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SUPPORTING INFORMATION

A high efficient Z-scheme B-doped g-C_3N_4/SnS_2 photocatalyst for CO_2 reduction reaction: A computational study

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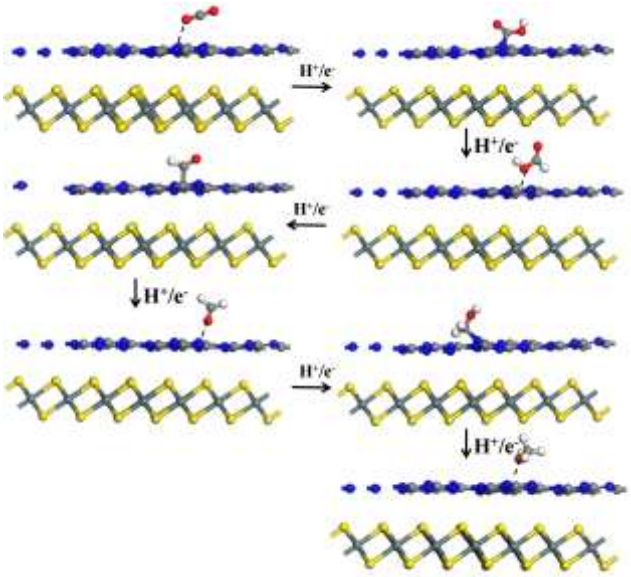
Table S1 Calculated free energy to the reaction path followed by the CO_2 conversion on Z-scheme g-C_3N_4/SnS_2 and B-doped g-C_3N_4/SnS_2 heterostructures.

		g-C_3N_4/SnS_2 ΔG (eV)	B-doped g-C_3N_4/SnS_2 ΔG (eV)
$1e^-$	$CO_2+e^-+H^++* \rightarrow COOH*$	1.10	-0.21
$2e^-$	$COOH*+e^-+H^+ \rightarrow CO+H_2O+*$	-0.52	-0.47
	$COOH*+e^-+H^+ \rightarrow HCOOH+*$	-0.86	0.45
$3e^-$	$HCOOH+e^-+H^++* \rightarrow HCO*+H_2O$	0.37	—
	$CO+e^-+H^++* \rightarrow HCO*$	—	0.22
	$CO+e^-+H^++* \rightarrow COH*$	—	0.24
$4e^-$	$HCO*+e^-+H^+ \rightarrow HCHO+*$	-0.20	0.97
	$HCO*+e^-+H^+ \rightarrow CHOH*$	0.32	-0.36
	$COH*+e^-+H^+ \rightarrow CHOH*$	—	-0.38
	$COH*+e^-+H^+ \rightarrow C*+H_2O$	—	1.00
$5e^-$	$HCHO+*+e^-+H^+ \rightarrow CH_3O*$	1.52	—
	$HCHO+*+e^-+H^+ \rightarrow CH_2OH*$	-0.21	—
	$CHOH*+e^-+H^+ \rightarrow CH*+H_2O$	-1.17	-0.30
	$CHOH*+e^-+H^+ \rightarrow CH_2OH*$	-0.73	0.83
$6e^-$	$CH_2OH*+e^-+H^+ \rightarrow CH_3OH+*$	-0.44	-0.12
	$CH_2OH*+e^-+H^+ \rightarrow CH_2*+H_2O$	0.24	-2.3
	$CH*+e^-+H^+ \rightarrow CH_2*$	0.65	-1.01
$7e^-$	$CH_2*+e^-+H^+ \rightarrow CH_3*$	-1.82	0.40
$8e^-$	$CH_3*+e^-+H^+ \rightarrow CH_4+*$	-0.54	0.39

Table S2. The calculated adsorption energies (E_{ads}) of various CO_2RR species with Z-scheme g-C_3N_4/SnS_2 and B-doped g-C_3N_4/SnS_2 heterostructures.

	CO_2 E_{ads} (eV)	COOH E_{ads} (eV)	HCOOH E_{ads} (eV)	CO E_{ads} (eV)	CH_3OH E_{ads} (eV)	CH_4 E_{ads} (eV)
g-C_3N_4/SnS_2	-0.11	-1.93	-0.27	-0.13	-0.27	-0.17
B-doped g-C_3N_4/SnS_2	-0.14	-3.25	-0.31	-2.17	-0.24	-0.20

(a)



(b)

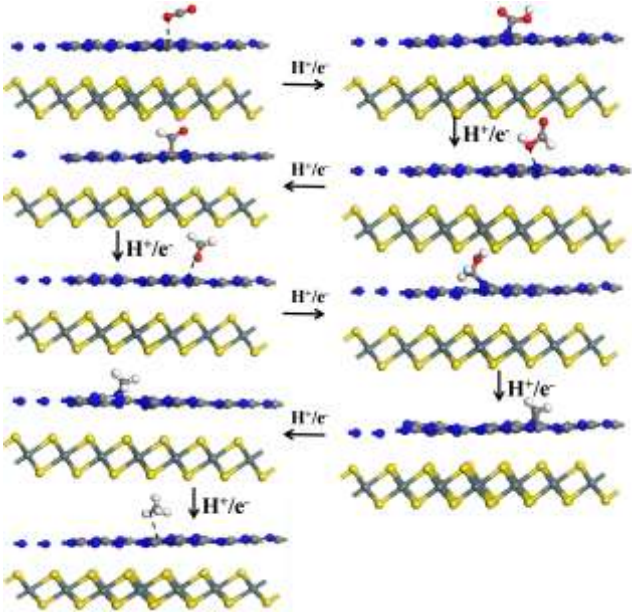


Fig. S1 Calculated the structures corresponding to the optimal reaction path followed by the CO_2 conversion on g-C_3N_4/SnS_2 (a,b).

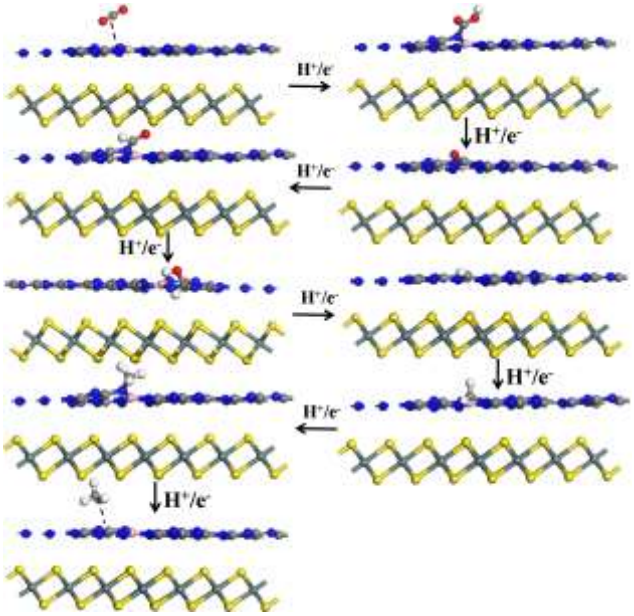


Fig. S2 Calculated the structures corresponding to the optimal reaction path followed by the CO_2 conversion on B-doped g-C_3N_4/SnS_2.