Electronic Supplementary Material (ESI) for Nanoscale.

Prediction of 2D IV-V semiconductors: Flexible monolayers with tunable bandgap and strong optical absorption as water-splitting photocatalysts

Luqi Liu[1], Xuxin Kang[1], Shan Gao[1,2], Xiangmei Duan[1,2*]

[1] School of Physical Science and Technology, Ningbo University, Ningbo, P. R. China
E-mail: duanxiangmei@nbu.edu.cn
[2] Laboratory of Clean Energy Storage and Conversion, Ningbo University, Ningbo, P. R. China

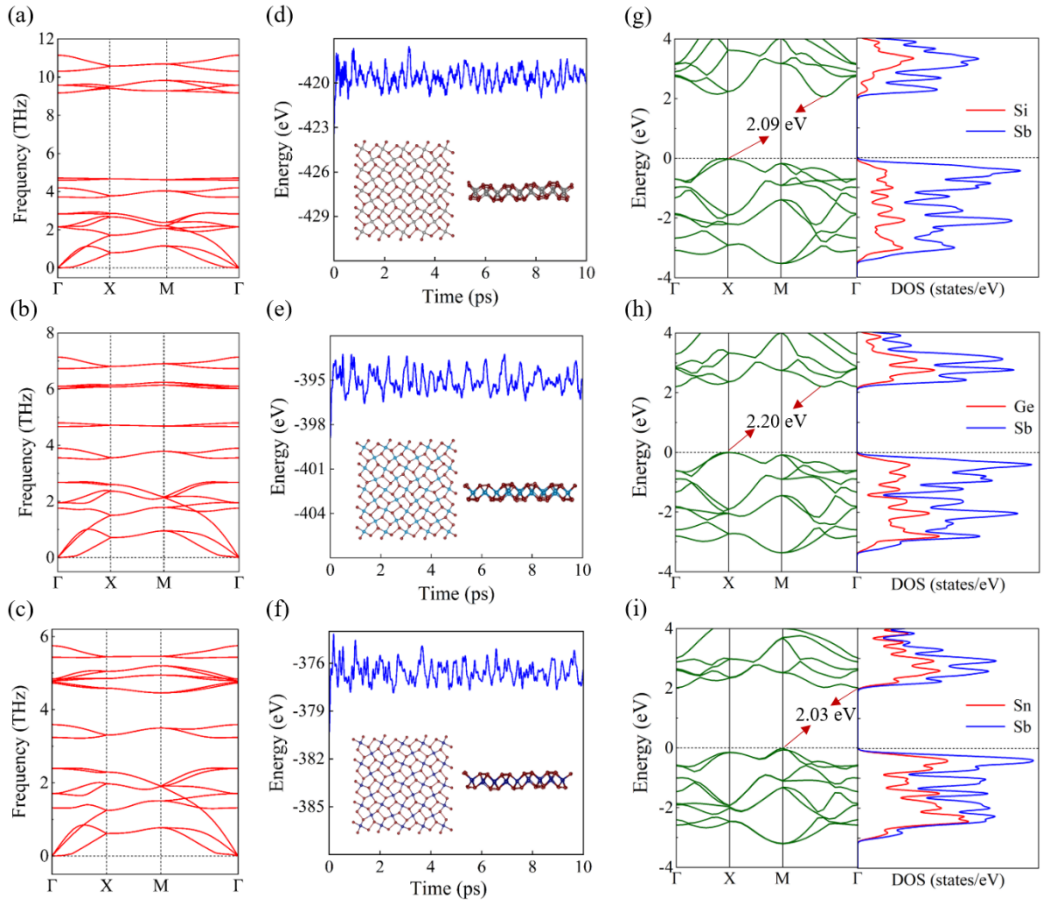

Fig. S1 The phonon spectra (a-c), Energy fluctuations in AIMD simulations at 300 K (d-f), HSE06 band structures and the corresponding partial density of states (g-i) of $SiSb_2$, $GeSb_2$ and $SnSb_2$ monolayers. The insets in (d-f) are the snapshots taken from the end of each simulation.

Table S1. Elastic constants (in Jm^{-2}), Young's modulus (Y, in Jm^{-2}), and Poisson's ratio (v) of XY_2 sheets. The reported data for pentagonal CP_2, CAs_2, CSb_2 and GeP_2 are included for comparison.

XY_2	$C_{11}=C_{22}$	C_{12}	C_{66}	Y	v
$SiSb_2$	30.97	11.45	21.20	42.42	0.37
$GeAs_2$	38.51	10.19	23.26	35.82	0.26
$GeSb_2$	27.11	9.63	18.13	36.50	0.36
SnP_2	37.48	7.60	20.14	35.94	0.20
$SnAs_2$	29.99	8.31	16.84	27.69	0.28
$SnSb_2$	22.13	7.56	13.20	19.54	0.34
CP_2[5]	84.11	44.72	79.18	60.33	0.53
CAs_2[5]	63.77	41.07	61.46	37.32	0.64
CSb_2[5]	40.78	36.20	44.94	8.65	0.89
GeP_2[6]	47.41	9.42	16.88	45.53	0.20

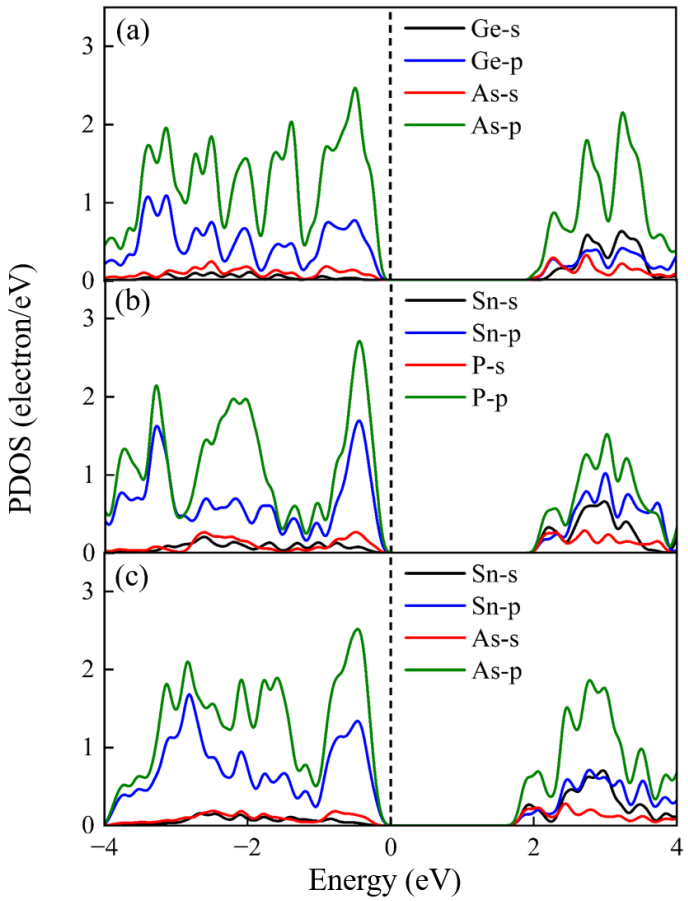

Fig. S2 The partial density of states (PDOS) of $GeAs_2$ (a), SnP_2 (b), and $SnAs_2$ (c).

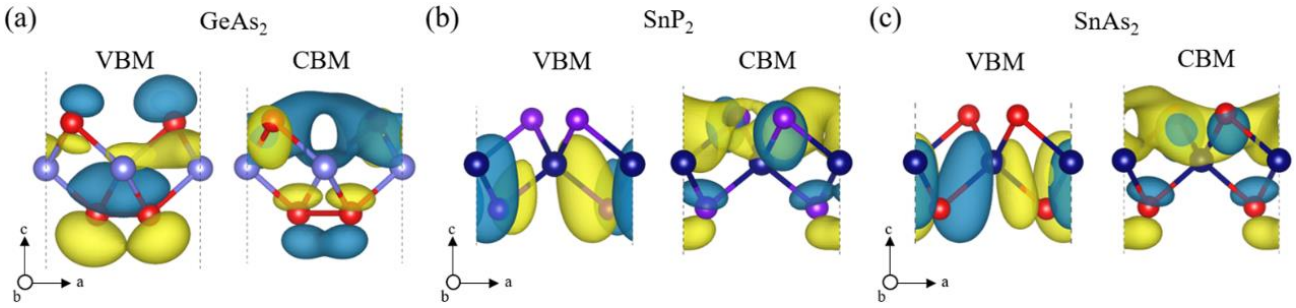

Fig. S3 The spatial charge density of VBM and CBM of the pentagonal $GeAs_2$ (a), SnP_2 (b), and $SnAs_2$ (c). The isolevels are set to be 0.004 $eÅ^{-3}$.

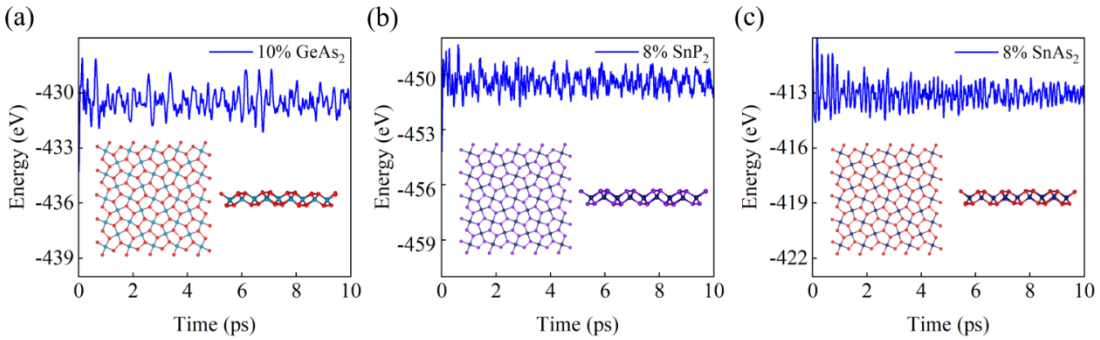

Fig. S4 Energy fluctuations for strained monolayers $GeAs_2$ (a), SnP_2 (b), and $SnAs_2$ (c) by MD simulations at 300 K. The insets are the snapshots taken from the end of each simulation.

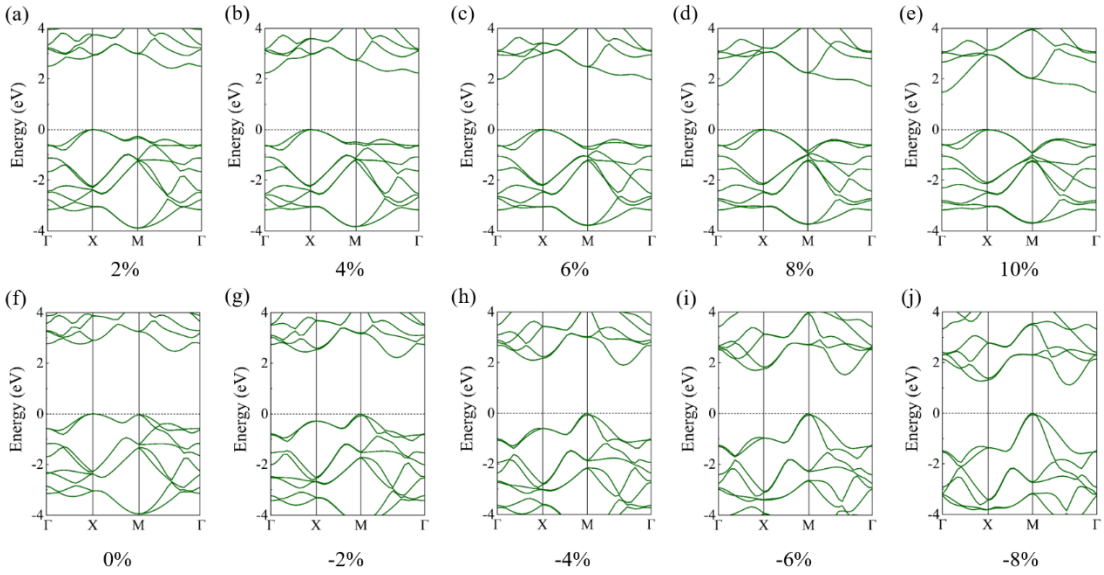

Fig. S5 (a-j) Band structure of $GeAs_2$ under different biaxial strains.

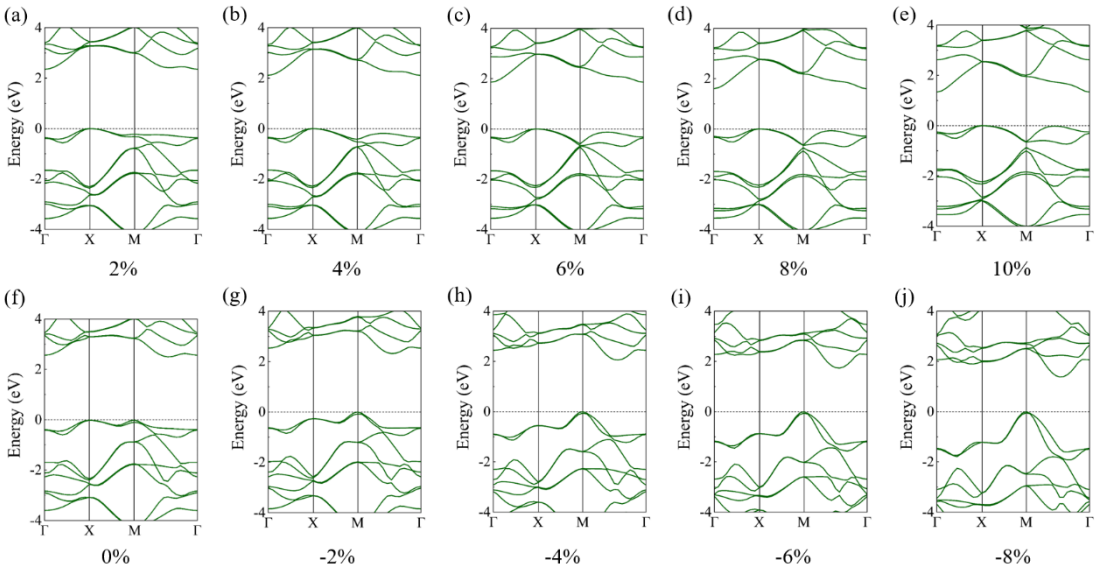

Fig. S6 (a-j) Band structure of SnP_2 under different biaxial strains.

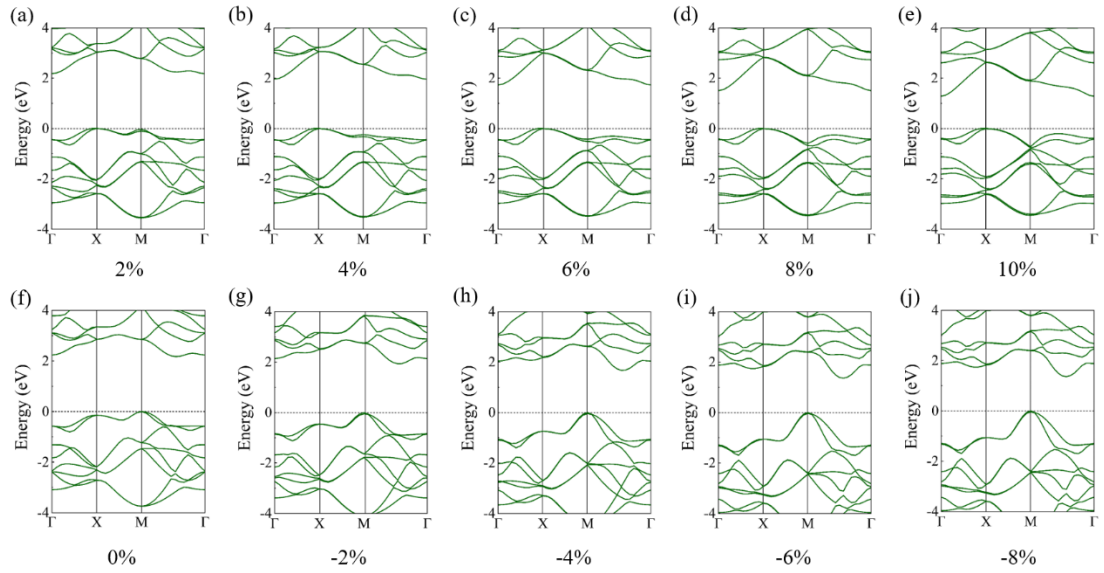

Fig. S7 (a-j) Band structure of $SnAs_2$ under different biaxial strains.

References

1 S. Sun, F. Meng, Y. Xu, J. He, Y. Ni and H. Wang, J. Mater. Chem. A, 2019, 7, 7791–7799.

2 F. Shojaei, J. R. Hahn and H. S. Kang, J. Mater. Chem. A, 2017, 5, 22146–22155.