

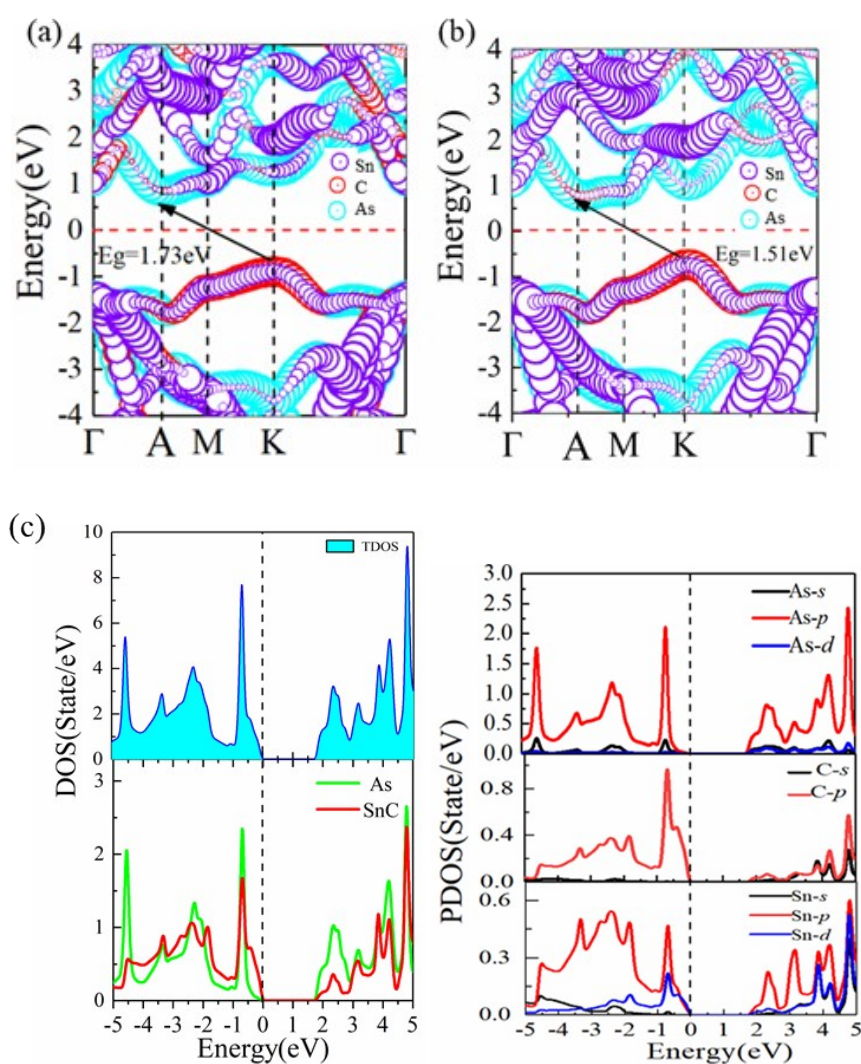
# Investigation on the mechanism of overall water splitting in UV-visible and infrared region with SnC/Arsenene vdW heterostructures in different configurations

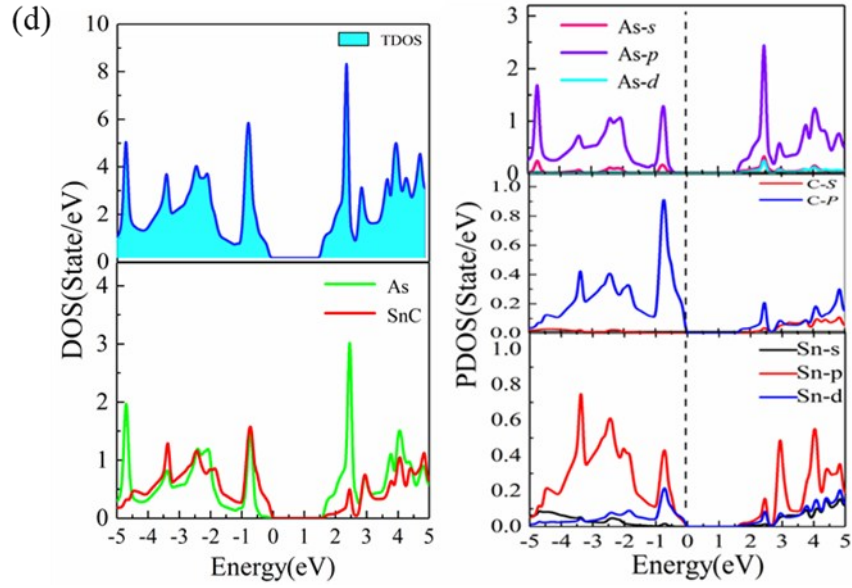
Jian Chai, Zhong Wang\*, Yuee Li\*

School of information science and engineering, Lanzhou University, China

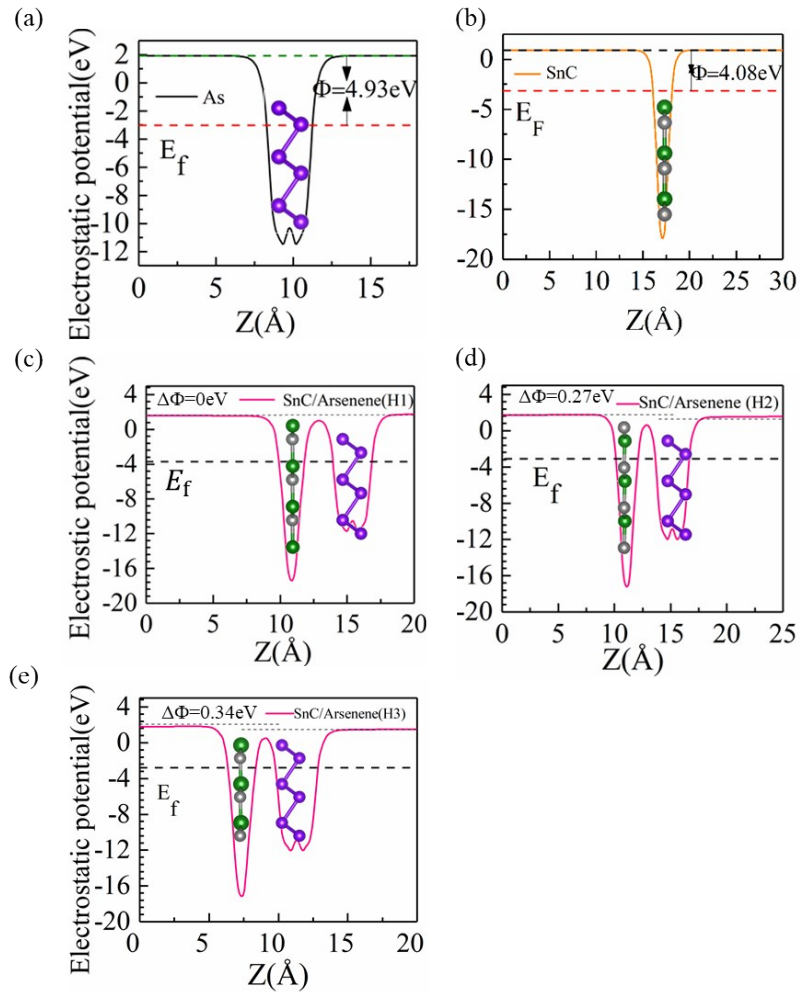
[\\*liyuee@lzu.edu.cn](mailto:liyuee@lzu.edu.cn) [wangzhong@lzu.edu.cn](mailto:wangzhong@lzu.edu.cn)

## Supporting information

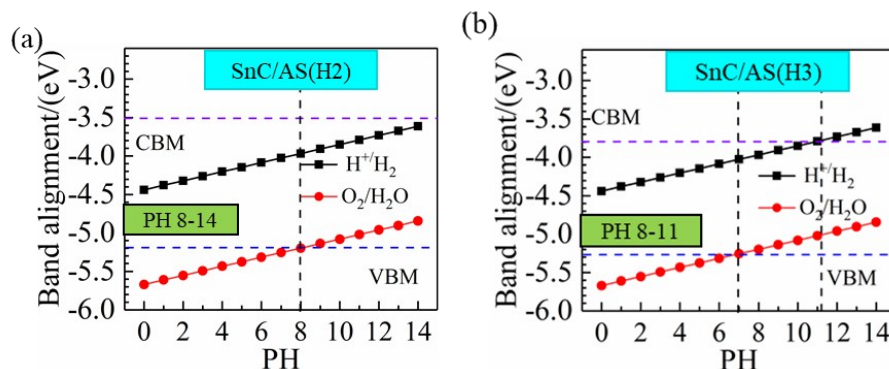




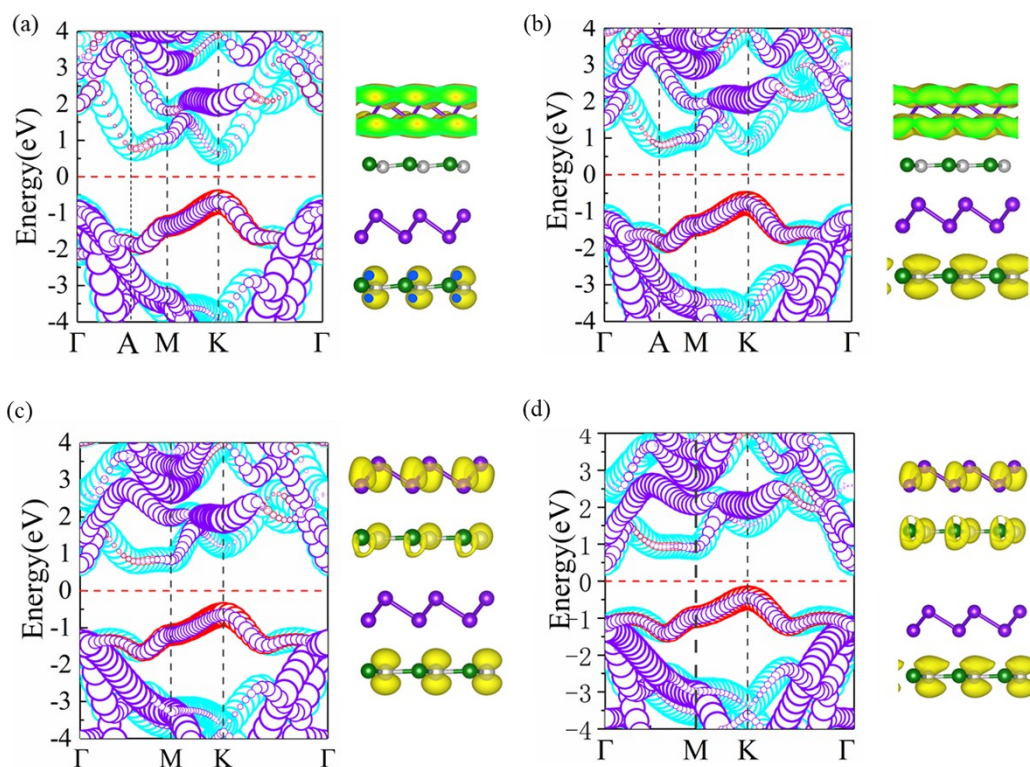
**Fig. S1** Flat band based on the atoms of with SnC/Arsenene heterostructure in (a) H2 , (b)H3 configuration based on the HSE06 functional. The PDOS of SnC/Arsenene heterostructure in (c) H2, (d) H3 configuration



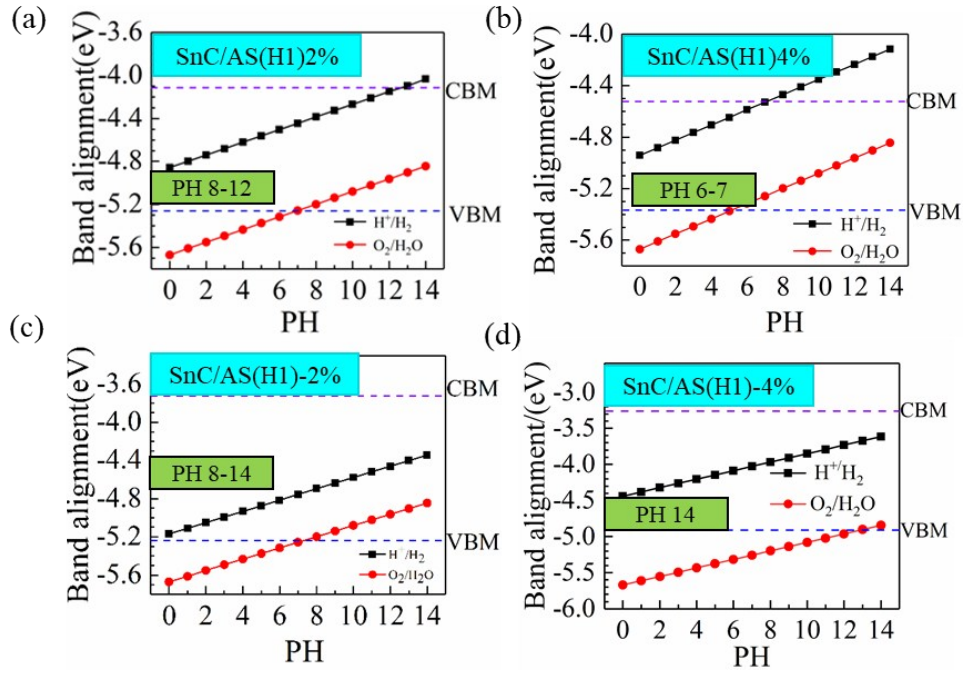
**Fig. S2** Calculated electrostatic potentials for monolayer (a) As, (b) SnC, SnC/Arsenene heterostructure in (c)H1, (d)H2, (e)H3 configuration



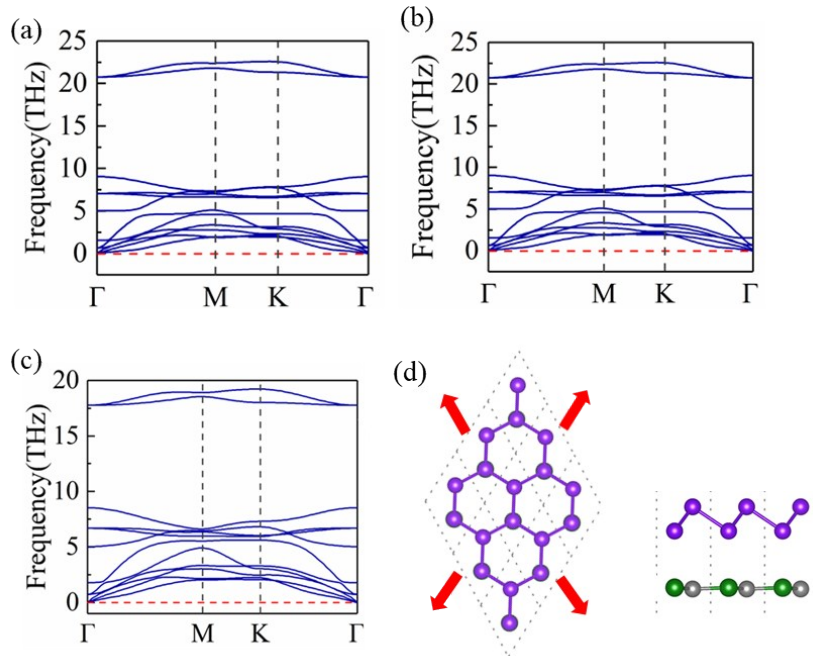
**Fig. S3** The relationship between oxidation potential and reduction potential of water splitting corresponding to different PH values and CBM and VBM of SnC/Arsenene heterostructure in (a) H2,(b) H3 configuration



**Fig. S4** Flat band based on the atoms(left) and the partial charge density of CBM and VBM(right), (the isovalue is  $0.002e/A^{-3}$ ) of SnC/Arsenene heterostructure in H3 configuration as functions of the in-layer biaxial strain: (a) -2%, (b) -4%, (c) 2%, (d)4%



**Fig. S5** The relationship between oxidation potential and reduction potential of water splitting as functions of PH values and CBM and VBM of SnC/Arsenene heterostructure in H3 configuration corresponding to different in-layer biaxial strains: (a) -2%, (b) -4%, (c) 2%, (d) 4%



**Fig. S6** The phonon spectrum of SnC/Arsenene heterostructure in H3 configuration at (a) 0% , (b) +2% , (c) +4% biaxial strain, respectively, (d) biaxial Strain applied on SnC/Arsenene heterostructure in H3 configuration