Electronic Supporting Information

Synergetic microstructure engineering by induced ZB/WZ twin boundaries and S vacancies in $Zn_{0.5}Cd_{0.5}S$ solid solution containing ZIF-8 as substrate for highly efficient photocatalytic hydrogen production

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Experimental section

Table S1. The preparation detail information of ZCS, ZCS-V, T-ZCS and T-ZCSv.

Samples	Materials	Solvent	Reaction conditions
ZCS	cadmium acetate dihydrate zinc acetate dihydrate thiourea	water	220 °C, 12 h
ZCS-V	cadmium acetate dihydrate zinc acetate dihydrate thiourea	water and $N_2H_4{\cdot}H_2O$	220 °C, 12 h
T-ZCS	cadmium acetate dihydrate zinc acetate thioacetamide	alcohol	160 °C, 24 h.
T-ZCSv	cadmium acetate dihydrate zinc acetate dihydrate thioacetamide	water and NaOH (4M)	180 °C, 24 h.

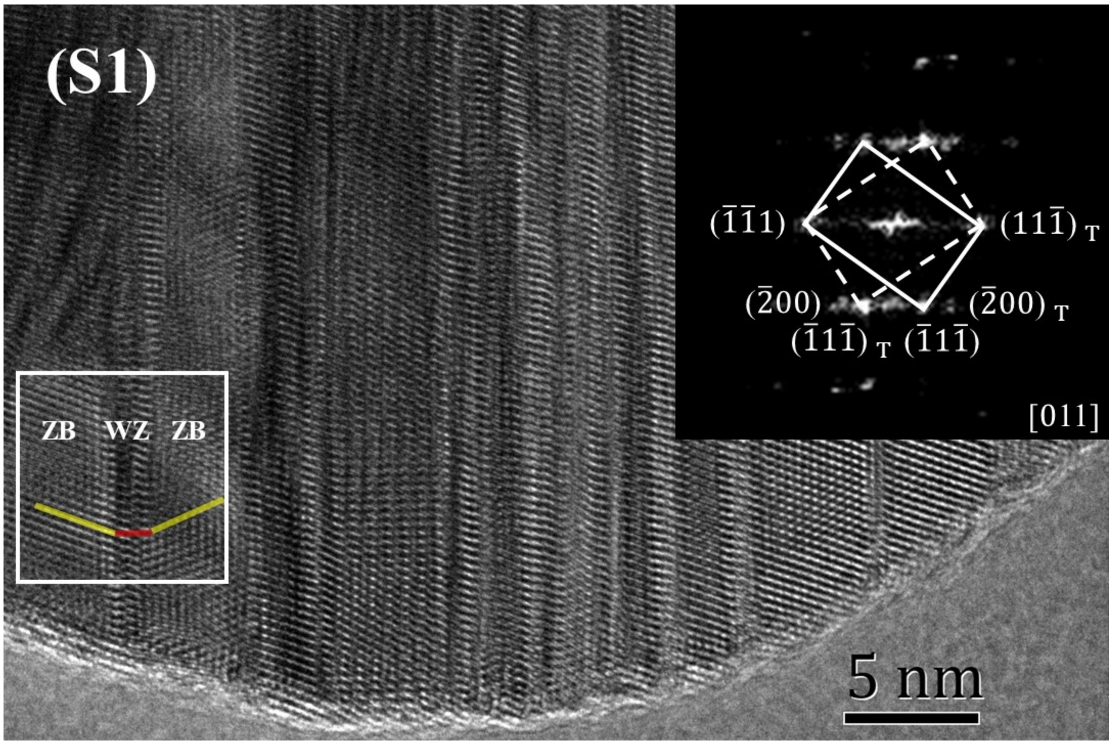

Figure S1. The wurtzite structure with two or three diatomic layers for T-ZCSv nanocrystals.

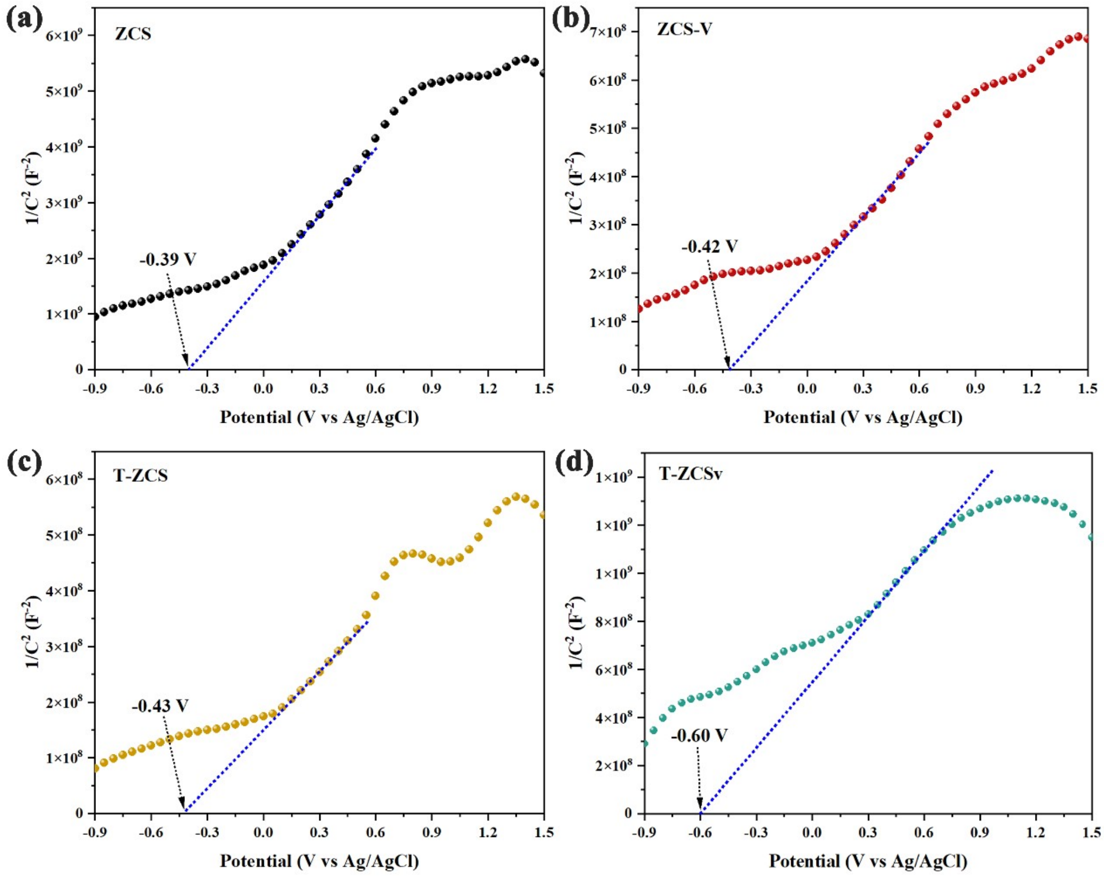

Figure S2. Mott-Schottky curves of (a) ZCS, (b) ZCS-V, (c) T-ZCS and (d) T-ZCSv samples

Table S2. The corresponding energy band structure of various samples

Samples	E_g (eV)	E_{CB} (V)	E_{VB} (V)
ZCS	2.31 eV	-0.39 V	1.92 V
ZCS-V	2.51 eV	-0.42 V	2.09 V
T-ZCS	2.47 eV	-0.43 V	2.04 V
T-ZCSv	2.60 eV	-0.60 V	2.00 V

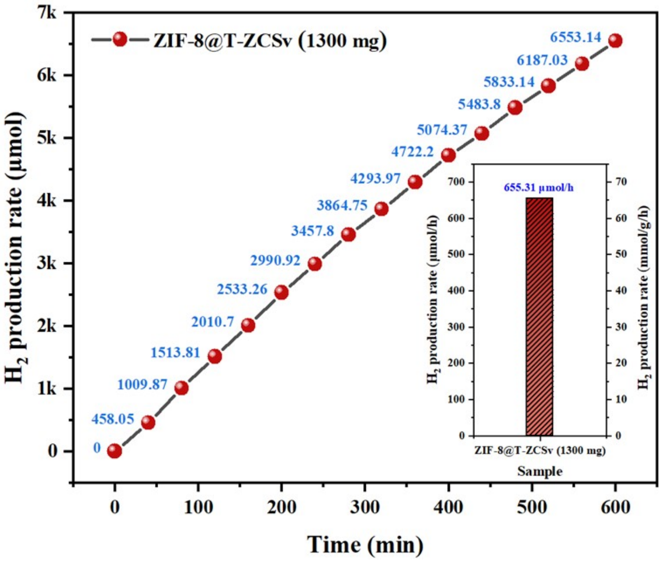

Figure S3. long-term activity and photocatalytic hydrogen generation rate of the ZIF-8@T-ZCSv (1300 mg) with 10 hours

Table S2. Comparison of the H_2 revolution rates (HER) of ZnCdS based composites.

Samples	Light Sources			Catalyst (mg)	Water (mL)	Sacrificial reagent	HER (μmol/h)	Ref
	(W)	Type	(nm)					
ZIF-8@T-ZCSv (1300mg)	300	Xe	420	10	50	0.25 M Na_2SO_3 and 0.35M $Na_2S·9H_2O$	583.25	This work
$Zn_{0.5}Cd_{0.5}S/ZnO/Zn_{0.5}Cd_{0.5}S$ cages	300	Xe	-	20	50	1.05 M Na_2SO_3 and 0.75M Na_2S	572	1
$Cd_{0.6}Zn_{0.4}S$ twinned crystals	300	Xe	420	50	80	0.15 M Na_2SO_3 and 0.15 M Na_2S	472	2
2Ni/4NiS/ZCS	300	Xe	420	100	75	25 mL lactic acid	415.1	3
3%$MoS_2/Zn_{0.5}Cd_{0.5}S$	300	Xe	420	50	50	0.25 M Na_2SO_3 and 0.35M $Na_2S·9H_2O$	388.2	4
CZS/NMF-4	5	LED	-	10	-	30 mL 10% lactic acid	346.24	5
NBZ-3	5	Xe	-	10	-	30 mL 10% lactic acid	304.2	6
T-ZCS	300	Xe	420	10	100	0.25 M Na_2SO_3 and 0.35 M Na_2S	302.9	7
ZIF-67/$Zn_{0.5}Cd_{0.5}S$	5	LED	-	10	-	30 mL 10% lactic acid	232.64	8
$C_{0.42}Z_{0.58}S$-3 polyhedrons	300	Xe	400	50	100	0.50 M Na_2SO_3 and 0.75M Na_2S	205	9
ZnCdS–NiCoP10	5	LED	-	10	-	30 mL 10% lactic acid	157.94	10
hollow $Zn_{0.6}Cd_{0.4}S$ cage	350	Xe	420	25	50	1.05 M Na_2SO_3 and 0.75M Na_2S	142	11
8 Pt-$Zn_{0.5}Cd_{0.5}S$ with ZB/WZ	500	Xe	400	30	120	0.1 M Na_2SO_3 and 0.1 M Na_2S	114.3	12
$Zn_{0.5}Cd_{0.5}S$ QDs	300	Xe	400	25	50	1.05 M Na_2SO_3 and 0.75M Na_2S	92.5	13
P-ZnCdS nanocages	300	Xe	400	20	100	0.45 M Na_2SO_3 and 0.25M Na_2S	57.21	14
ZnCdS-CdS-3	350	Xe	420	10	100	Na_2S (1.2 g) and Na_2SO_3 (0.63 g)	27	15

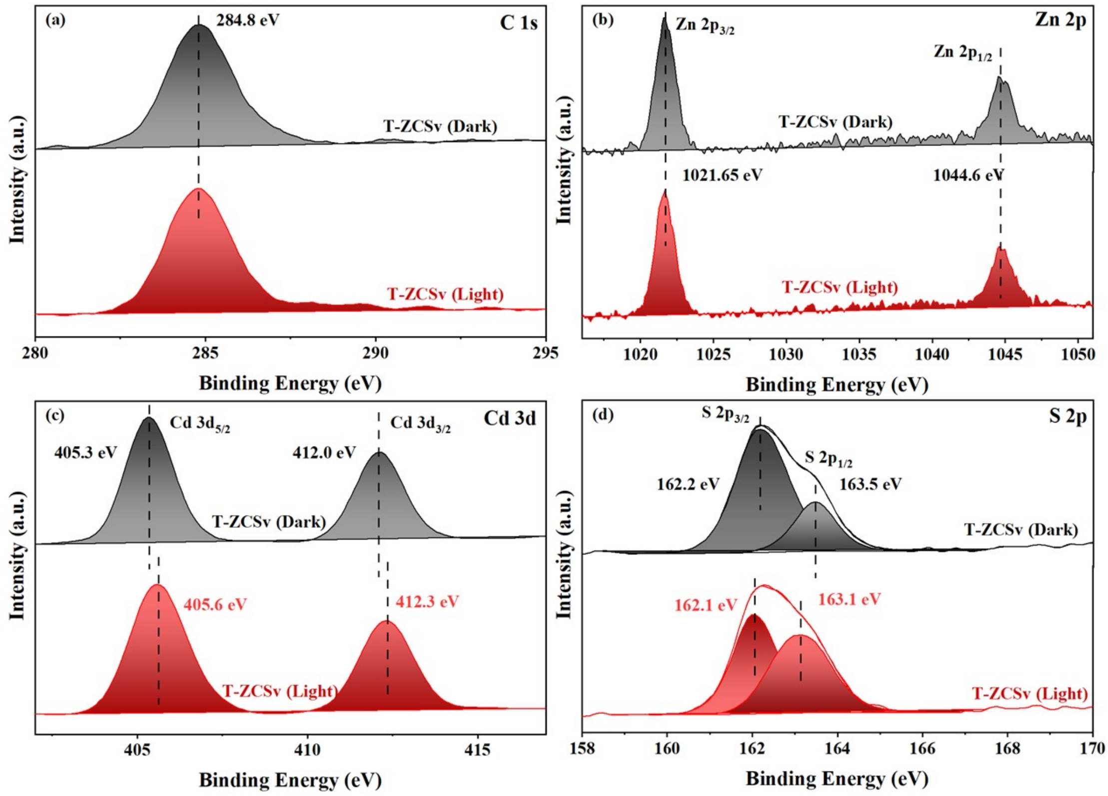

Figure. S4. The high-resolution in situ XPS spectra of pristine T-ZCSv for C 1s (a), Zn 2p (b), Cd 3d (c), S 2p (d).

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