Supporting Information

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

Ya-Nan Liu,ᵃ Xiao Zhou,ᵃ Cong-Cong Shen,ᵃ Zhi-Wei Zhao,ᵃ Yi-Fan Jiang,ᵃ Liu-Bo Ma,ᵃ Xiao-Xiang Fang,ᵃ Zeb, Akif,ᵃ Tuck-Yun Cheag,ᵇ and An-Wu Xuᵃ

ᵃDivision of Nanomaterials and Chemistry, Hefei National Laboratory for Physical Sciences at Microscale, Department of Chemistry Physics, University of Science and Technology of China, Hefei, Anhui 230026, People’s Republic of China.

ᵇDepartment of Breast and Thyroid Surgery, The First Affiliated Hospital of Sun Yat-Sen University, Guangzhou 510080, China

*To whom correspondence should be addressed.
Email: anwuxu@ustc.edu.cn
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 (1695-1670 cm$^{-1}$) in the spectrum of FcDA/CN composite, indicating that the hydrogen bonding has been formed between FcDA and g-C$_3$N$_4$.$^2$ The broad peak at 3000-3700 cm$^{-1}$, attributed to the unpolymerized N-H vibration of g-C$_3$N$_4$, shifts to large wave-number slightly, which is induced by the effect from hydrogen bonding of N-H groups in the g-C$_3$N$_4$ with carboxylic groups in the FcDA.$^3$

![Fig. S1](image)

**Fig. S1** The FTIR spectra of FcDA, g-C$_3$N$_4$ and FcDA/CN composite.

![TEM images](image)

**Fig. S2** TEM images of (a) pure g-C$_3$N$_4$ 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 (λ ≥ 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 g-C₃N₄ 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, sanned 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, HOMO = $-(4.80_{(\text{Fc})} + E_{\text{OX}})$ eV.⁴
Notes and references


