Electronic Supplement Information for

Strain-induced excellent photocatalytic performance in Z-scheme BlueP/γ-SnS heterostructures for water splitting

Quan Li[a], Jiabao Wang[a], Hao Hang[a], Guangting Zhao[a], Ling-Ling Wang[b] and Xiaojun Zhu[*c]

[a] School of Energy and Mechanical Engineering, Jiangxi University of Science and Technology, Nanchang 330013, China.

[b] School of Physics and Electronics, Hunan University, Changsha 410082, China.

[c] School of Software Engineering, Jiangxi University of Science and Technology, Nanchang 330013, China.

[*] Corresponding author.
E-mail address: zhuxiaojun@jxust.edu.cn.

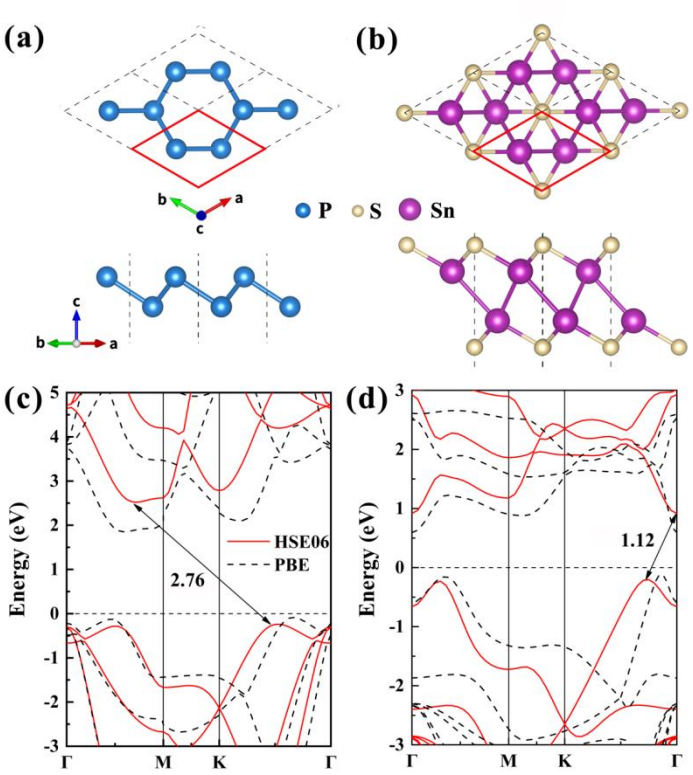

Figure S1 Top (upper) and side (downside) views of (a) BlueP and (b) γ-SnS monolayers. Blue, brownish yellow and purple balls represent P, S and Sn atoms, respectively. Band structure of (c) BlueP and (d) γ-SnS monolayers calculated with PBE and HSE06 functionals. The Fermi level was set to zero.

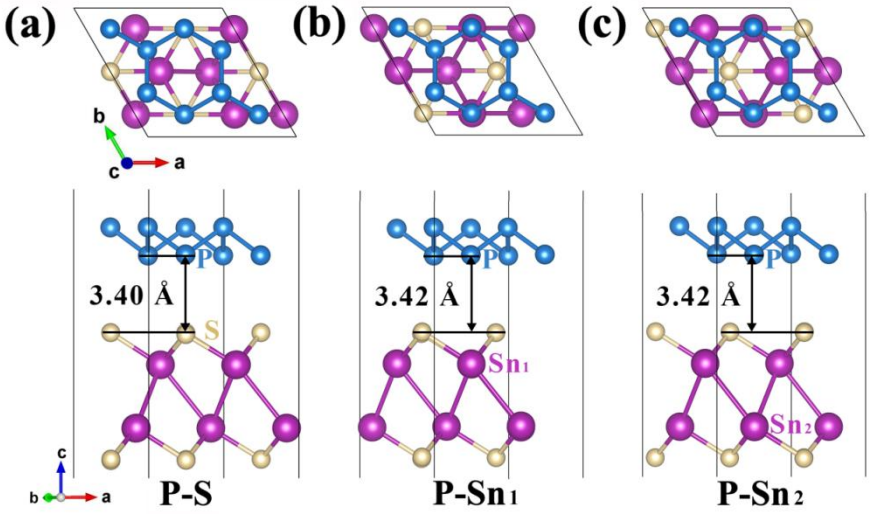

Figure S2 Top (upper) and side (downside) views of the three stacking patterns with different atom-alignment types for BlueP/γ-SnS heterobilayers. The interlayer distance is given in the corresponding configuration.

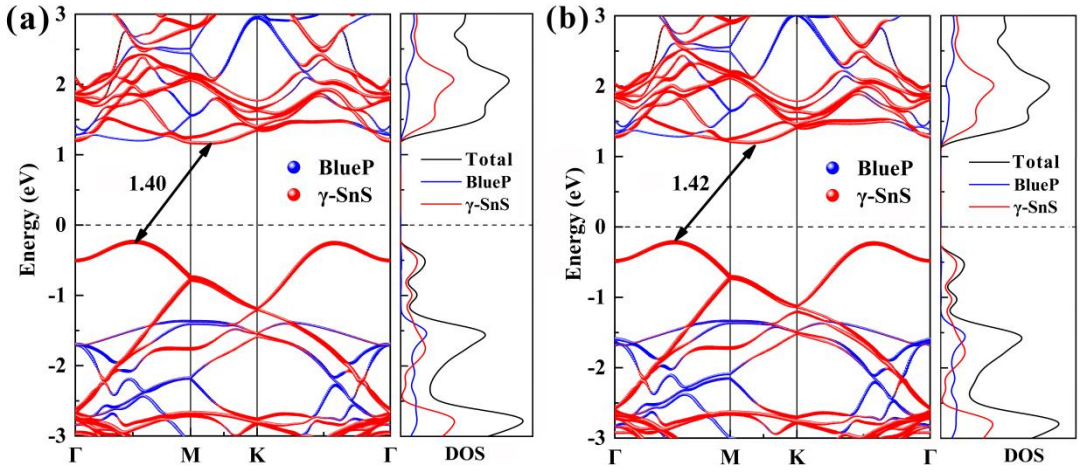

Figure S3 Projected band structures (left) and PDOS (right) of (a) P-Sn_1 and (b) P-Sn_2. The blue and red patterns in band structures denote the weight of BlueP and γ-SnS monolayers, respectively. The black, blue, and red lines in the DOS represent the density of states for the heterojunction, BlueP monolayer and γ-SnS monolayer, respectively. The dashed lines represent the Fermi level.

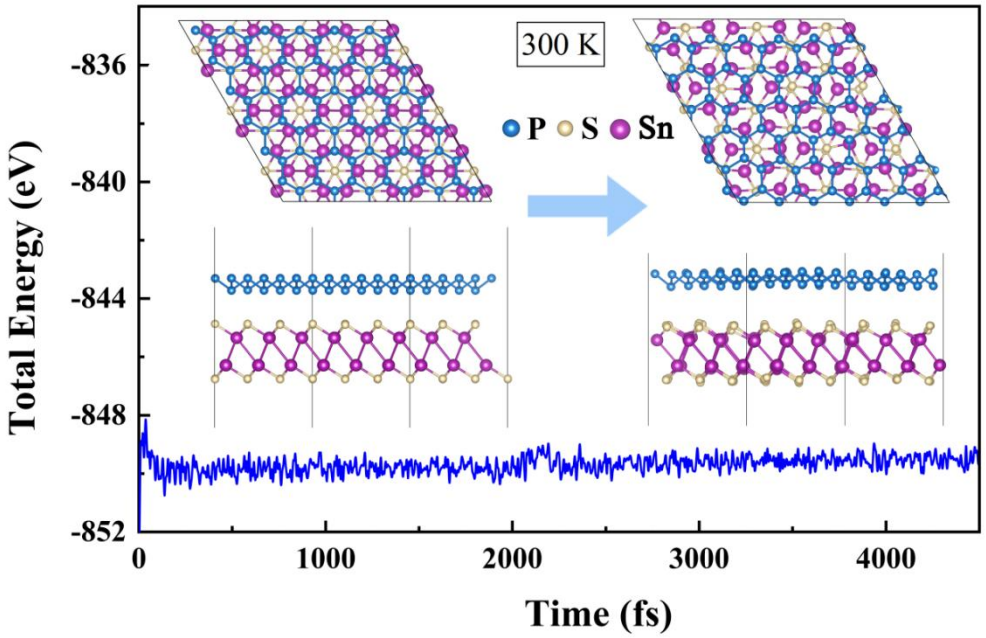

Figure S4 Total potential energy fluctuation with the AIMD simulation time at 300 K for the BlueP/γ-SnS heterobilayer. The insets show the initial and final structures in AIMD simulation, respectively.

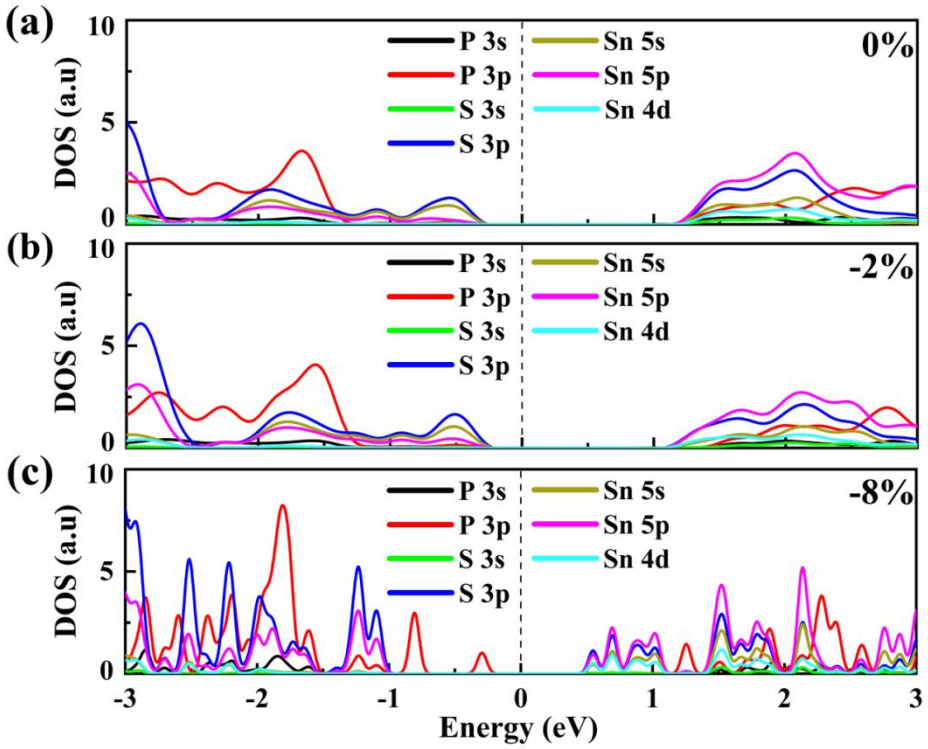

Figure S5 Atom-resolved density of states (DOS) of the BlueP/γ-SnS heterojunction under (a) 0%, (b) -2%, and (c) -8% strains.

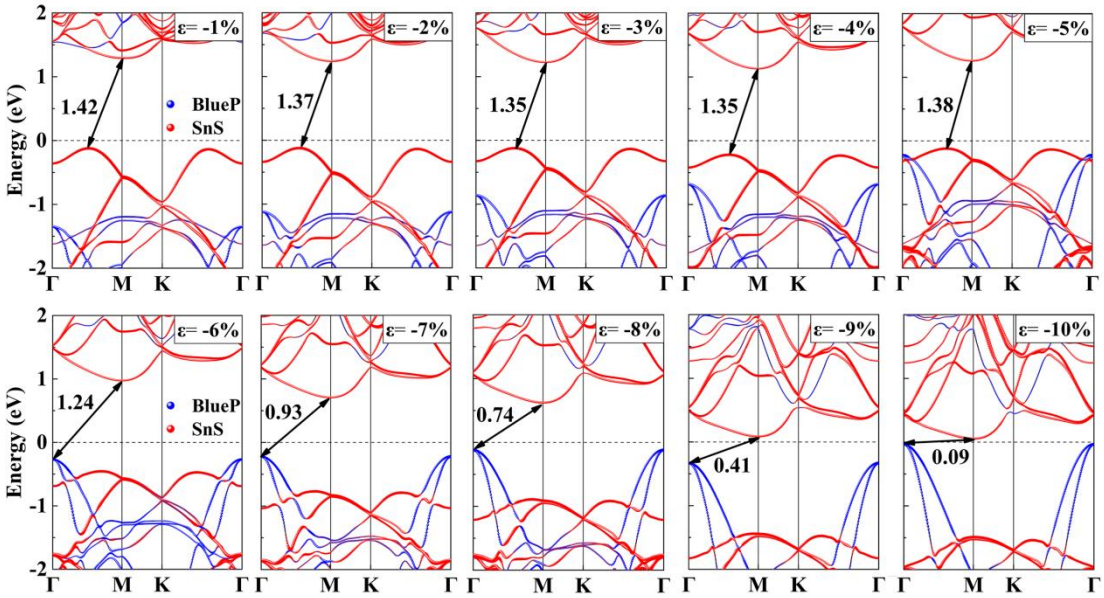

Figure S6 The projected band structures of BlueP/γ-SnS bilayer under different compressive strains (-10% ≤ ε ≤ -1%). The curves highlighted by blue and red spheres represent the BlueP and γ-SnS components, respectively. The Fermi level was set to zero.

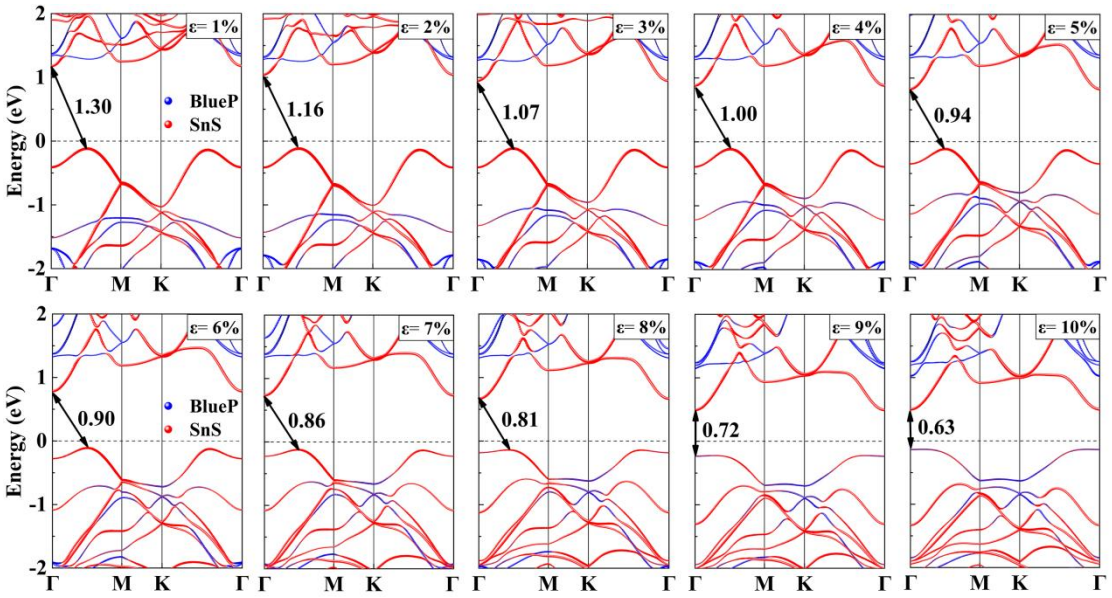

Figure S7 The projected band structures of BlueP/γ-SnS heterobilayer under different tensile strains (1% ≤ ε ≤ 10%). The curves highlighted by blue and red spheres represent the BlueP and γ-SnS components, respectively. The Fermi level was set to zero.

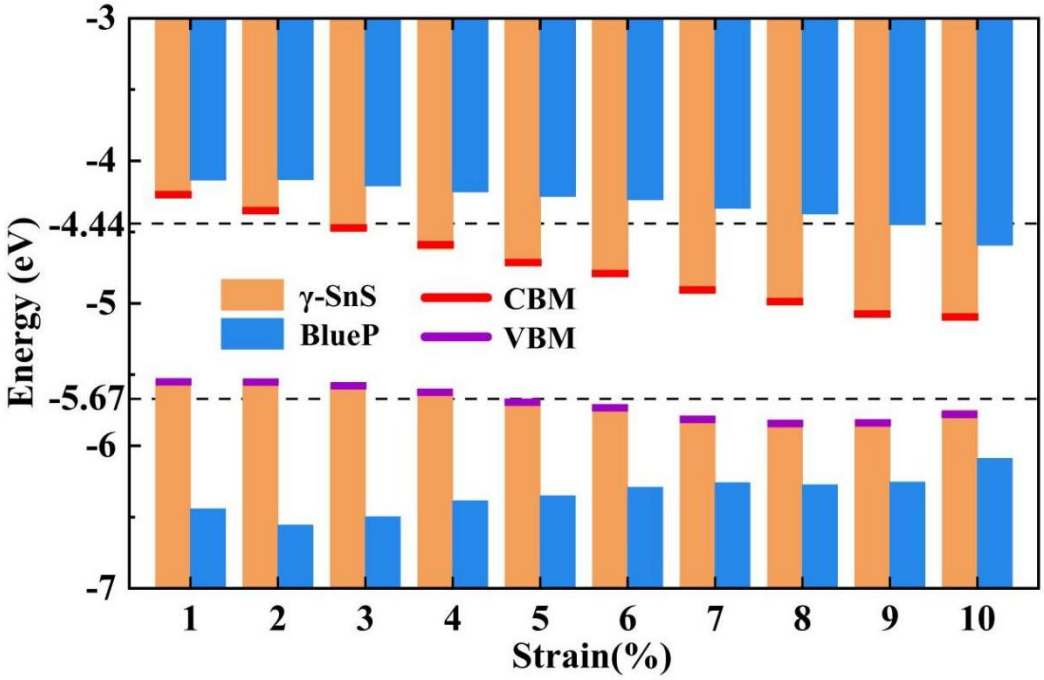

Figure S8 The band edge positions of BlueP and γ-SnS monolayers in BlueP/γ-SnS bilayer under various tensile strains (1% ≤ ε ≤ 10%), with respect to water redox potentials at pH=0. The blue and orange columns stand for the BlueP and γ-SnS, respectively.

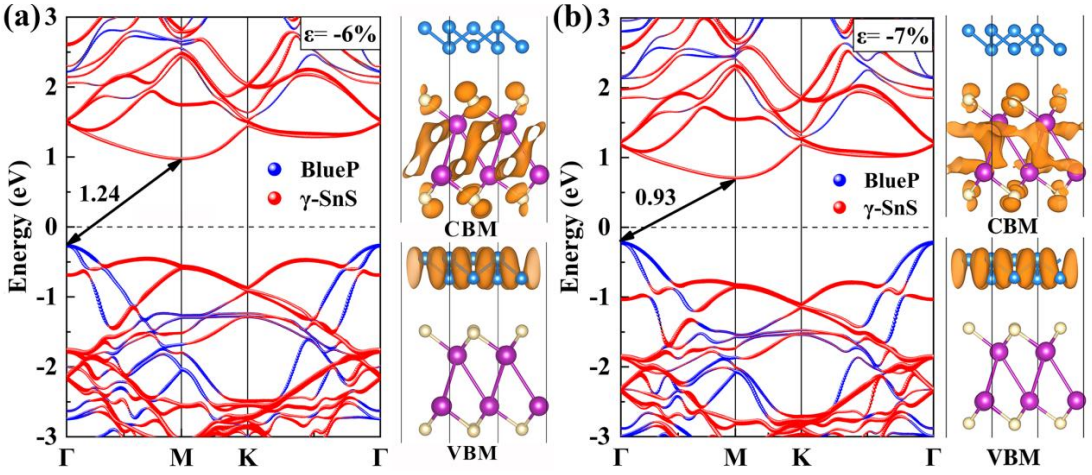

Figure S9 The projected band structures and the partial charge density (VBM and CBM) of the BlueP/γ-SnS heterojunction under (a) -6% and (b) -7% strains.

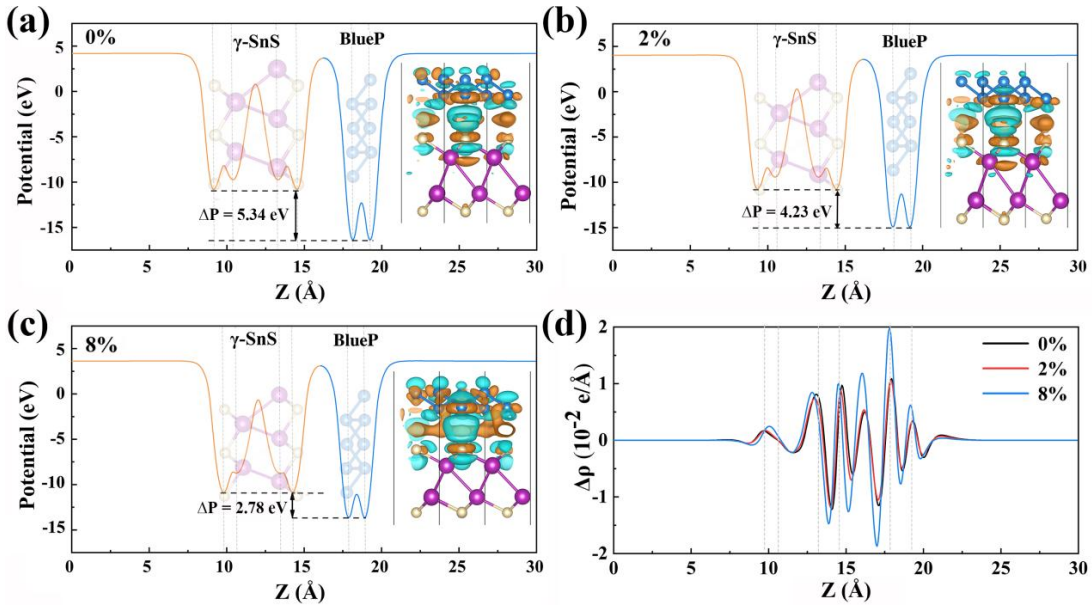

Figure S10 , The electrostatic potential and three-dimensional charge density difference along the z-direction for the BlueP/γ-SnS heterojunction at (a) 0%, (b) 2%, and (c) 8% strains. The contour values were set at 2×10^{-4} e/Å^3. The orange and blue contours respectively denote the accumulation and depletion of electrons in space. (d) The planar-averaged charge density difference of the BlueP/γ-SnS heterojunction under 0%, 2%, and 8% strains.

Table S1 Different stacking modes, lattice constants (a and b), interface area (Area), interface binding energy (E_b), interlayer distance (Distance), and band gap of BlueP/γ-SnS heterostructures.

System	Lattice constant (Å)		Area (Å^2)	E_b (meV/Å^2)	Distance (Å)	Band gap (eV)	
	a	b				PBE	HSE06
P-S	6.63	6.63	38.03	-8.92	3.40	0.90	1.41
P-Sn_1	6.63	6.63	38.06	-8.89	3.42	0.89	1.40
P-Sn_2	6.63	6.61	37.95	-8.82	3.42	0.94	1.42

Table S2 Reduced effective masses (m), 2D elastic moduli (C), deformation potential constant (E) and carrier mobilities (μ) of BlueP and γ-SnS monolayers along different directions.

Carrier type	System	m_x (m_0)	m_y (m_0)	C_x (N/m)	C_y (N/m)	E_x (eV)	E_y (eV)	μ_x (cm^2 V^{-1} S^{-1})	μ_y (cm^2 V^{-1} S^{-1})
Electron	BlueP	0.92	1.05	78.15	78.26	2.26	7.42	360.83	29.40
	γ-SnS	0.21	0.21	129.92	128.32	-6.42	-5.96	1546.88	1725.86
Hole	BlueP	0.89	0.80	78.15	78.26	2.00	1.40	548.67	1246.55
	γ-SnS	0.31	0.31	129.92	128.32	-3.26	-3.73	2704.89	2144.52