Supporting Information

COF in situ growing on CdS nanorods as core-shell heterojunction for improving the charge-separation efficiency

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Part S1

Characterization

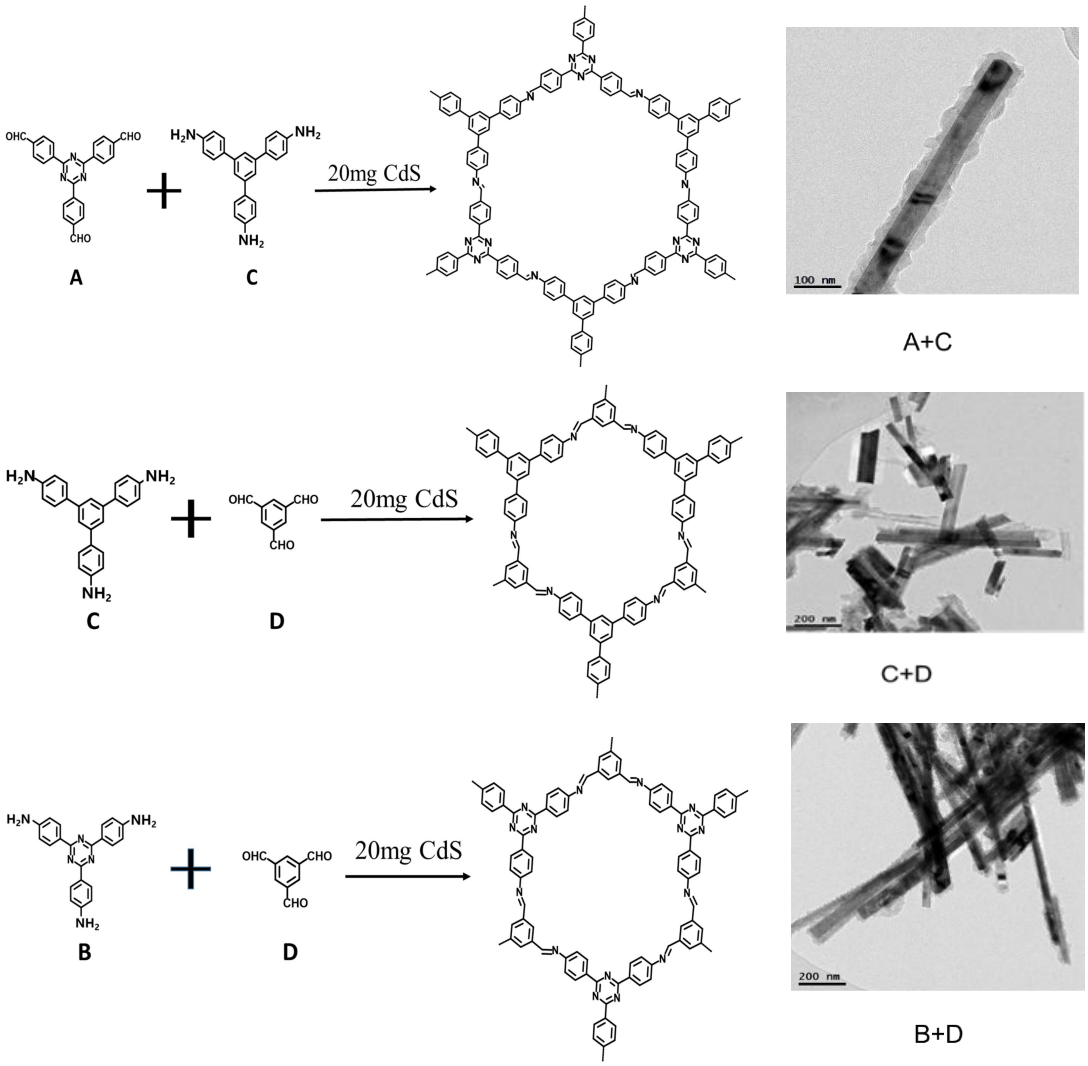

Fig. S1 Synthetic process and TEM images of CdS@COF_{A+C}, CdS@COF_{C+D} and CdS@COF_{B+D}, respectively.

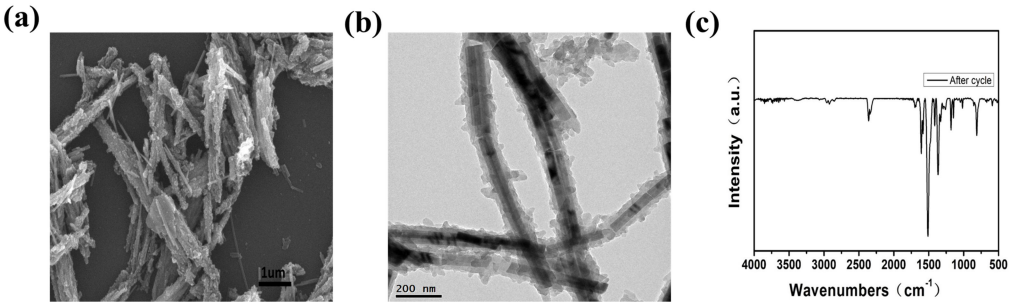

Fig. S2 SEM, TEM and FT-IR after hydrogen evolution cycling reaction of CdS@TTI-COF-60

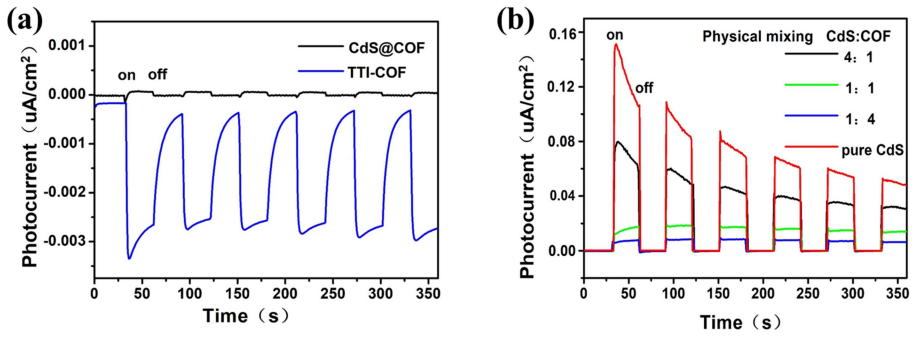

Fig. S3 Photocurrent response of (a)TTI-COF and CdS@TTI-COF-60 (b)pure CdS and physical mixing of CdS and TTI-COF

Part S2

Calculation of apparent quantum yield

The apparent quantum yield (AQY) of CdS@TTI-COF-60 was calculated based on the H_2 production under simulated solar irradiation by a Xe lamp equipped with a 420nm monochromatic optical filter, the ILT 950 spectroradiometer was used to measure the intensity of incident monochromatic illumination . The AQY is calculated by using the following equation

$$AQY = \frac{2MN_Ahc}{AIt\lambda} \times 100\%$$

Where M is molar amounts of H_2 during irradition 1 h ($M=4.25\times10^{-6}$mol/h), N_A is Avogadro constant (6.022×10^{23} mol^{-1}). h is Planck constant (6.626×10^{-34} J·s). c is the light velocity (3×10^8 m/s). A is the irradiation area (1.6×10^{-3} m^2). I is the intensity of irradation light (281.46 W/m^2). t is the reaction time (3600 s). λ is the wavelength of the monochromatic light (λ= 420 nm). Finally, AQY=0.15%

Part S3

Carrier density calculation

The carrier density (N_D) is calculated using this formula: [1-3]

$$N_D=(2/e\varepsilon\varepsilon_0)[d(U_{FL})/d(1/C^2)]$$

where e = 1.6×10^{-19} C, ε_0= 8.86×10^{-12} F m^{-1}, ε is the dielectric constant, and C is the

capacitance. The dielectric constants of TTI-COF and CdS are about 3.67 and 6.56, respectively. The slopes of TTI-COF and CdS are 6.4×10^{10} and 3×10^{10}. Therefore, the N_D values of TTI-COF and CdS are about 5.99×10^{18} cm^{-3} and 7.16×10^{18} cm^{-3}, respectively.

References

1 X. Fang-Xing, S.F. Hung, J.W. Miao, H.Y. Wang, H.B. Yang, B. Liu, *Small*, 2015, **11**, 554-567.

2 Z.H. Zhang, P. Wang, *Energy Environ. Sci.*, 2012, **5**, 9948-9948.

3 G. Wang, Q. Wang, W. Lu, J.H. Li, *J. Phys. Chem. B*, 2006, **110**, 22029-22034.