

Supporting Information

Hydrogen-Bonding-Assisted Charge Transfer: Significantly Enhanced Photocatalytic H₂ Evolution over g-C₃N₄ Anchored with Ferrocene-based Hole Relay

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In the FT-IR spectrum of FcDA, the band at 1695 cm^{-1} is assigned to the stretching mode of C=O.¹ When the C=O group is involved in hydrogen bonds, the resonance will take place and then influence their stretching wave-numbers.² The vibration of C=O moves to low wave-number ($1695\text{--}1670\text{ cm}^{-1}$) in the spectrum of FcDA/CN composite, indicating that the hydrogen bonding has been formed between FcDA and g-C₃N₄.² The broad peak at $3000\text{--}3700\text{ cm}^{-1}$, attributed to the unpolymerized N-H vibration of g-C₃N₄, shifts to large wave-number slightly, which is induced by the effect from hydrogen bonding of N-H groups in the g-C₃N₄ with carboxylic groups in the FcDA.³

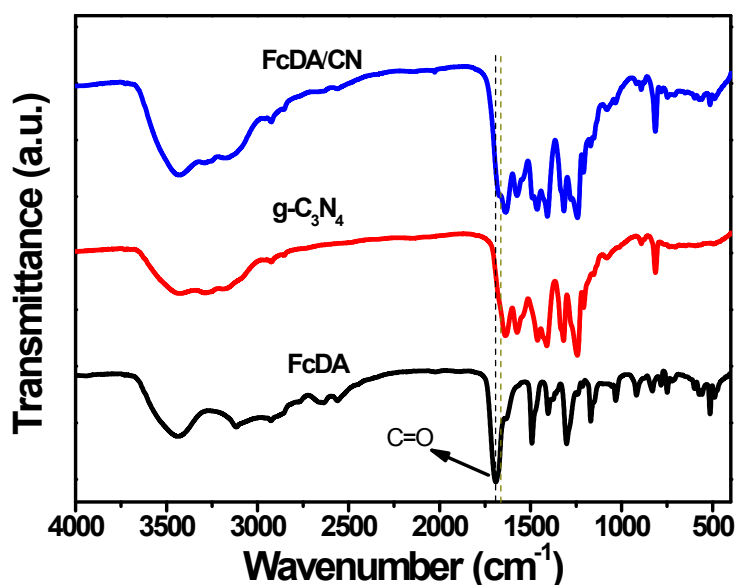


Fig. S1 The FTIR spectra of FcDA, g-C₃N₄ and FcDA/CN composite.

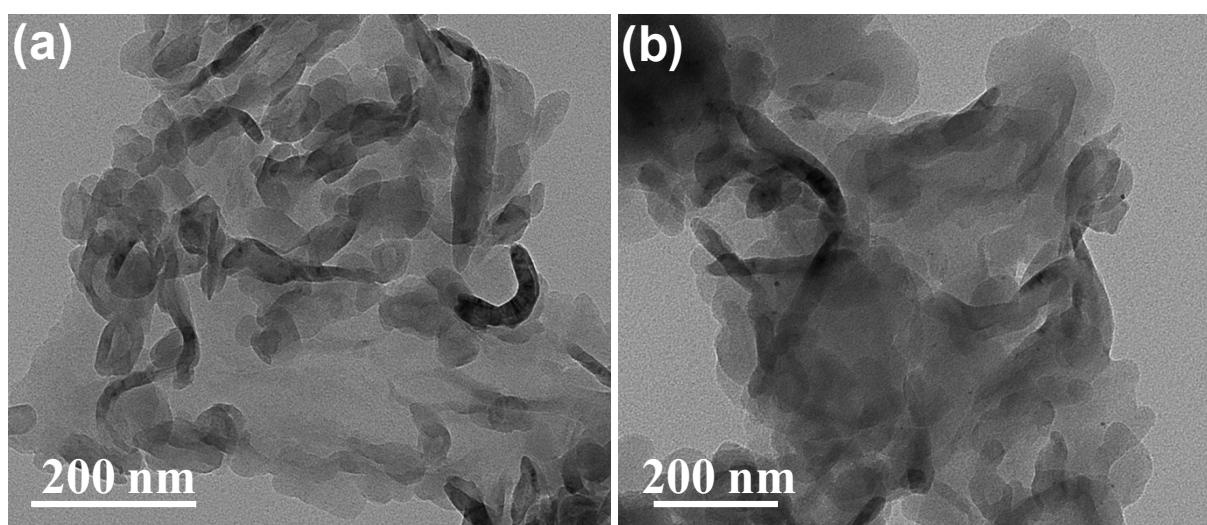


Fig. S2 TEM images of (a) pure g-C₃N₄ and (b) FcDA/CN with 1 wt % Pt loading.

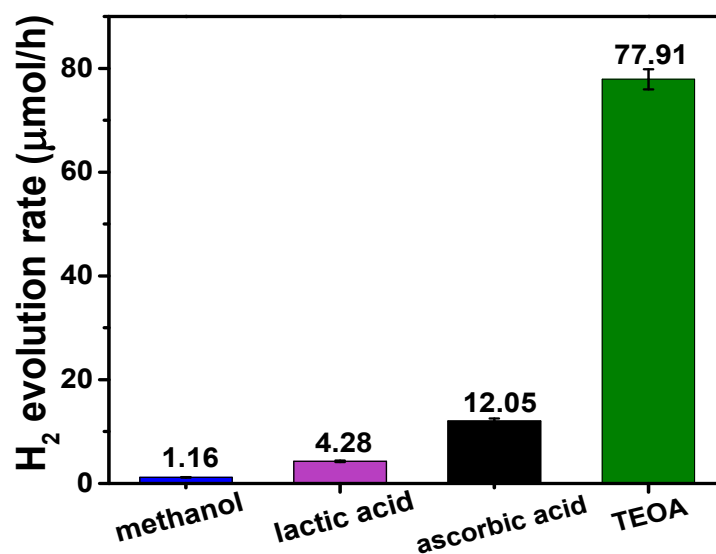


Fig. S3 Comparison of photocatalytic hydrogen evolution rates on 4 wt% FcDA/CN photocatalyst in the presence of different sacrificial reagents under visible light ($\lambda \geq 420$ nm). Reaction conditions: catalyst, 50 mg; 100 mL of solution containing sacrificial reagents; light source, xenon lamp (300 W) with a cutoff filter; temperature, 10 °C.

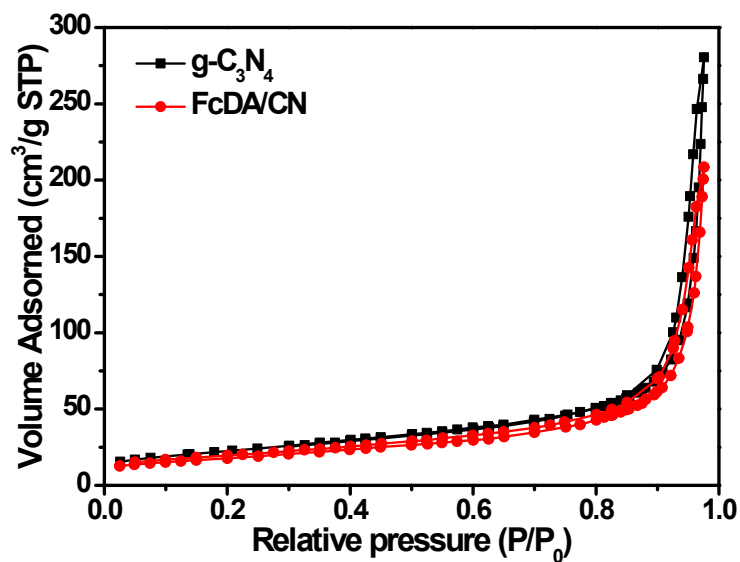


Fig. S4 The nitrogen adsorption/desorption isotherms of $\text{g-C}_3\text{N}_4$ and FcDA/CN composite.

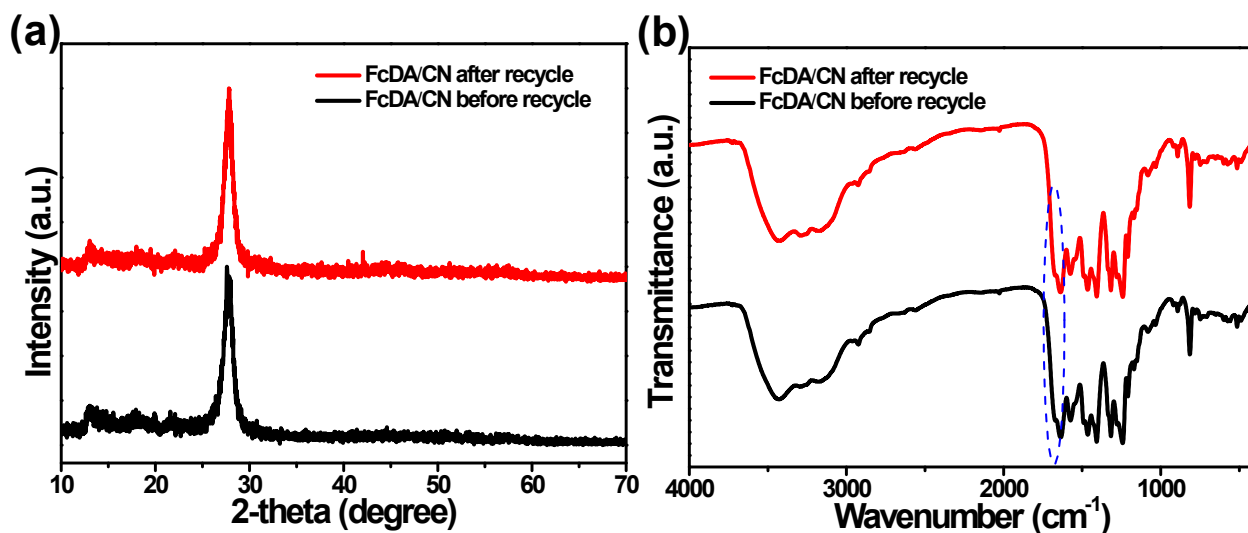


Fig. S5 The XRD patterns (a) and FT-IR spectra (b) of FcDA/CN composite before and after cycle test.

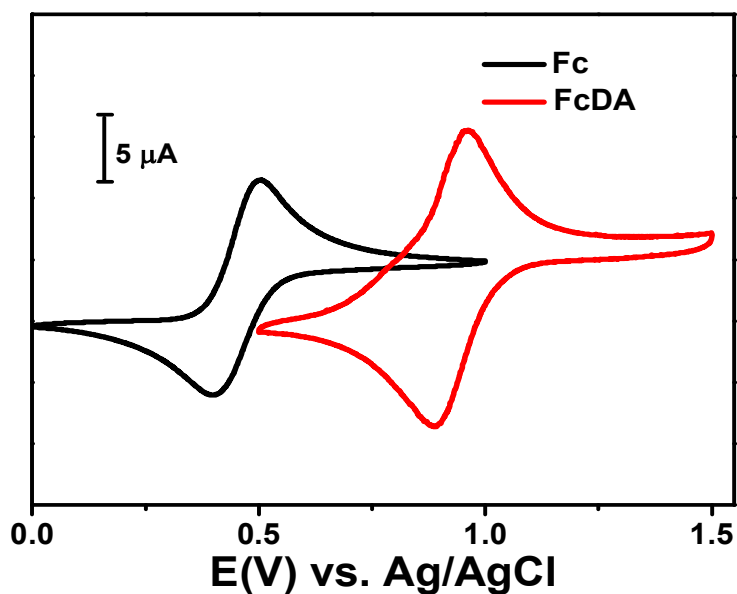


Fig. S6 Cyclic voltammograms of the Fc and FcDA collected in 0.1 M of Bu₄NPF₆ in acetonitrile, scanned at 50 mV s⁻¹, Ag⁺/AgCl as a reference electrode, freshly polished 3.0 mm diameter glassy carbon button electrode served as the working electrode, Pt wire as a counter electrode. The concentration of FcDA in solution was approximately 1 mM. Onset potential with reference to Fc, $E_{\text{OX}} = E_{\text{Ag}^+/\text{AgCl}} - E_{\text{Fc}}$; Calculated from the equation, $\text{HOMO} = -(4.80_{(\text{Fc})} + E_{\text{OX}})$ eV.⁴

Notes and references

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2. Z. H. Sun, W. M. Sun, C. T. Chen, G. H. Zhang, X. Q. Wang and D. Xu, *Spectrochimica Acta Part A*, 2011, **83**, 39–45.
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4. J. Lee, M. M. Byranvand, G. Kang, S. Y. Son, S. Song, G. –W. Kim, T. Park, *J. Am. Chem. Soc.*, 2017, **139**, 12175–12181.