (b) Penta-As$_2$C (c) Penta-Sb$_2$C 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 $\varepsilon$ 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$_2$C (X=P, As, Sb) family, the strain $\varepsilon$ parallel to the $\theta$ ($\theta$ is the angle respect to a direction) direction $\varepsilon_{\parallel}$ and the strain $\varepsilon$ perpendicular to the $\theta$ 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 ($Y(\theta)$) and Poisson’s ratio ($\nu(\theta)$) can be obtained via the following equations:

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

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

![Graph showing lattice constant expansion ratio versus tensile ratio tested by tensile strain](image)

**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\(_2\)C, Penta-As\(_2\)C, and Pena-Sb\(_2\)C, respectively.

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The orbital-projected band structures and density of states for Penta-X\(_2\)C family

The elastic constant and deformation potential constant of Penta-X\(_2\)C family

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Fig.S3 Illustration for Penta-X$_2$C 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$_2$C (b) Penta-As$_2$C (c) Penta-Sb$_2$C, respectively.

Fig. S5 (a)(b) (c) Projected electronic density of states of Penta-X$_2$C (X = P, As, Sb), respectively.
Fig. S6 The polynomial fitting total energy for elastic constant of (a) Penta-P$_2$C (b) Penta-As$_2$C (c) Penta-Sb$_2$C, respectively.

Fig. S7 The linear fitting of VBM and CBM locations of (a) Penta-P$_2$C (b) Penta-As$_2$C (c) Penta-Sb$_2$C corresponding to the applied strain along \( a \) and \( b \) direction, respectively.