

Supplementary Materials

Designing a 0D/1D S-Scheme Heterojunction of Cadmium Selenide and Polymeric Carbon Nitride for Photocatalytic Water Splitting and Carbon Dioxide Reduction

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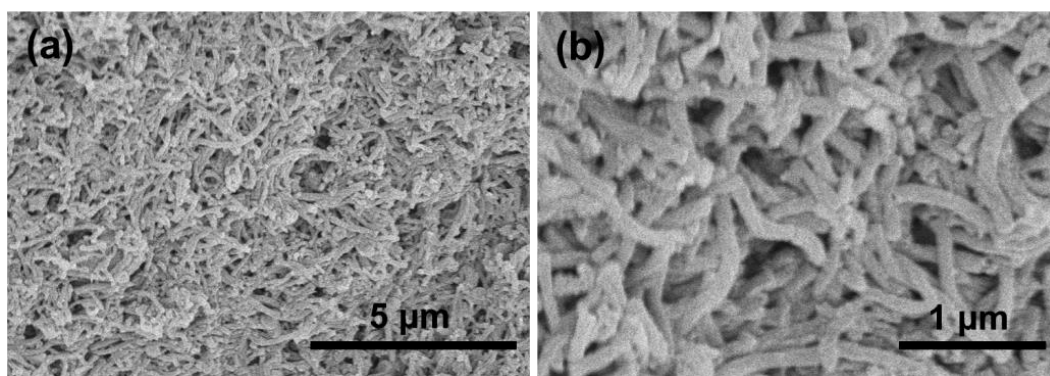


Figure S1. SEM images of CN nanorods.

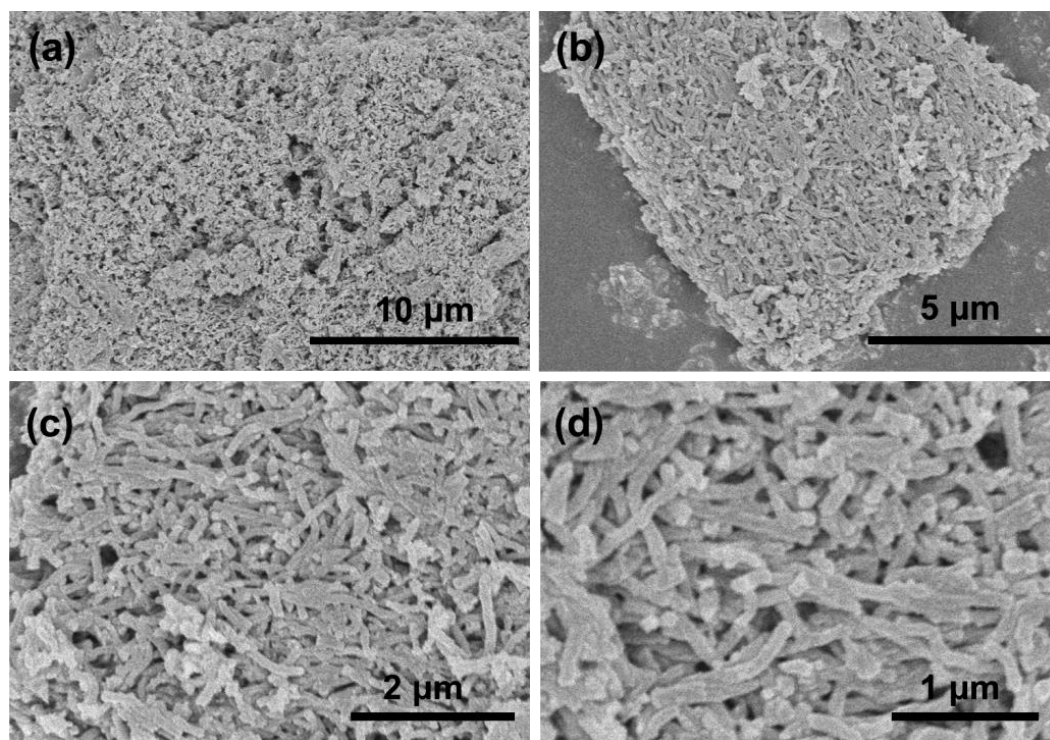


Figure S2. SEM images of 5% CdSe/CN hybrid.

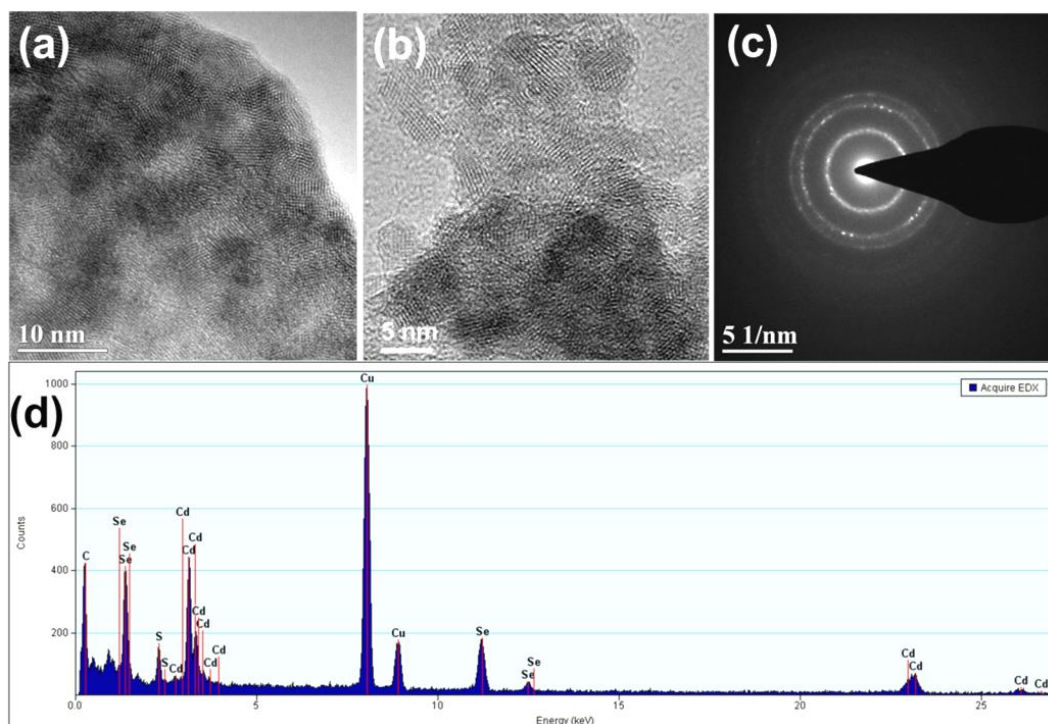


Figure S3. (a) TEM image, (b) HRTEM image, (c) SAED image, and (d) EDX image of CdSe QD solutions.

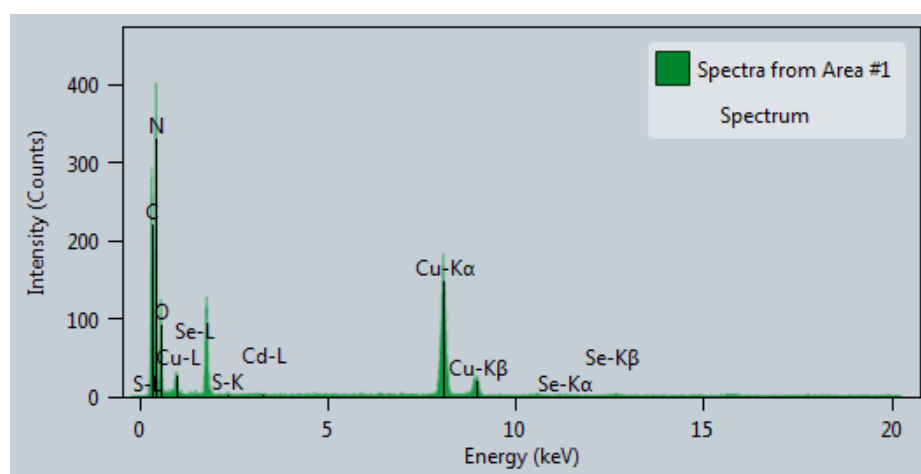


Figure S4. TEM-EDX images of 5% CdSe/CN hybrid.

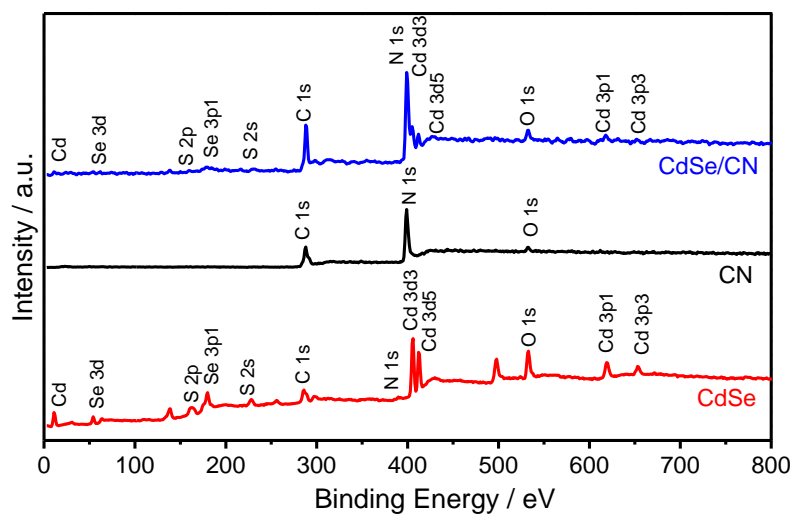


Figure S5. XPS survey spectra of CN, CdSe and 5% CdSe/CN hybrid.

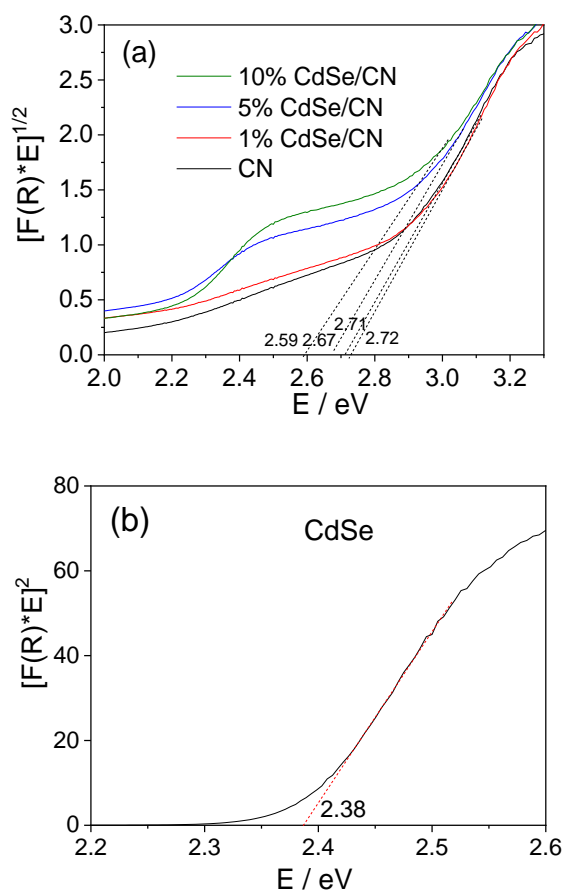


Figure S6. Tauc plots of (a) CN nanorods, CdSe/CN hybrids and (b) CdSe QDs.

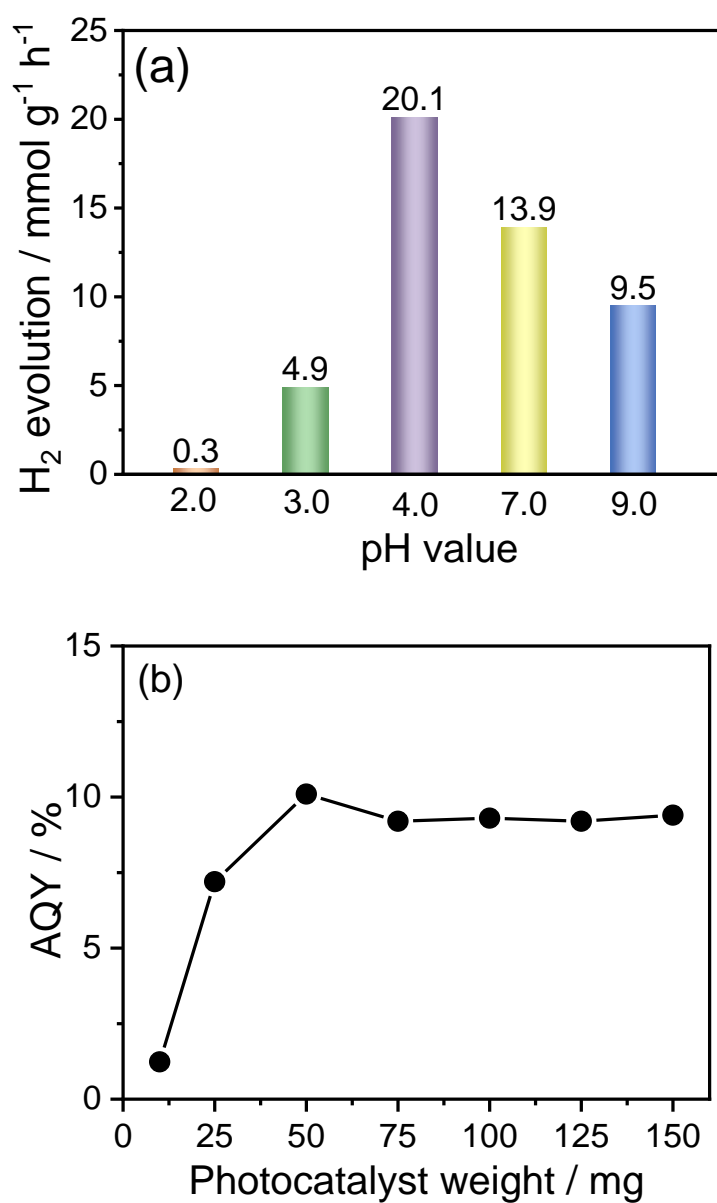


Figure S7. (a) Amount of hydrogen evolved from 5% CdSe/CN using ascorbic acid (H₂A) as sacrificial reagent by changing pH value. (b) AQY of 5% CdSe/CN for photocatalytic H₂ evolution with different photocatalyst weight.

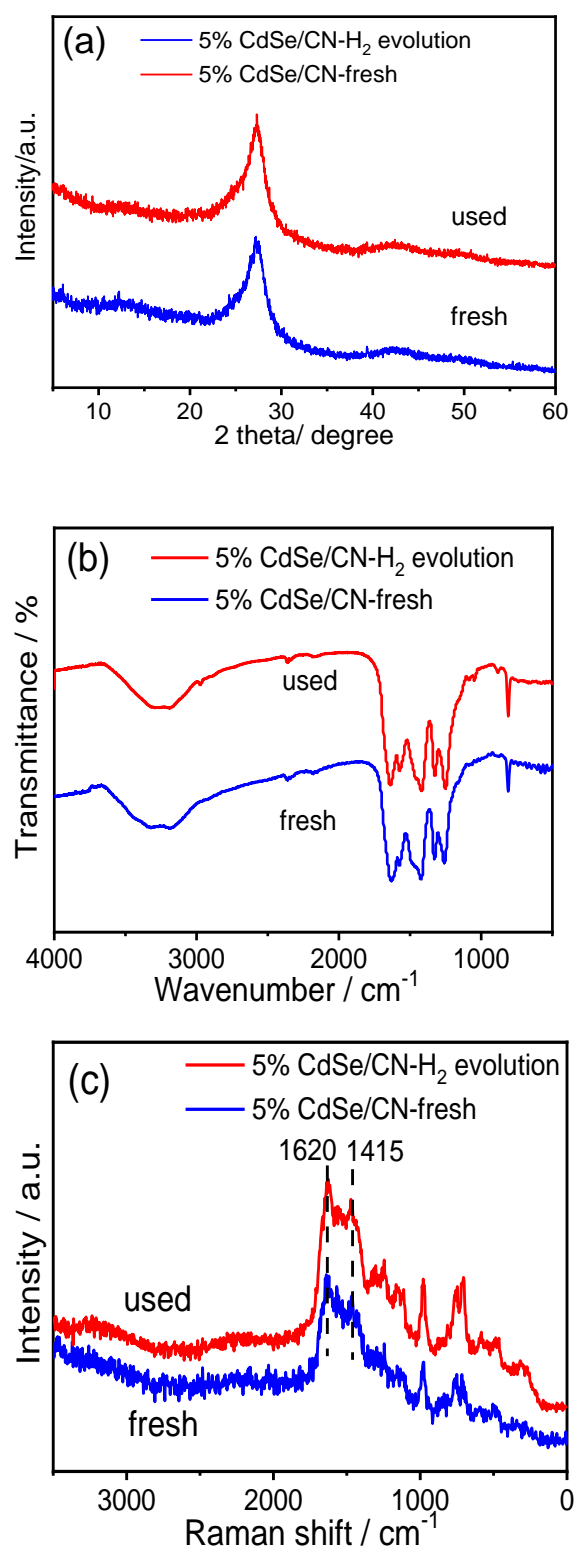


Figure S8. (a) XRD pattern, (b) FT-IR spectra and (c) UV-Raman spectra of 5% CdSe/CN before and after the hydrogen evolution reaction.

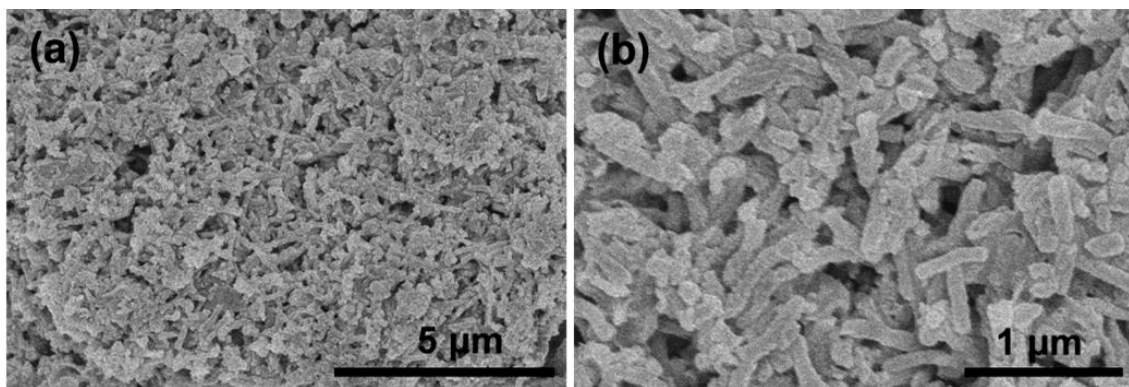


Figure S9. SEM images of 5% CdSe/CN after photocatalytic reactions.

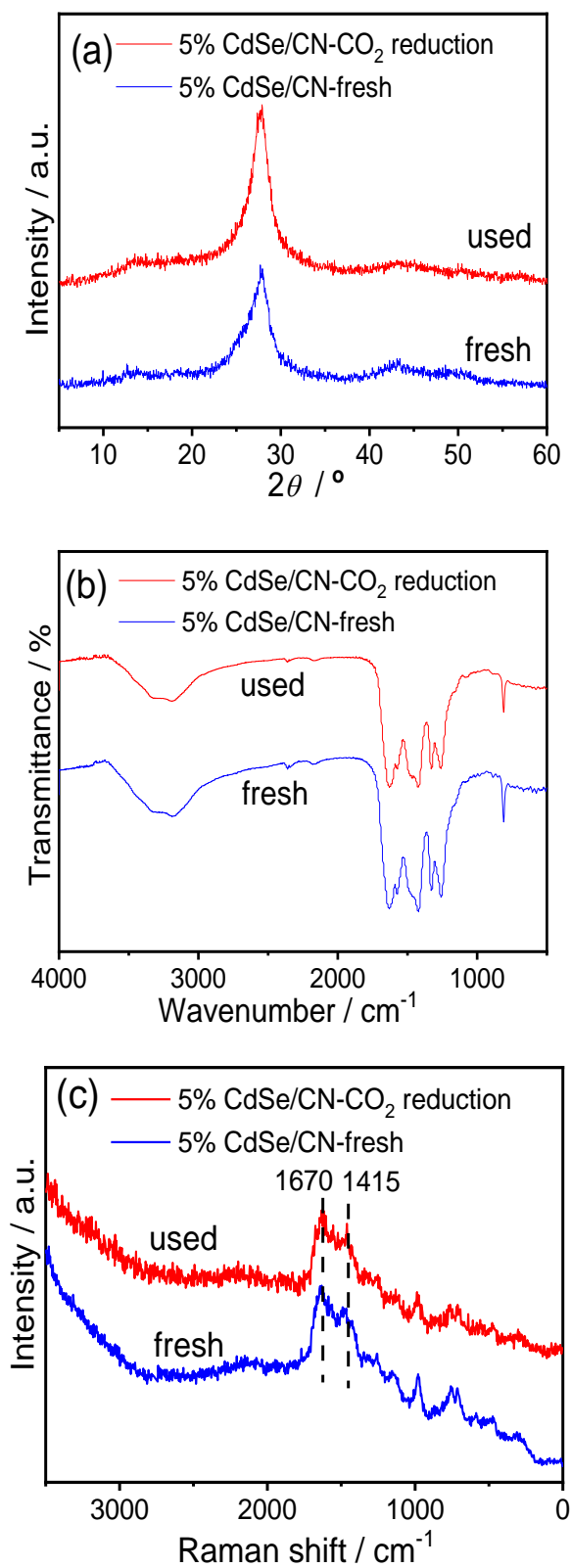


Figure S10. (a) XRD pattern, (b) FT-IR spectra, and (c) UV-Raman spectra of 5% CdSe/CN before and after the CO_2 conversion reaction.

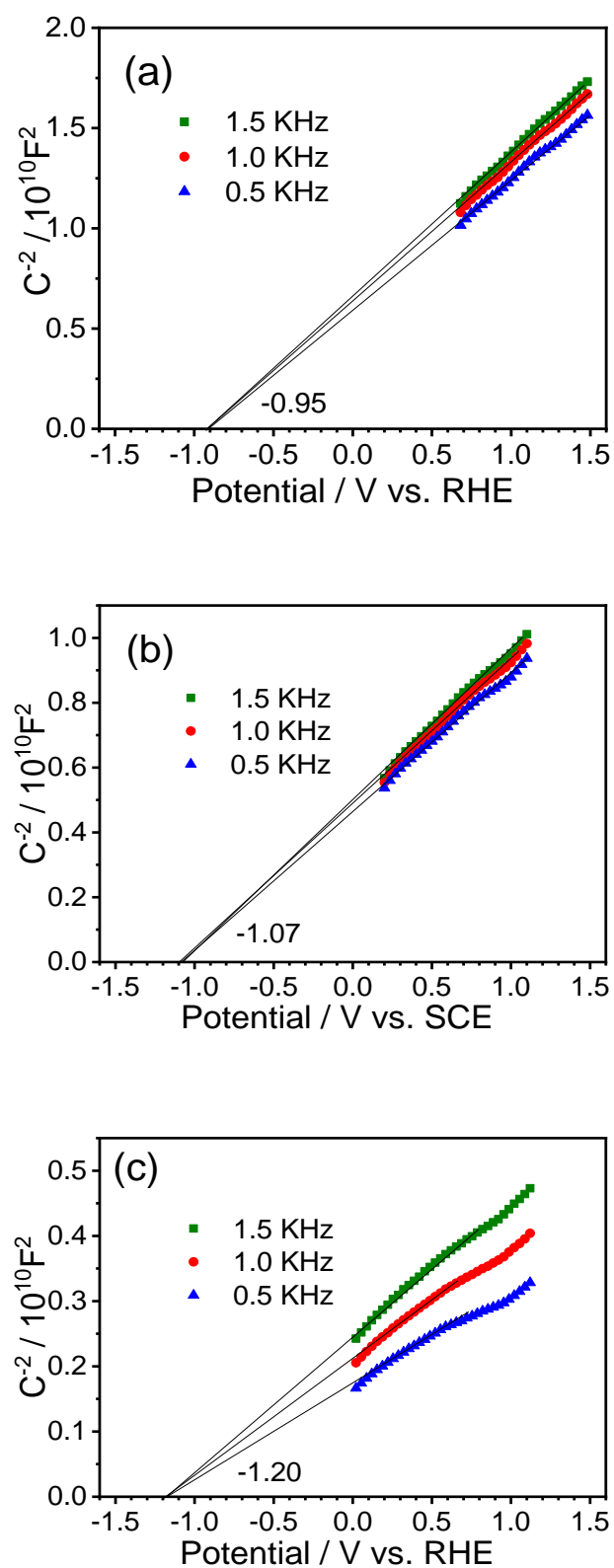


Figure S11. Mott-Schottky plots of (a) CN nanorods, (b) 5% CdSe/CN and (c) CdSe QDs.

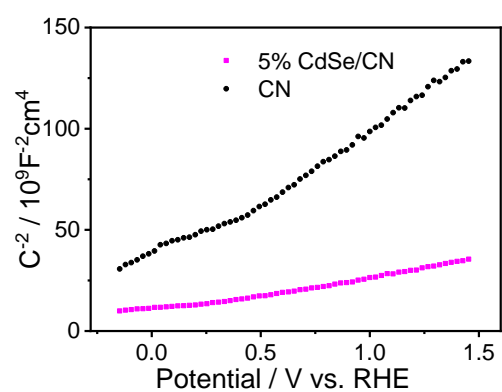


Figure S12. Mott-Schottky plots of CN nanorods and 5% CdSe/CN to calculate the charge carrier density.

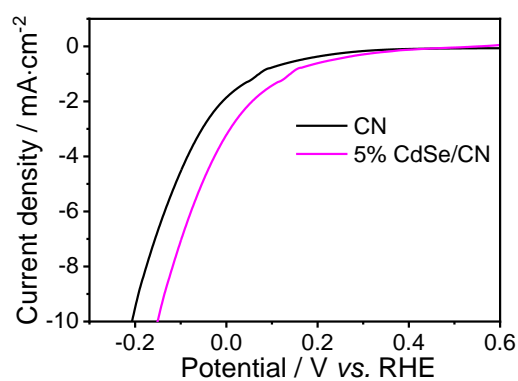


Figure S13. Linear sweep voltammetry for CN and 5% CdSe/CN.

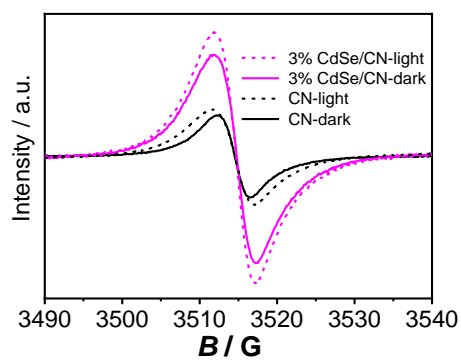


Figure S14. EPR spectra of CN and 5% CdSe/CN.

Table S1. Fitted fluorescence decay components of CN nanorods and 5% CdSe/CN ($\lambda = 375$ nm).

Sample	τ_1 (ns)	τ_2 (ns)	τ_{average} (ns)	χ^2
CN nanorods	1.15 (86.3%)	9.71 (13.7%)	2.32	0.986
5% CdSe/CN	1.03 (76.9%)	5.83 (23.1%)	2.14	0.993

short lifetime (τ_1), long lifetime (τ_2) and average lifetime (τ_{average}).

Table S2. Literature values of AQY for CN-based photocatalysts in hydrogen evolution.

Photocatalyst	Photocatalyst loading (mg)	Co-catalysts	Incident wavelength; λ_i (nm)	AQY (%)	Reference
CdSe/CN	20	3 wt % Pt	420 nm	10.2	This work
18 wt% CdSe-TF-g-C ₃ N ₄ sheet	5	/	460 nm	13.9	[39]
Porous g-C ₃ N ₄ sheet	50	3 wt % Pt	420 nm	1.5	[68]
			580nm	6.3	
			680nm	4.4	
Carbon QDs on g-C ₃ N ₄ nano tubes	50	3 wt % Pt	420 nm	10.9	[69]
P-doped g-C ₃ N ₄ nanoflakes	10	3 wt % Pt	420 nm	6.7	[70]
			600nm	0.2	
Crystalline g-C ₃ N ₄ nanosheet	50	3 wt % Pt	420 nm	9.0	[71]
Thin, porous g-C ₃ N ₄ sheet	50	3 wt% Pt	425 nm	6.8	[72]
Defect-rich amorphous carbon nitride (DACN)	50	3 wt% Pt	400 nm	34.4	[73]
			425nm	31.9	
CdS QDs on WS ₂ /g-C ₃ N ₄ nanosheets	10	/	400 nm	5.4	[74]
Few-layered polymeric CN	50	3 wt% Pt	405 nm	11.3	[75]
C ₃ N ₄ sheet/MnO ₂	100	/	420 nm	3.8	[76]

Table S3. Various controlled experiments for CO₂ reduction.

Entry	Reaction Conditions	CO [μmol]	H ₂ [μmol]	CO+H ₂ [μmol]
1	(a)	7.0	1.1	8.1
2	Without catalyst	n.d. ^(b)	n.d.	-
3	In dark	n.d.	n.d.	-
4	Using Ar instead of CO ₂	n.d.	0.5	0.5
5	Without triethanolamine	n.d.	n.d.	-
6	Without bipyridine	n.d.	<0.1	<0.1
7	Without CoCl ₂ ·6H ₂ O	n.d.	<0.1	<0.1

(a) Reaction conditions: 5% CdSe/CN catalyst (20 mg), 2,2'-bipyridyl (15 mg), H₂O (1 mL), acetonitrile (3 mL), triethanolamine (1 mL), CoCl₂·6H₂O (1 μmol), CO₂ (1 bar), 40 °C, 1 h, and λ > 420 nm; (b) Not detectable.

Table S4. The reactivity of photocatalysts for CO₂ reduction.

Entry	Catalyst	CO [μmol]	H ₂ [μmol]	CO+H ₂ [μmol]	Turn over number ^(a)	Selectivity ^(b) / %
1	CN nanorods	8.9	0.3	9.2	9.2	96.7
2	CdSe	0.5	0.1	0.6	0.6	83.3
3	1% CdSe/CN	15.2	0.4	15.6	15.6	97.4
4	3% CdSe/CN	17.8	0.4	18.2	18.2	97.8
5	5% CdSe/CN	23.2	0.5	23.7	23.7	97.9
6	7% CdSe/CN	20.8	0.6	21.4	21.4	97.2
7	10% CdSe/CN	18.5	0.6	19.1	19.1	96.9

Reaction conditions: catalyst (30 mg), 2,2'-bipyridyl (15 mg), H₂O (1 mL), acetonitrile (3 mL), triethanolamine (1 mL), CoCl₂·6H₂O (1 μmol), CO₂ (1 bar), 30 °C, 1 h, and λ > 420 nm. (a) Turn over number = (mol amount of CO and H₂)/(mol amount of cobalt ion); (b) Selectivity = $n_{\text{CO}}/n_{(\text{CO}+\text{H}_2)} \times 100$; (c) Not detectable.

Table S5. Calculated values of equivalent circuit elements for CN and 5% CdSe/CN samples.

Samples	R ₁ [Ω]	R ₂ [Ω]	C ₂ [F]
CN	145.8	1.09×10 ⁶	1.52×10 ⁻⁶
5% CdSe/CN	124.2	9.73×10 ⁵	3.57×10 ⁻⁶