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Supporting Information

Charge Migration in CdS/NiS Schottky junction composites for benzylalcohol oxidation coupled with hydrogen production

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COMPUTATIONAL DETAILS

All the DFT calculations in our work were performed by the Vienna ab initio simulation package (VASP)[1, 2], and the frozen-core projector augmented wave (PAW) approach was used to describe the interaction between the core and valence electrons. The generalized gradient approximation of Perdew-Burke-Ernzerhof (PBE)[3, 4] was used to optimize the geometric structures, and the van der Waals (vdW) correction DFT-D2 proposed by Grimme was chosen to describe the interaction, because of its good description of the long-range vdW interactions[5]. The cutoff energy of 450 eV was employed and Monkhorst-Pack meshs with 2×4×1 k-points were used to sample the two-dimensional Brillioiun zone of the super-cell calculations. A unit cell with Lz = 35 Å (the vacuum space is larger than 15 Å for our all models) was used to separate the interactions between neighboring slabs in a perpendicular direction. Meanwhile all geometry structures were fully relaxed until the convergence criteria of force and energy were less than 0.02 eV/Å and 10^{-4} eV, respectively.

Supplementary Figures

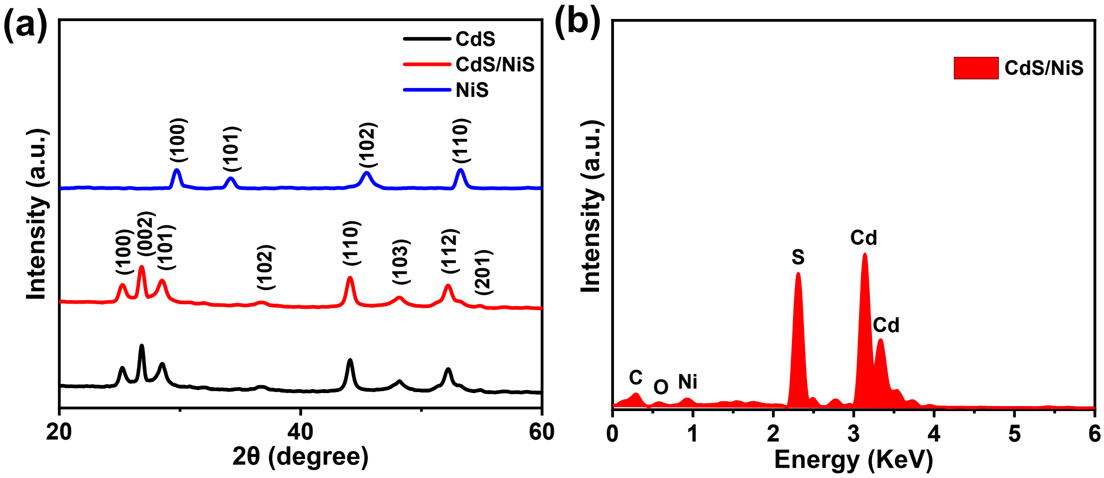

Figure S1. (a) Powder XRD patterns of as-synthesized CdS, 1% CdS/NiS and NiS; (b) EDX spectrum of of CdS/NiS.

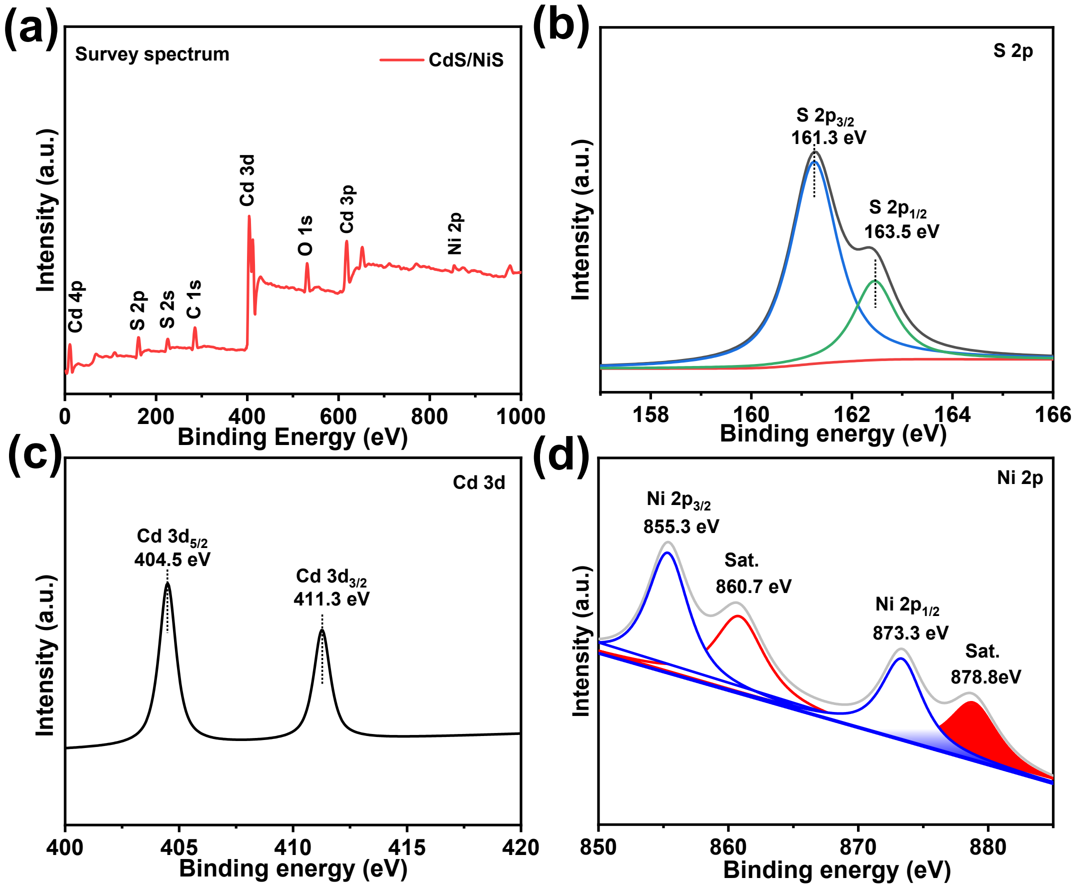

Figure S2. XPS spectra of (a) survey; (b) S 2p; (c) Cd 3d and (d) Ni 2p in CdS/NiS.

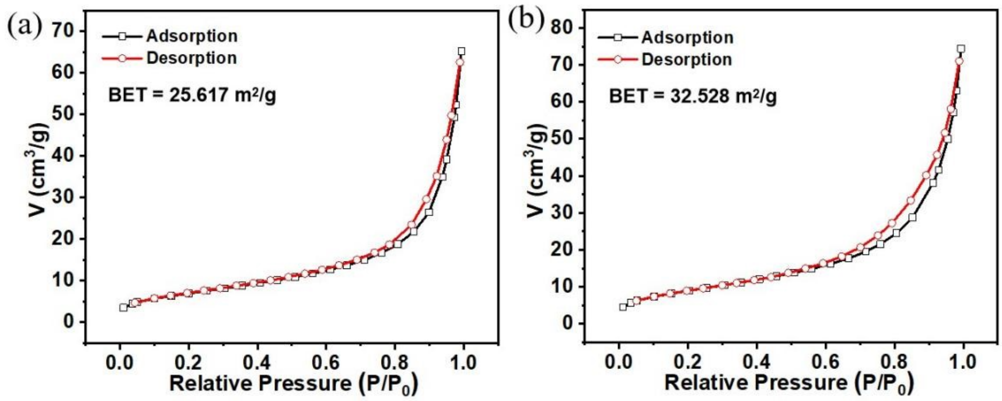

Figure S3. The BET measurements of the (a) CdS and (b) CdS/NiS.

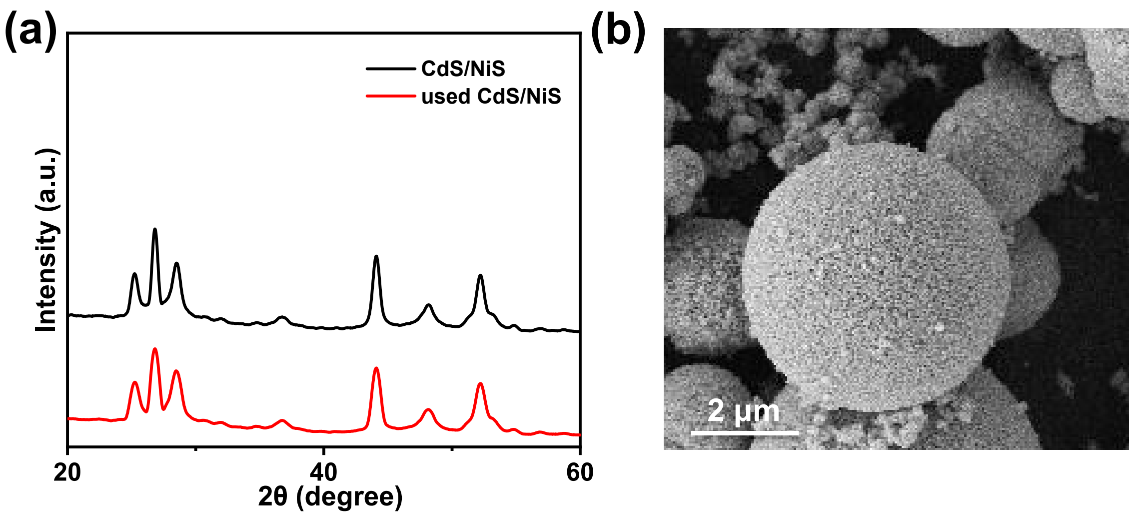

Figure S4. Powder XRD patterns and SEM of CdS/NiS after photocatalytic reaction.

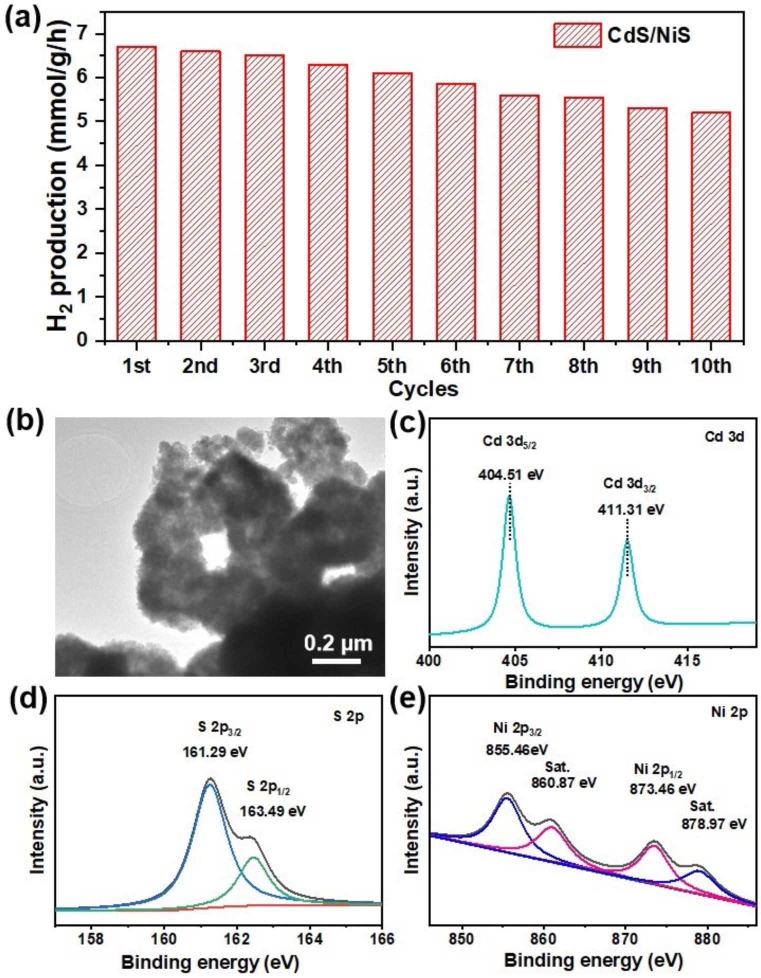

Figure S5. (a) Photocatalytic cycling tests of 1% CdS/NiS; (b) TEM of CdS/NiS after photocatalytic reaction; XPS spectra of (c) Cd 3d; (d) S 2p; (e) Ni 2p in CdS/NiS.

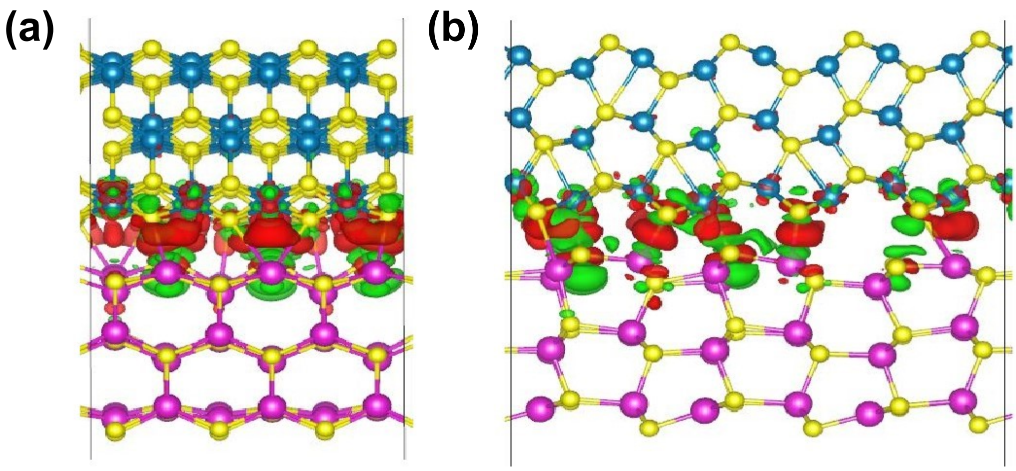

Figure S6. Side view and top view of the charge density difference of CdS@NiS composite with an isovalue of 0.02 e Å^{-3}. The green and red areas indicate electron accumulation and depletion, respectively.

References

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Supplementary Tables

Table S1 Comparisons of H_2 and aldehyde production rates with recently reports.

Year	**Photocatalyst**	**Light source**	**Substrate**	**Solvent**	**BAD/BZ/HB (mmol g^{-1} h^{-1})**	**H_2 evolution (mmol g^{-1} h^{-1})**	**Ref.**
This work	1%CdS/NiS	300 W Xe lamp (λ>400 nm)	BA	H_2O	BAD:5.8; Sel: 91.2%	6.7	
2024	PtO-CdS	300 W Xe lamp	BA	CH_3CN	BAD：90.6 %	29.1	1
2023	HC-CdS2/Co	Visible light	BA	CH_3CN	BAD: Sel: 3% HB: Sel: 97%	1.22	2
2023	$Zn_{0.6}Cd_{0.4}S$	300 W Xe lamp (λ≥420 nm)	BA	H_2O CH_3CN	HB: Sel: 81.2%(4 h) 98.8%(10 h)	0.55(4 h)	3
2022	CdS(ZB)/CdS(WZ)/Ni-BTC	300 W Xe lamp (λ>420 nm)	BA	H_2O	BAD: Sel: 90.2%	2.89	4
2022	CdS/WO_3-20	300 W Xe lamp	BA	H_2O	BAD: 3.98	5.48	5
2022	25%MO-ZnCdS	300 W Xe lamp (420 nm≤λ≤780 nm)	BA	CH_3CN	BAD: 0.50	0.50	6
2022	30%NiS/CdS	300 W Xe lamp (λ≥420 nm)	BA	H_2O	BAD: 8.19	10.39	7

2021	CdS/MIL-53(Fe)	300 W Xe lamp (λ>420 nm)	BA	CH_3CN	BAD: 2.83	2.33	8
2020	CdS/SiO_2	300 W Xe lamp	BA	CH_3CN	BAD: 0.15; Sel: 0.9% HB: 17; Sel: 99.1%	17.9	9
2020	$CdS@MoS_2$	300 W Xe lamp (λ > 420 nm)	BA	CH_3CN	BAD: Sel: 94%	4.23	10
2019	Ni/ZnCdS	300 W Xe lamp (λ ≥420 nm)	BA	BA	BAD: 7.46	9.49	11

BA: benzyl alcohol; BAD: benzaldehyde; BZ: benzoin; HB: hydrobenzoin.'

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