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Ultrafast carrier recombination in BC_6N/SnXY Z-scheme heterostructure for water splitting: insights from ground- and excited-state carrier dynamics

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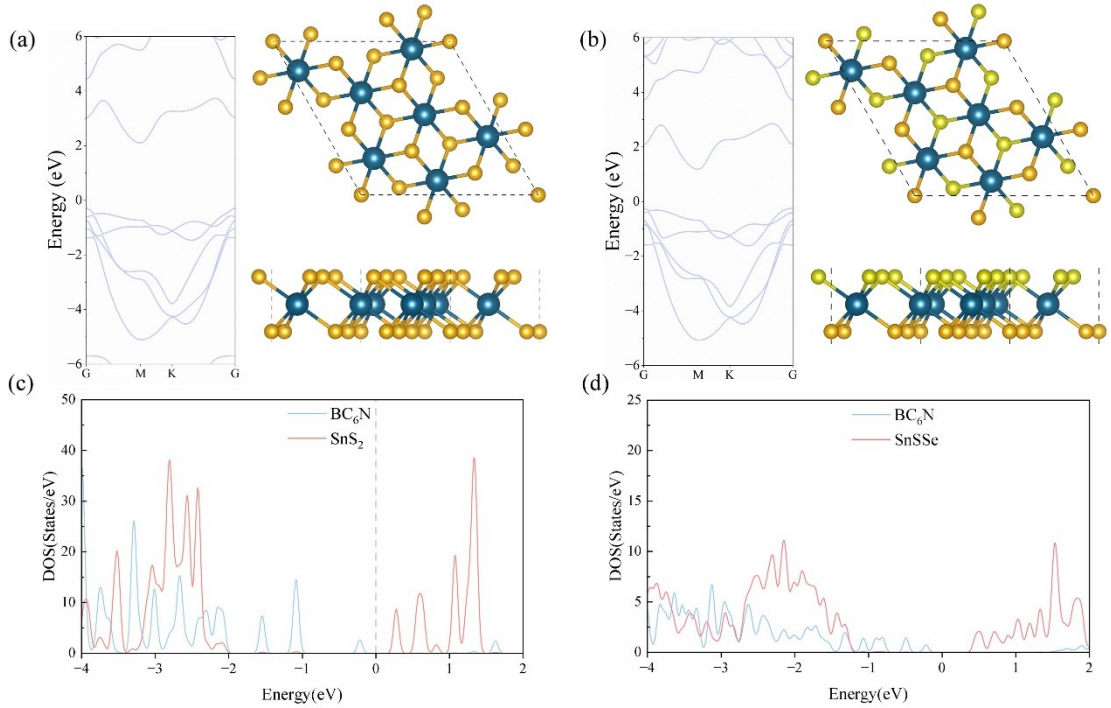

Fig. S1 The band structure and structure diagram of (a)BC_6N/SnS_2 and (b) BC_6N/SnSSe. The calculated of corresponding DOS for monolayers in heterojunction of (c) BC_6N/SnS_2 and (d) BC_6N/SnSSe.

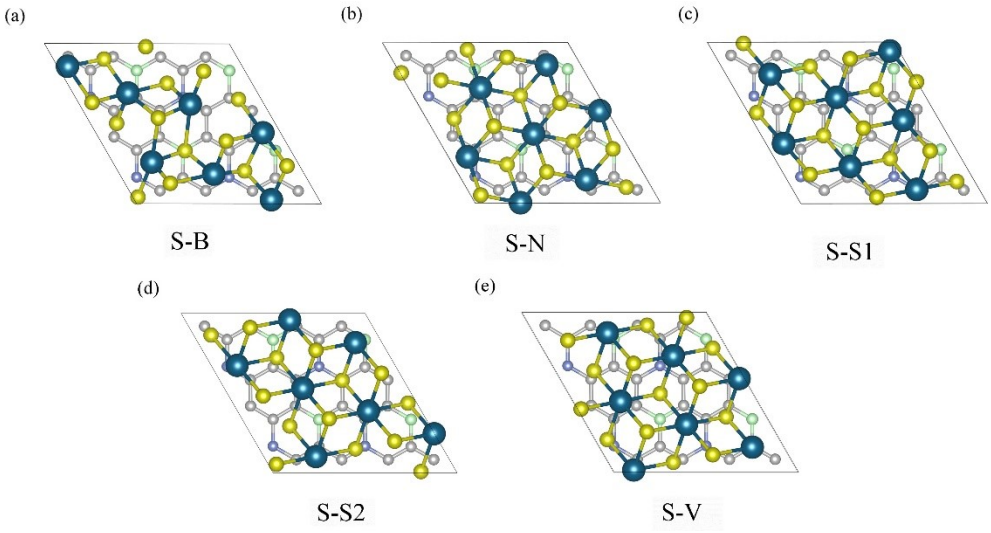

Fig. S2 The different stacking configuration for $BC_6N/SnXY$

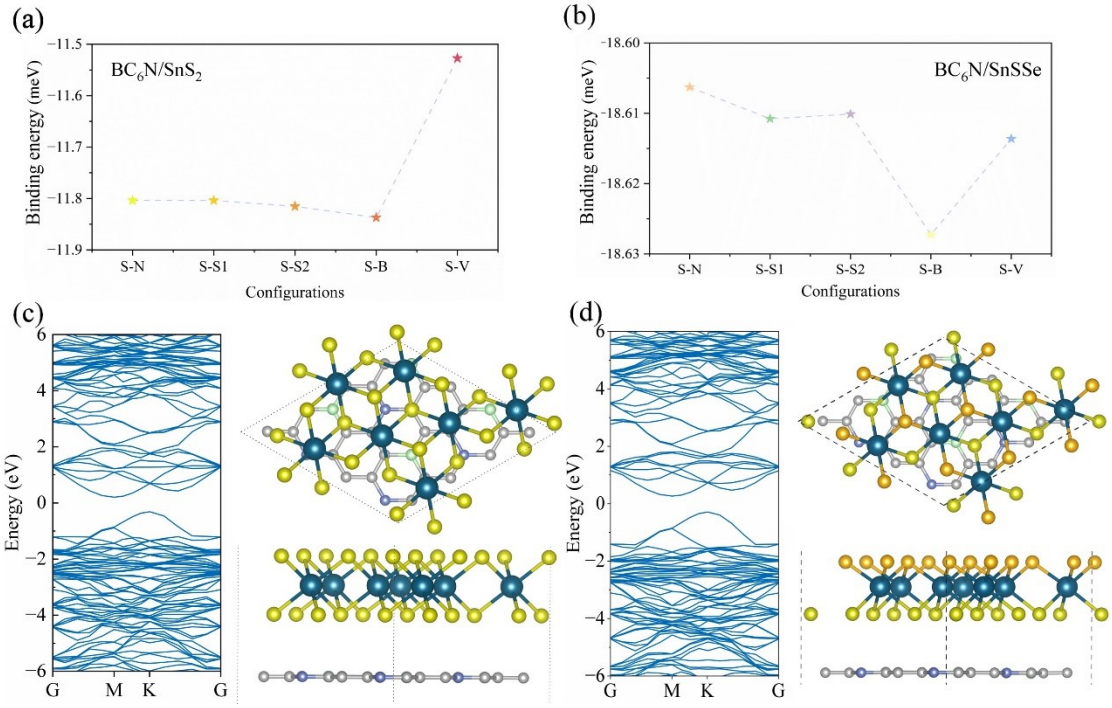

Fig. S3 The binding energy of (a) BC_6N/SnS_2 and (b) $BC_6N/SnSSe$. (c)(d) are the band structure and structural schematic for $BC_6N/SnSe_2$ and $BC_6N/SnSSe$.

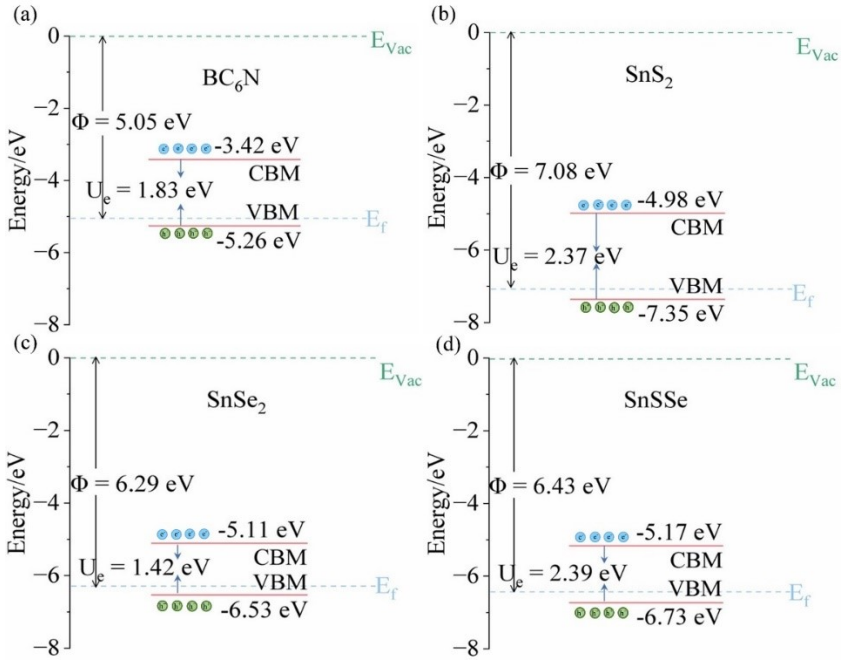

Fig. S4 The band alignment of BC_6N and SnXY monolayers.

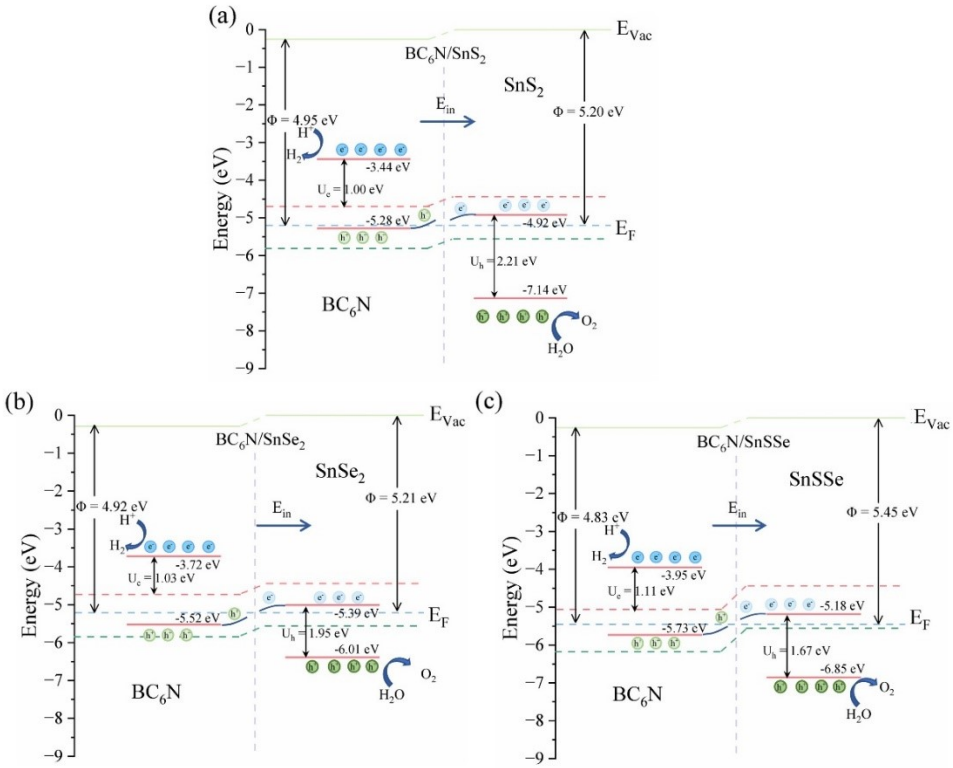

Fig. S5 The band alignment of (a)BC_6N/SnS_2, (b) $BC_6N/SnSe_2$ and (c) BC_6N/SnSSe heterojunction. Here, Φ (work function) represent the difference of vacuum and Fermi level.

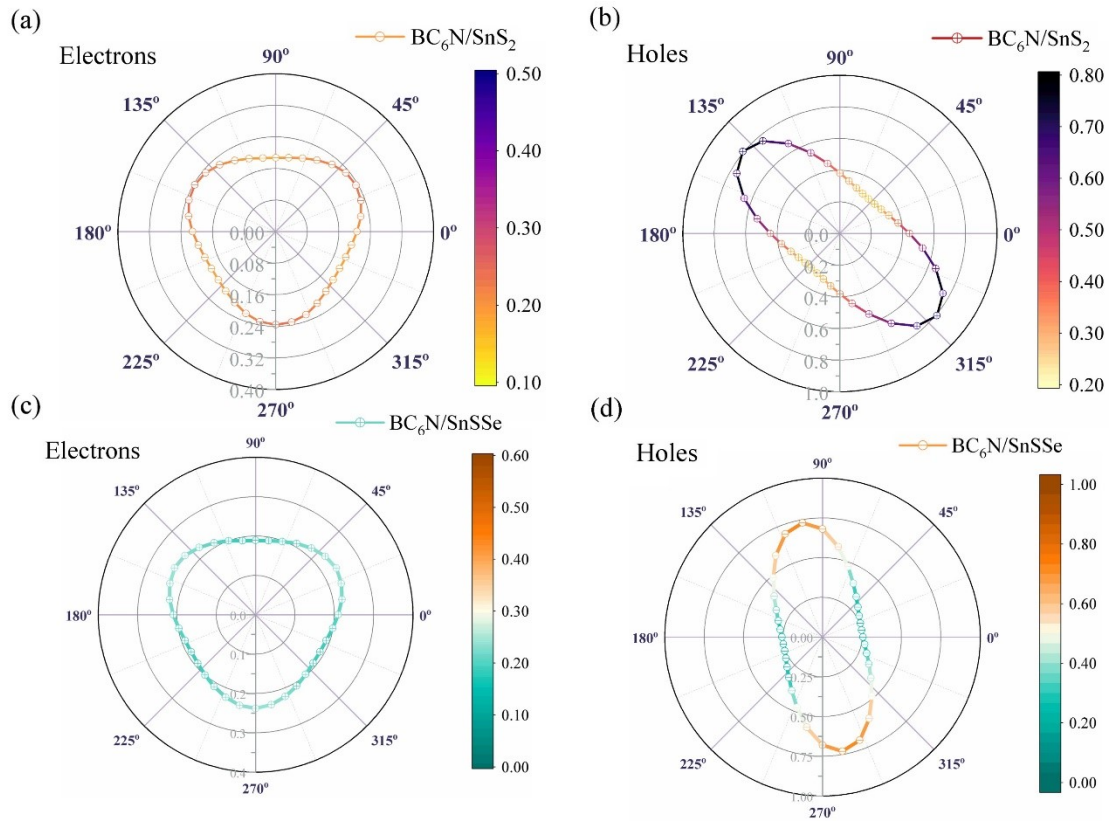

Fig. S6 The angular dispersion of hole effective mass for BC_6N/SnS_2 and $BC_6N/SnSSe$.

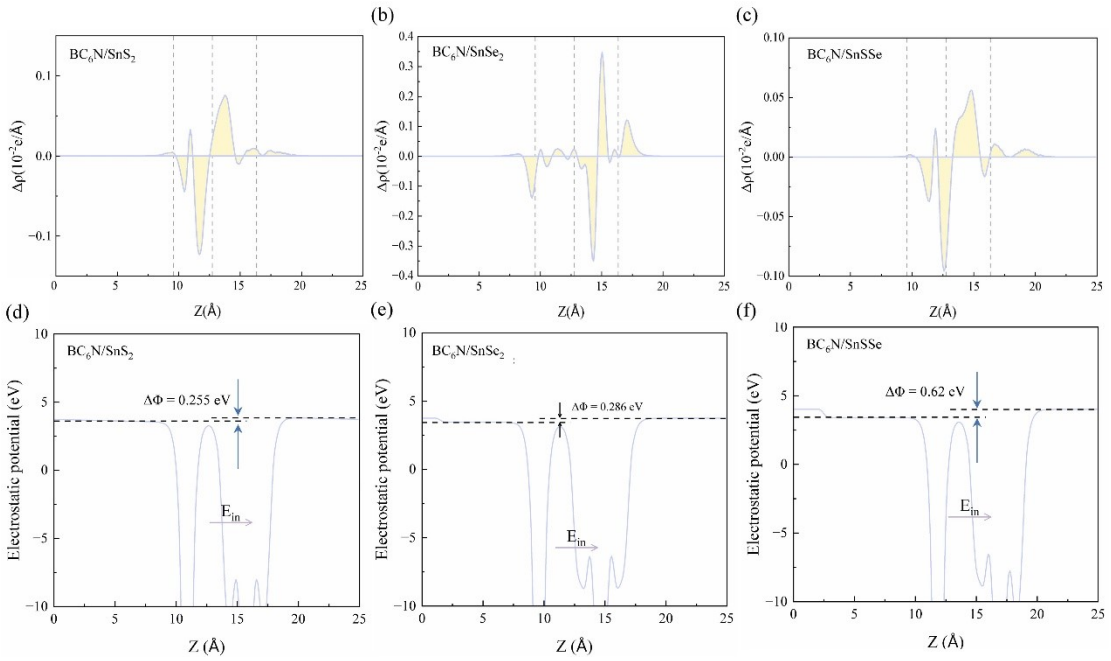

Fig. S7 The calculated average charge density difference and electronic potential for three kinds of heterojunctions.

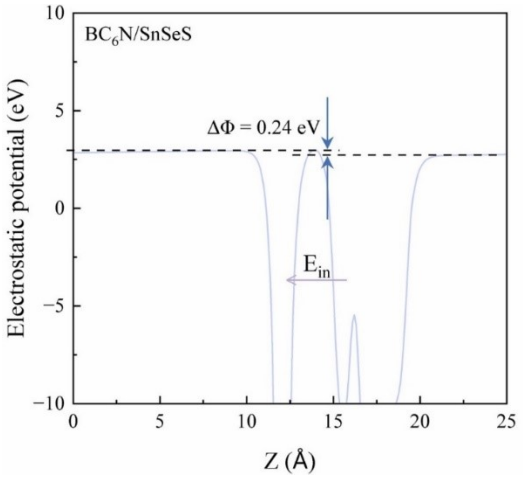

Fig. S8 The calculated average electronic potential for BC_6N/SnSeS.

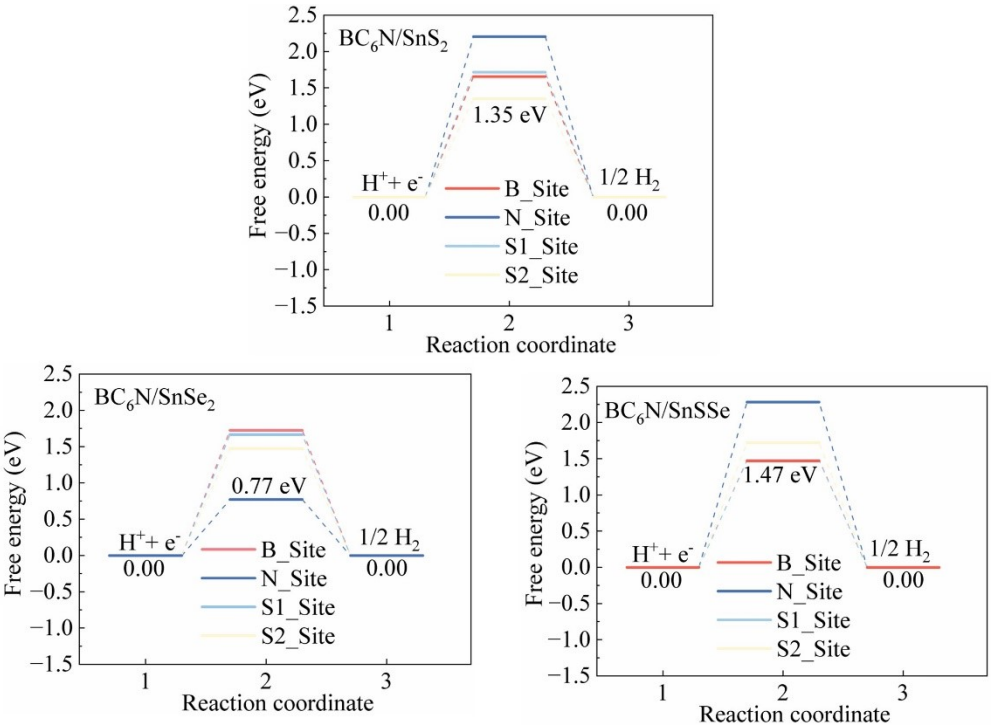

Fig. S9 The calculated free energy changes of HER for different adsorption sites on BC_6N/SnXY

Table S1 The structural parameters of monolayers materials

Monolayers	α(Å)	β(Å)	$d_{C\text{-}C}$	$d_{C\text{-}B}$	$d_{B\text{-}N}$	$d_{Sn\text{-}S}$	$d_{Sn\text{-}Se}$	Φ(eV)	E_g^{HSE} (eV)
BC_6N	4.975	4.975	1.416	1.475	1.456	—	—	5.05	1.83
SnS_2	3.663	3.663	—	—	—	2.583	—	7.08	2.39
$SnSe_2$	3.823	3.823	—	—	—	—	2.730	6.43	1.42
SnSSe	3.740	3.740	—	—	—	2.611	2.704	6.29	1.56

Table S2 The interlayer distances of BC_6N/SnXY heterostructure

Monolayers	X-B	X-S1	X-S2	X-N	X-V
BC_6N/ SnS_2	3.378	3.432	3.413	3.383	3.338
BC_6N/$SnSe_2$	3.325	3.421	3.450	3.384	3.456
BC_6N/SnSSe	3.408	3.483	3.447	3.446	3.426

The Gibbs free energy

The method proposed by Nørskov was used to calculate the Gibbs free energy (ΔG), and the formula for every elemental step was shown below:

$$\Delta G = \Delta E + \Delta E_{ZPE} - T\Delta S \quad (1)$$

where ΔE is the electronic energy difference between the reactants and products, $\Delta E_{ZPE}$and ΔS are the variation of the zero-point energy and entropy at room temperature (T = 298.15 K), respectively.