Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Construction of MoS_2/CdS heterojunction with crystal plane modulation for photocatalytic coupling of benzylamine under aerobic and anaerobic conditions

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Characterization

The morphology, microstructure, and element distribution of the photocatalysts were analyzed by field emission scanning electron microscope (SEM, FeI-F50), energy dispersive spectrometer (EDS) and transmission electron microscope (TEM, FEI Tecnai G2 F30). The crystal structure of the photocatalysts was determined using X-ray diffractometer (SmartLab, Rigaku). X-ray photoelectron spectroscopy (XPS, Thermo Fisher Scientific) was conducted with an Al Kα X-ray source. The optical absorption properties of different photocatalysts were evaluated using a UV-Vis spectrophotometer (UV-3600, Shimadzu, Japan). Electrochemical performance was characterized by a CHI660E electrochemical workstation (Chenhua, Shanghai, China). The reactants and products were detected by gas chromatography (Agilent GC 7890B, FID), and the hydrogen generated under nitrogen atmosphere was detected by gas chromatography (GC 9790Ⅱ, FuLi, TCD). The superoxide radicals generated in photocatalytic system are analyzed by electron spin resonance (ESR) spectrometer (Bruker A300) using 5,5-dimethyl-1-pyrroline N-oxide (DMPO) as the radical trapping reagent.

Results and discussion

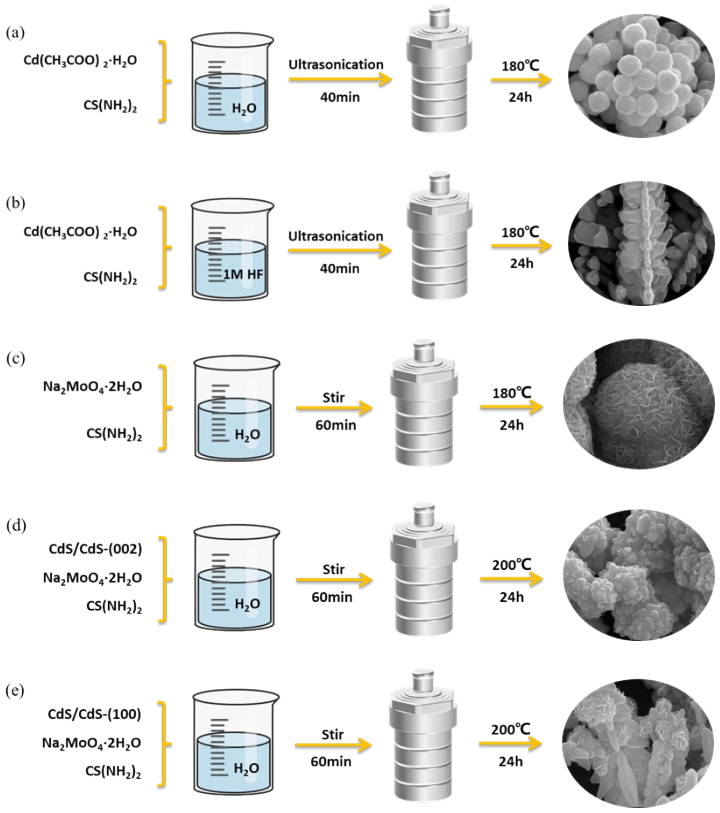

Fig. S1 Schematic illustration of the synthesis of (a) CdS-(002), (b) CdS-(100), (c)MoS_2, (d) MoS_2/CdS-(002) and (e) MoS_2/CdS-(100).

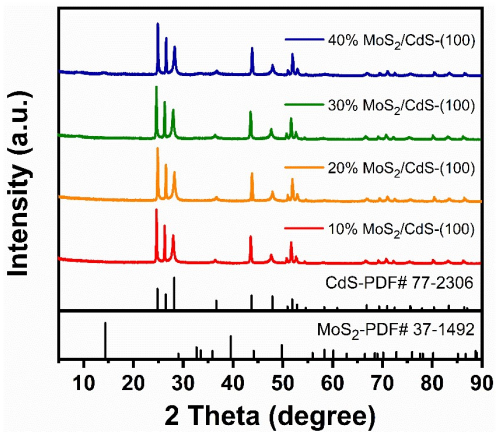

Fig. S2 XRD patterns of MoS_2/CdS-(100) with different mass ratios.

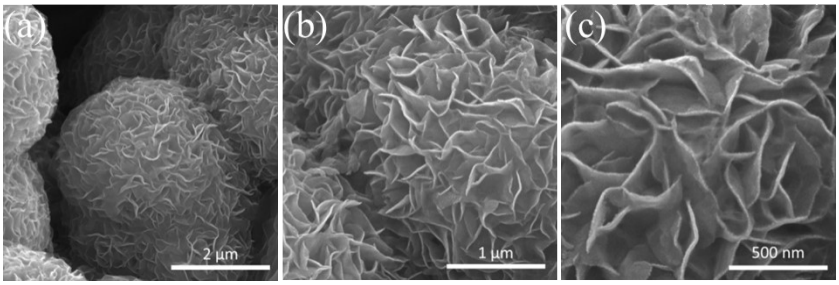

Fig. S3 SEM images of MoS_2.

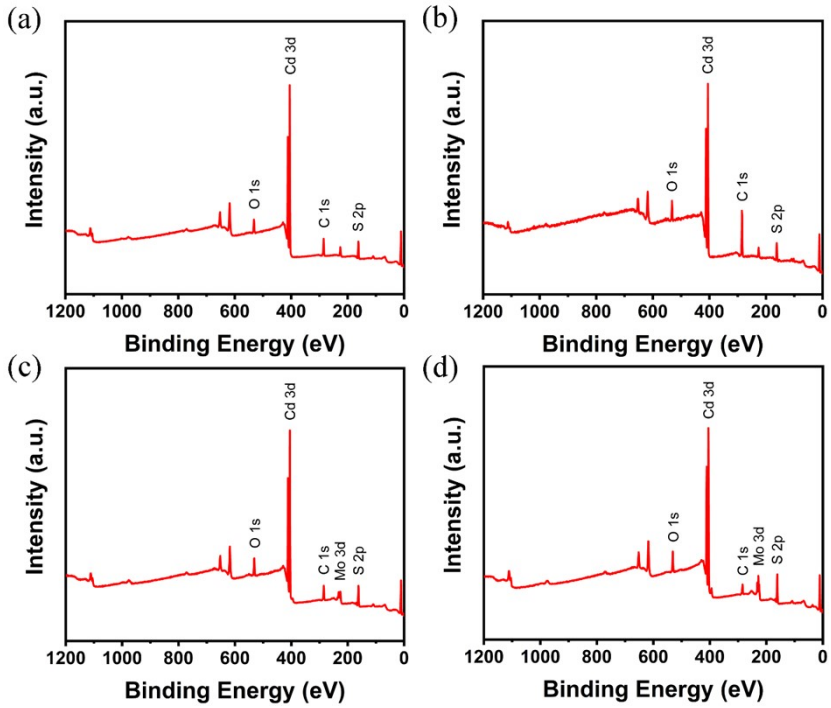

Fig. S4 XPS survey spectra of (a) CdS-(002), (b) CdS-(100), (c) 20% MoS_2/CdS-(002) and (d) 20% MoS_2/CdS-(100).

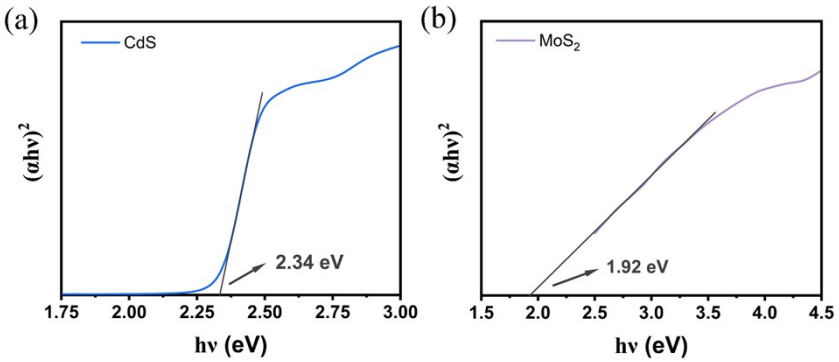

Fig. S5 Tauc plots of (a) CdS and (b) MoS_2.

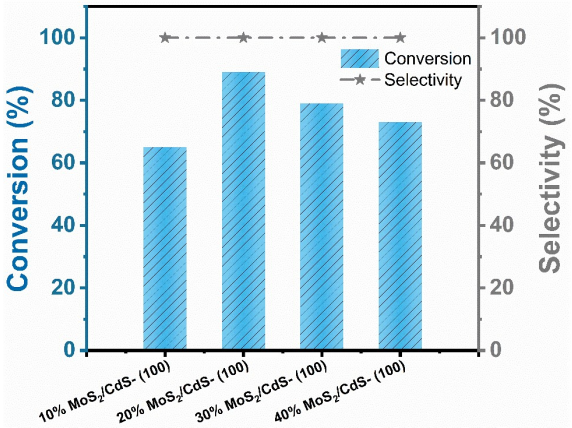

Fig. S6 Photocatalytic activity test of MoS_2/CdS-(100) with different mass ratios.

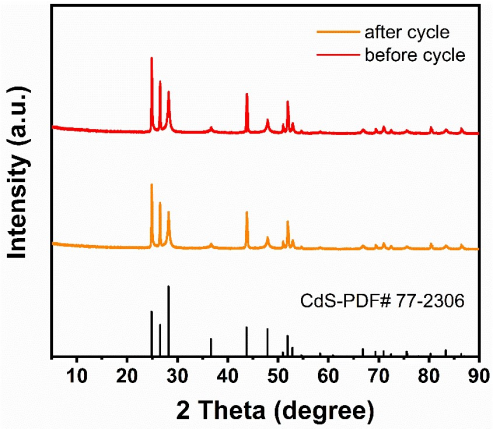

Fig. S7 XRD patterns of 20% MoS_2/CdS-(100) before and after stability test.

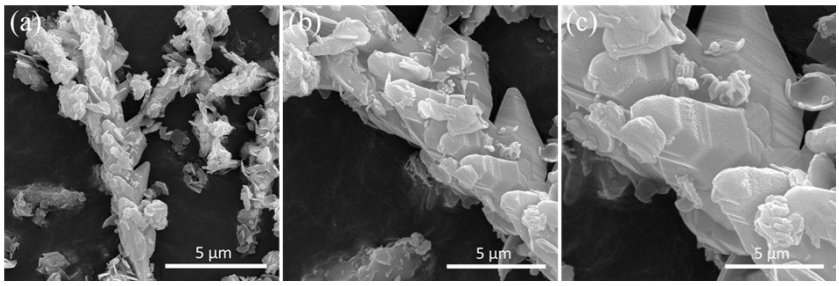

Fig. S8 SEM images of 20% MoS_2/CdS-(100) before and after stability test.

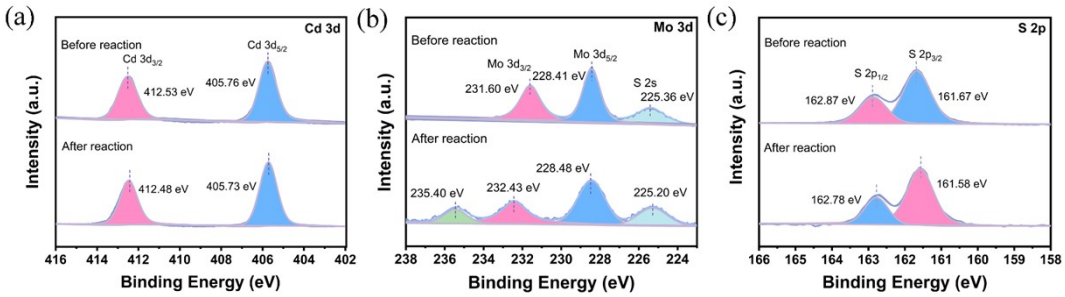

Fig. S9 XPS spectra of 20% MoS_2/CdS-(100) before and after stability test.

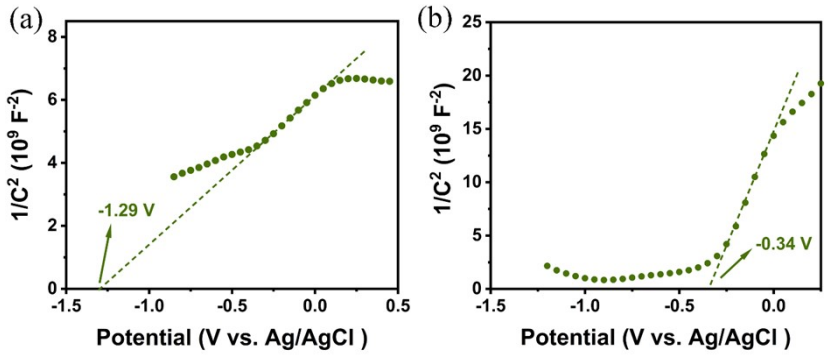

Fig. S10 Mott-Schottky plots measured at 1000 Hz of (a) CdS and (b) MoS_2.

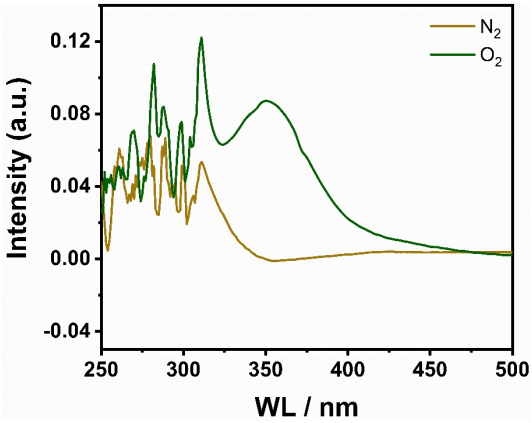

Fig. S11 The UV-Vis spectrum after adding iodide ions to the solution after the reaction of benzylamine.

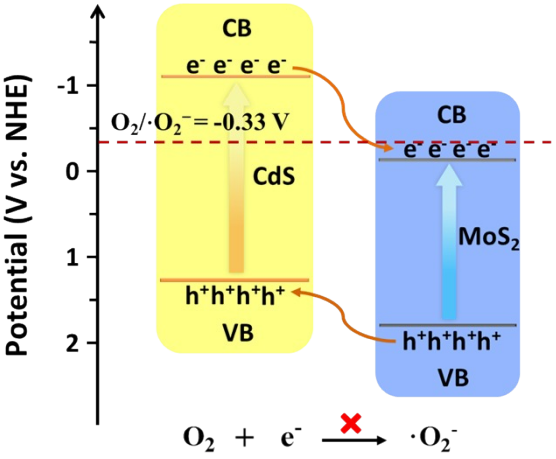

Fig. S12 Schematic diagram of the charge transfer in the type II heterojunction.

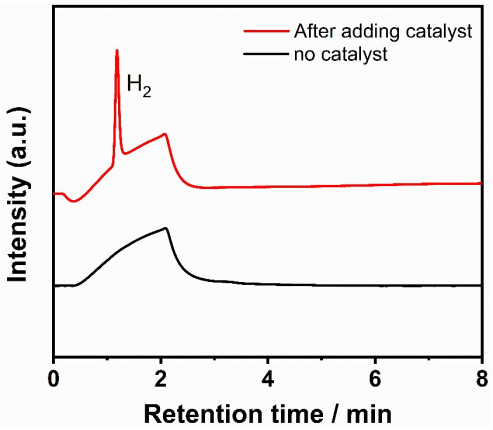

Fig. S13 GC spectra of H_2 produced in the reaction system under anaerobic condition.

Table S1 Photocatalytic activity test of CdS and MoS_2/CdS composites with different ratios[a].

Entry	Catalyst	Conv. (%)	Sel. (%)
1	MoS_2	2	>99
2	CdS-(002)	24	>99
3	CdS-(100)	35	>99
4	10% MoS_2/CdS-(100)	65	>99
5	20% MoS_2/CdS-(100)	89	>99
6	20% MoS_2/CdS-(002)	73	>99
7	30% MoS_2/CdS-(100)	79	>99
8	40% MoS_2/CdS-(100)	73	>99

[a]Reaction conditions: benzylamine (0.1 mmol), catalyst (10 mg), solvent (4 mL acetonitrile), 30 W White LED, reaction for 5 h, air atmosphere.

Table S2 Controlled experiment of photocatalyst visible-light photocatalytic benzylamine coupling[a].

Entry	Catalyst	Solvent	Atm.	Light	Conv. (%)	Sel. (%)
1	-	CH_3CN	Air	White LED	-	-
2[b]	20% MoS_2/CdS-(100)	CH_3CN	Air	-	-	-
3[c]	20% MoS_2/CdS-(100)	CH_3CN	Air	White LED	89	>99
4	20% MoS_2/CdS-(100)	CH_3CN	Air	White LED	>99	>99
5[d]	20% MoS_2/CdS-(100)	CH_3CN	Air	White LED	91	>99
6	20% MoS_2/CdS-(100)	CH_3OH	Air	White LED	87	>99
7	20% MoS_2/CdS-(100)	DMF	Air	White LED	>99	92
8	20% MoS_2/CdS-(100)	1, 2-Dichloroethane	Air	White LED	>99	97
9	20% MoS_2/CdS-(100)	THF	Air	White LED	85	34
10	20% MoS_2/CdS-(100)	DMSO	Air	White LED	>99	92
11	20% MoS_2/CdS-(100)	1,4-Dioxane	Air	White LED	22	>99
12	20% MoS_2/CdS-(100)	Toluene	Air	White LED	18	>99
13	20% MoS_2/CdS-(100)	CH_3CN	Air	Red LED	-	-
14	20% MoS_2/CdS-(100)	CH_3CN	Air	Green LED	92	>99
15	20% MoS_2/CdS-(100)	CH_3CN	Air	Blue LED	>99	>99
16	20% MoS_2/CdS-(100)	CH_3CN	O_2	White LED	>99	>99
17	20% MoS_2/CdS-(100)	CH_3CN	N_2	White LED	>99	>99

[a]Reaction conditions: benzylamine (0.1 mmol), catalyst (15 mg), solvent (4 mL), reaction for 5 h.
[b,c]The amount of catalyst is 10 mg.
[d]Reation for 4 h.

Table S3 Photocatalytic benzylamine coupling uses different catalysts.

photocatalysts	Light sources	Reaction conditions	Efficiencies (μmol g^{-1} h^{-1})	Ref.
MoS_2/CdS	30 W white LED	15 mg catalyst; 0.1mmol benzylamine; 4 mL CH_3CN	667	This work
g-C_3N_4/BiOBr	50 W white LED	100 mg catalyst; 5 mM benzylamine; 25 mL CH_3CN	313	1
TiO_2/g-C_3N_4	50 W halogen lamp	10 mg catalyst; 0.2mmol benzylamine; 2 mL toluene	375	2
CdS/$Ti_3C_2T_x$	300 W Xe lamp (λ > 420 nm)	10 mg catalyst; 5 mL DMF-based solution with H_2O	156	3
2D-MoS_2	45 W white LED	3 mg catalyst; 80°C; 0.1 mmol benzylamine	23	4
TiO_2(B)/anatase	300 W Xe lamp (λ > 420 nm)	50 mg catalyst; 0.25 mmol benzylamine; 10 mL CH_3CN	329	5
Pd/NH_2-MIL-125	300 W Xe lamp (λ > 420 nm)	5 mg catalyst; 0.1 mmol benzylamine; 2 mL CH_3CN	819	6
PCN	300 W Xe lamp (λ > 420 nm)	20 mg catalyst; 10 mL benzylamine; 50 mL deionized water	417	7
Pd/BiOCl	300 W Xe lamp (λ >420 nm)	10 mg catalyst; 0.2mmol benzylamine; 1.5 mL CH_3CN	833	8
Q-$BiVO_4$	300 W Xe lamp (λ > 420 nm)	10 mg catalyst; 0.1 mmol benzylamine; 5 mL CH_3CN	32	9
Bi_5O_7I-(010)	15 W Philips lamp	100 mg catalyst; 0.1 mmol benzylamine; 5 mL CH_3CN	28	10

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