

Supplementary information (SI) for

**Janus monolayer PXC (X= As and Sb) for photocatalytic
water splitting with negative poisson's ratio**

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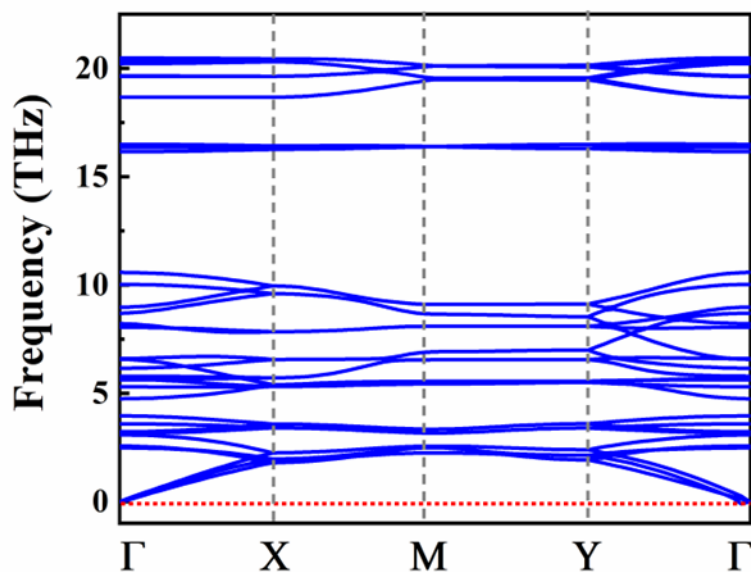


Fig. S1 The phonon spectra of monolayer PSbC.

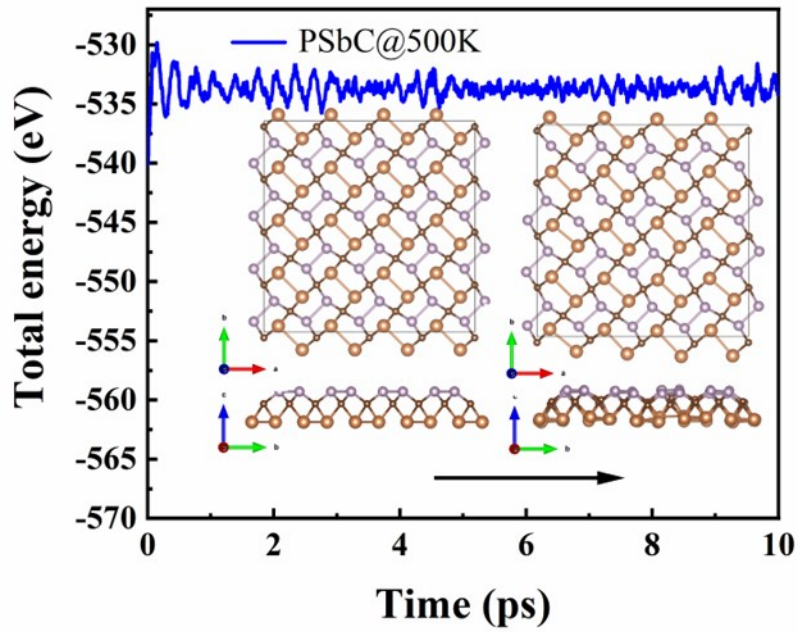


Fig. S2 The total energy of monolayer PSbC and corresponding supercells structure through 10 ps canonical ensemble (NVT) MD simulation with initial temperature set as 500 K.

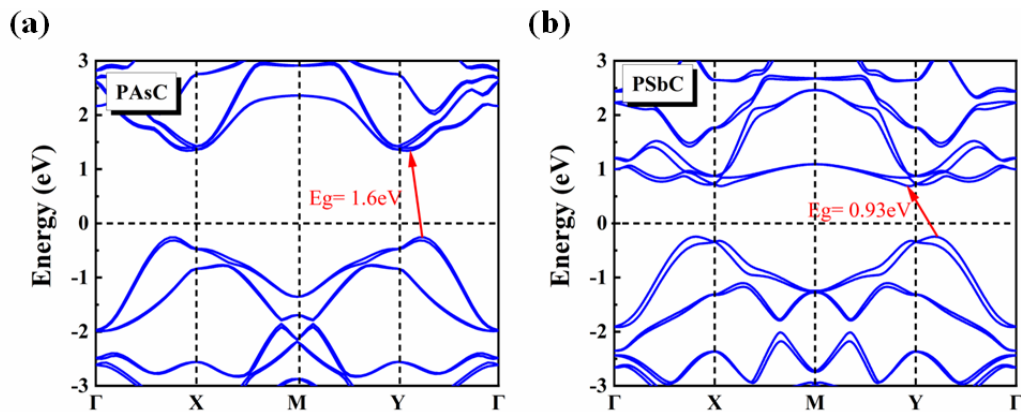


Fig. S3 Calculated band structures of for (a) PAsC and (b) PSbC monolayers employing the PBE + SOC method

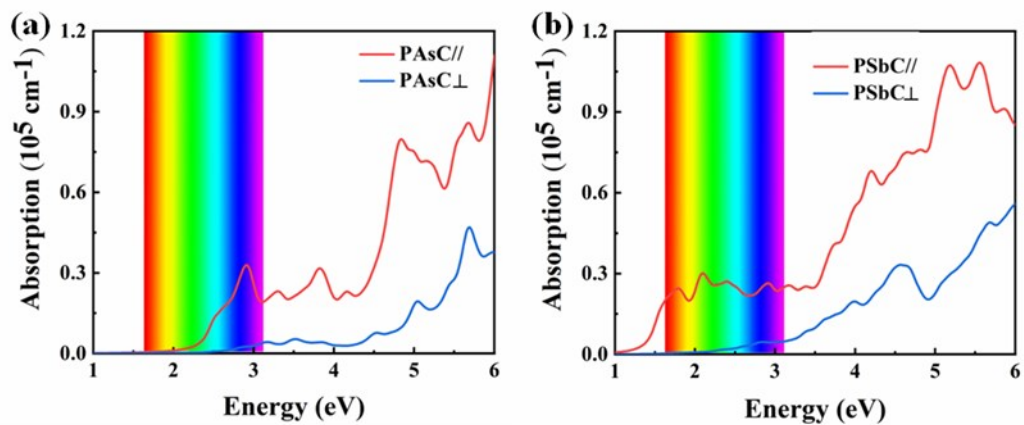


Fig. S4 The calculated optical absorption spectrum of (a) PAsC and (b) PSbC monolayers using HSE06 functional.