Enhancing Photocatalytic Water Splitting via GeC/SGaSnP Z-Scheme Heterojunctions with Built-in Electric Fields

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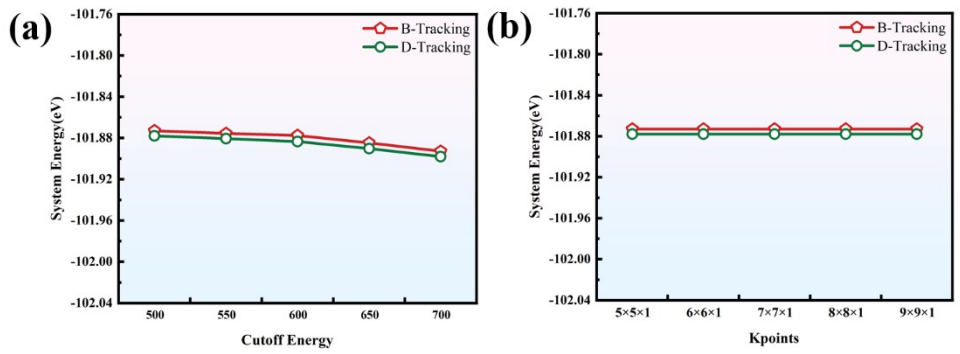

Fig. S1: Convergence Tests for B-stacking and D-stacking GeC/SGaSnP heterojunctions. (a) Total energy variations with different plane-wave energy cutoffs (500 eV, 550eV, 600 eV, 650eV, 700 eV) for B-stacking and D-stacking configurations. (b) Total energy variations with different k-point grid densities (5×5×1, 6×6×1, 7×7×1, 8×8×1, 9×9×1) for B-stacking and D-stacking configurations.

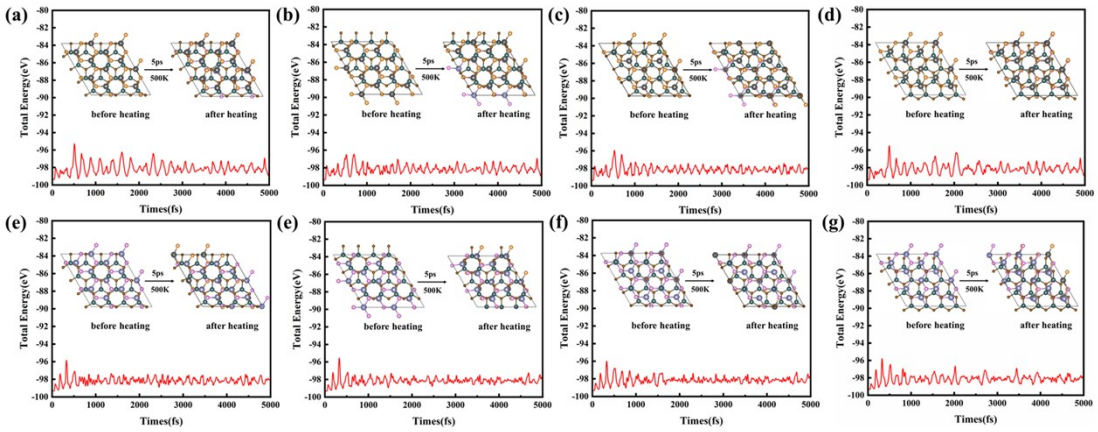

Fig. S2: Ab initio molecular dynamics (AIMD) simulations of (a) stacking mode A, (b) stacking mode B, (c) stacking mode C, (d) stacking mode D, (e) inverted stacking mode A', (f) inverted stacking mode B', (g) inverted stacking mode C', and (h) inverted stacking mode D' of GeC/SGaSnP. The temperature was set to 500 K with a time step of 2 fs, and a simulation time of 5 ps.

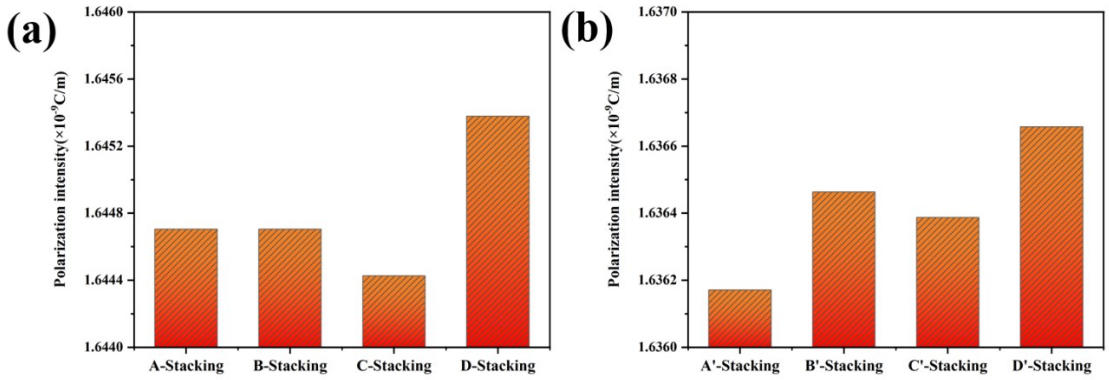

Fig. S3: Calculated polarization intensities of the GeC/SGaSnP heterostructures for stacking configurations A–D (a) and A'–D' (b), employing the Berry phase method.

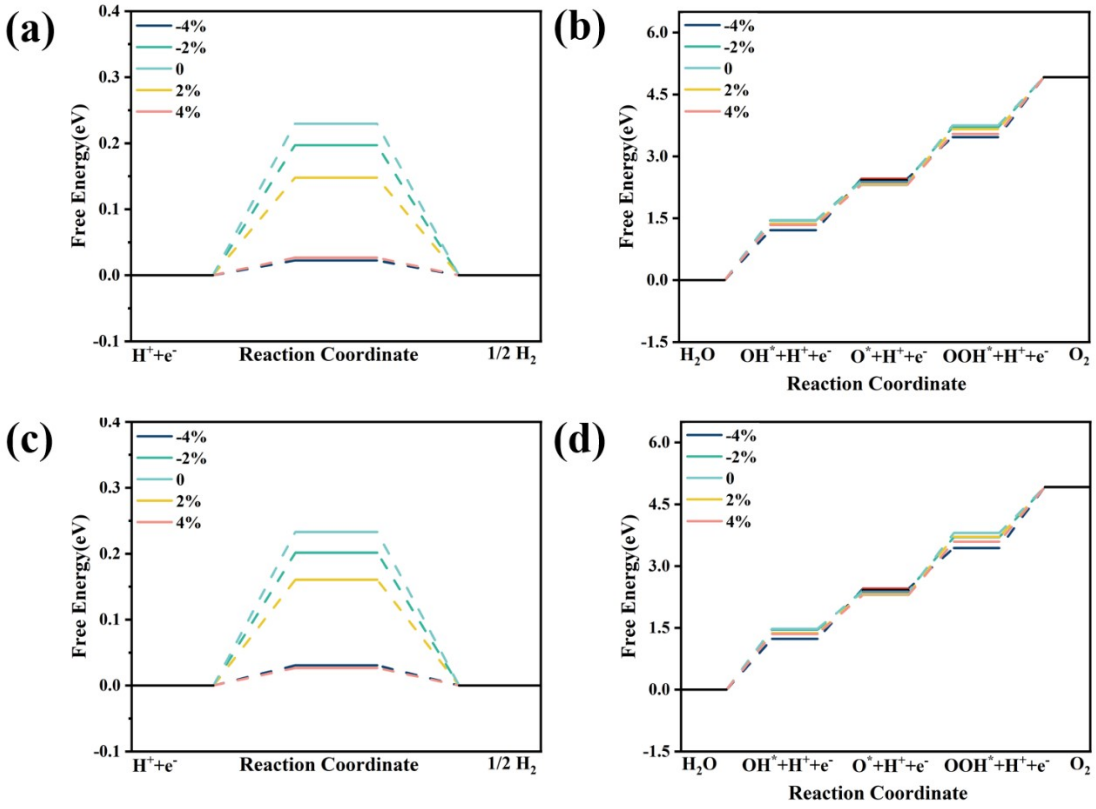

Fig. S4: Effect of strain on the HER and OER performance in the B-stacking and D-stacking configurations. Figure (a) and (b) present the HER and OER performance for the B-stacking configuration, respectively, while (c) and (d) illustrate the HER and OER performance for the D-stacking configuration. The color scale represents different applied strains: deep blue corresponds to 4% compressive strain, green to 2% compressive strain, cyan to no strain, light yellow to 2% tensile strain, and red to 4% tensile strain.

Table. S1: Comparative Analysis of Key Performance Metrics for Advanced Z-Scheme Heterojunction Photocatalysts

Structure	Lifetime(electron)/ps	Lifetime(hole)/ps	Energy Barrier (HER)/eV	Energy Barrier (OER)/eV	Ref
$MoSe_2/Ti_2CO_2$	0.5(100%-5%)	0.5(100%-15%)	-	1.98	[1]
MgO /g-C_3N_4	0.24	0.47	>0.3	>0.4	[2]
OH/OCN-PNR_s	1.5(90%-54%)	1.5(72%-32%)	>1	1.06	[3]
Se@CTF-0/β-Sb	0.21	0.6	1.04	0.72	[4]
g-C_3N_4/TiO_2	<0.3ps	<0.3ps	-	-	[5]
C_2N/BCN	< 1ps	< 1ps	-	-	[6]
Defective BP(5|9)/$SnSe_2$	4.01	8.46	0.47	0.32	[7]
β-As/Ti_2CO_2	0.2	0.8	0.57	0.63	[8]
B-Stacking GeC/SGaSnP	0.66	634.92	0.23	0.21	This work
D-Stacking GeC/SGaSnP	37.04	0.59	0.23	0.25	This work

Table S2: Ionic dipole moment, electronic dipole moment, total dipole moment, and polarization intensities of GeC/SGaSnP heterostructures with different stacking configurations calculated using the Berry phase method.

Type	Ionic dipole moment/(e×Å)	Electronic dipole moment/(e×Å)	Total dipole moment/(e×Å)	Polarization intensity(C/m)
A	17.1496	20.8743	38.0239	1.64471E-9
B	17.1496	20.8743	38.0239	1.64471E-9
C	17.1675	20.8499	38.0174	1.64443E-9
D	17.1161	20.9233	38.0394	1.64538E-9
A’	5.93069	31.8959	37.8266	1.63617E-9
B’	5.9217	31.9116	37.8333	1.63646E-9
C’	5.94633	31.8852	37.8316	1.63639E-9
D’	5.87369	31.9641	37.8378	1.63666E-9

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