Supporting Information

Fe-based MOFs for Photocatalytic CO_2 Reduction: Role of Coordination Unsaturated Sites and Dual Excitation Pathways

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Figure S1 TG of the as-prepared MIL-101(Fe).

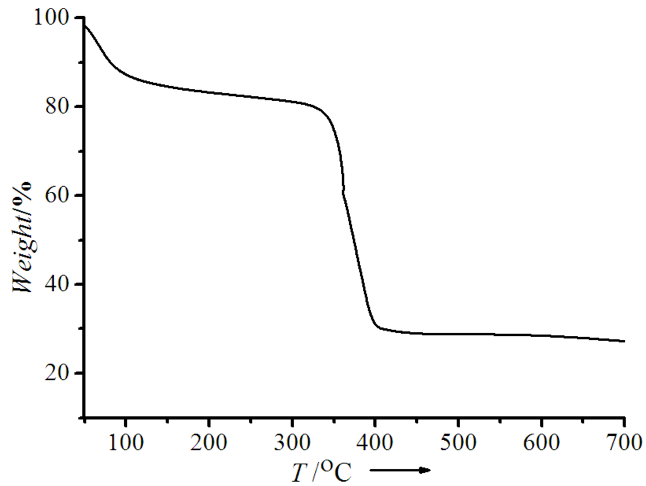

Figure S2 N_2 adsorption/desorption of the as-prepared MIL-101(Fe).

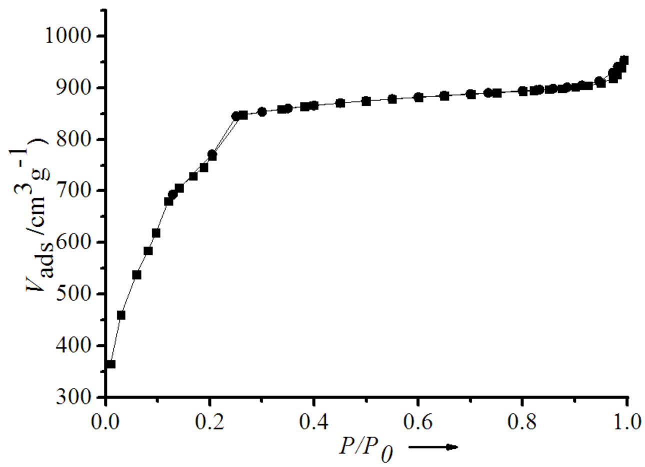

Figure S3 The ^{13}C NMR spectra for the product obtained from the reaction with $^{12}CO_2$

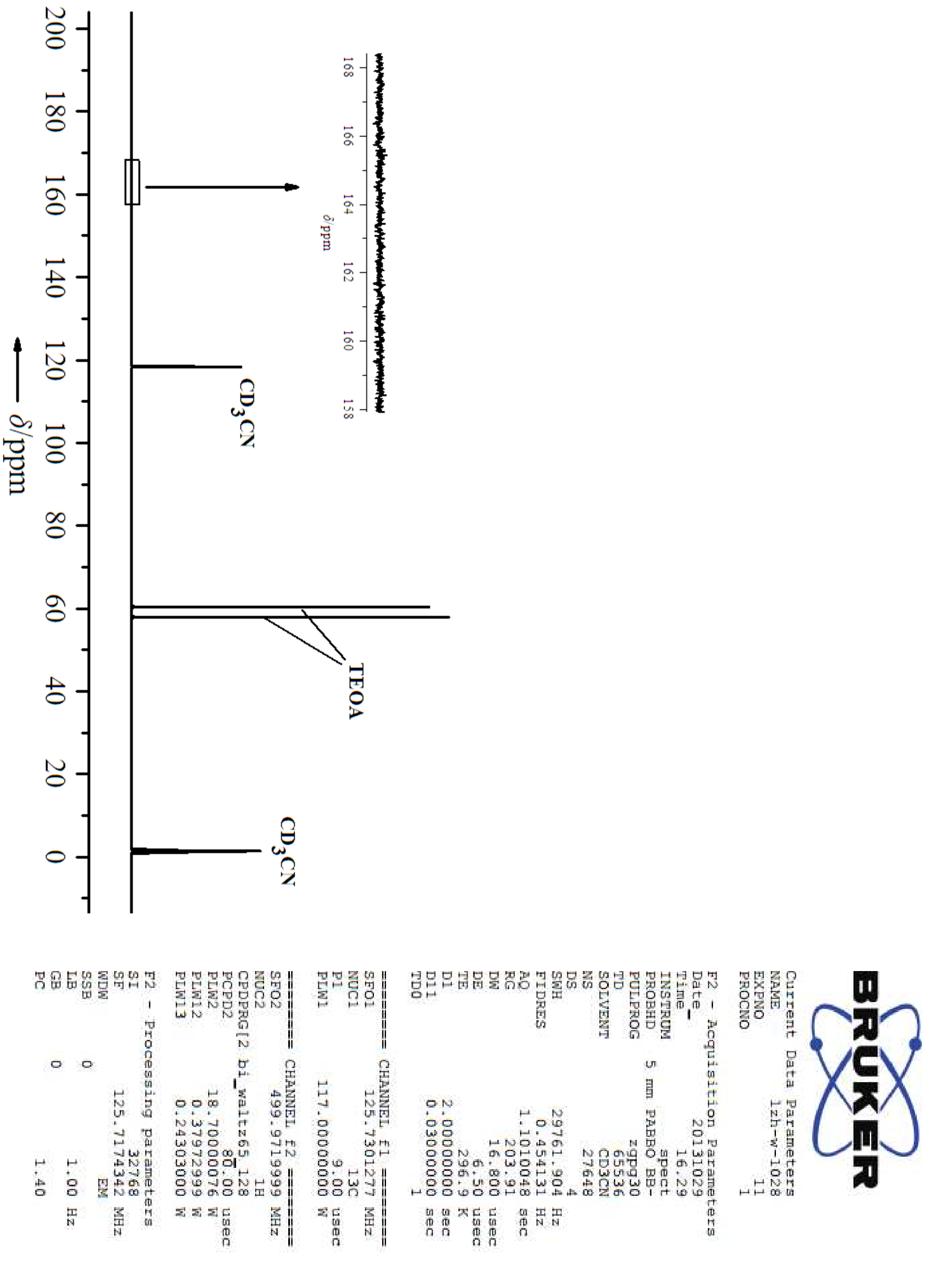

Figure S4 The ^{13}C NMR spectra for the product obtained from the reaction with $^{13}CO_2$

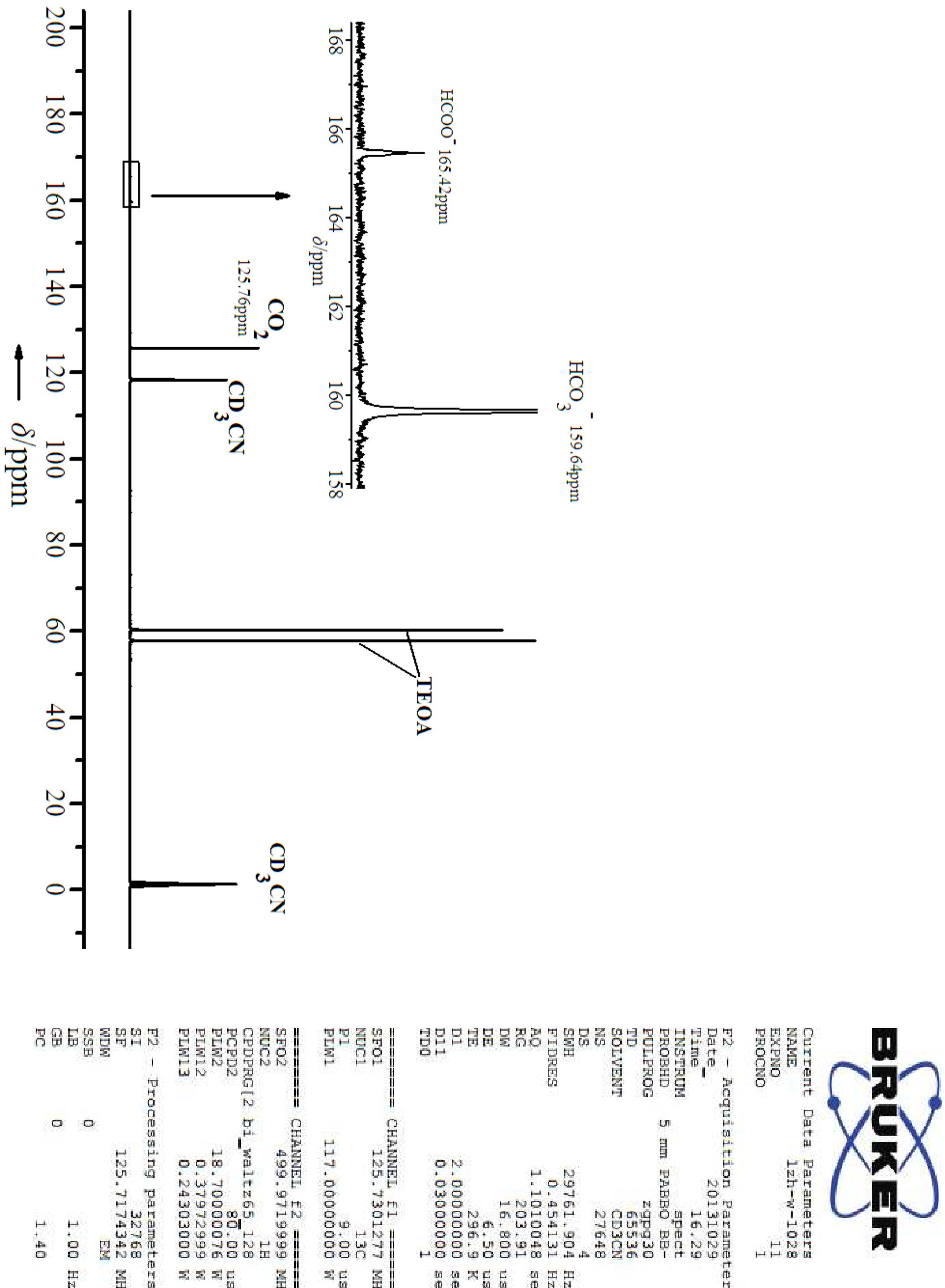

Figure S5 The amount of $HCOO^-$ produced as a function of the irradiation time over MIL-101(Fe) (at 8 h, the solid was removed from the reaction system)

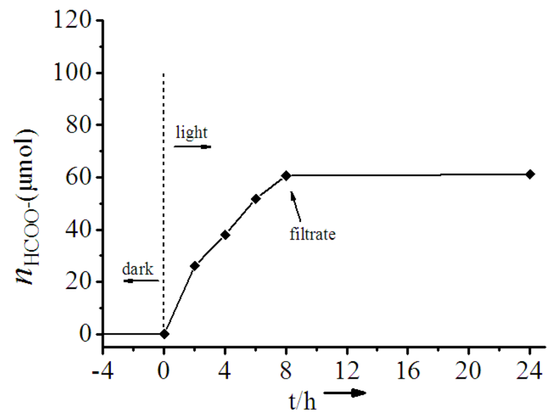

Figure S6 The recycling use of MIL-101(Fe) for photocatalytic CO_2 reduction

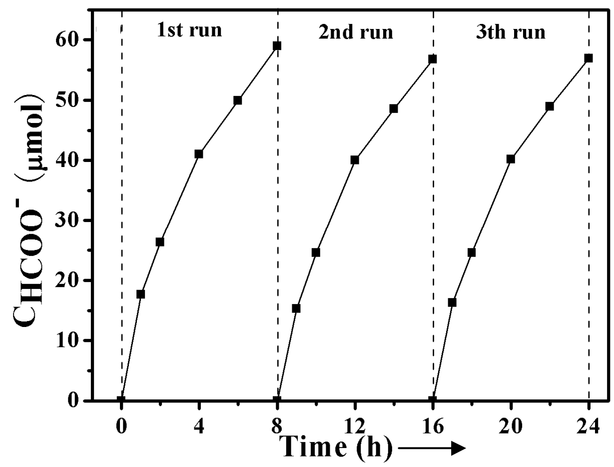

Figure S7 XRD of MIL-101(Fe) (fresh and after the photocatalytic reaction)

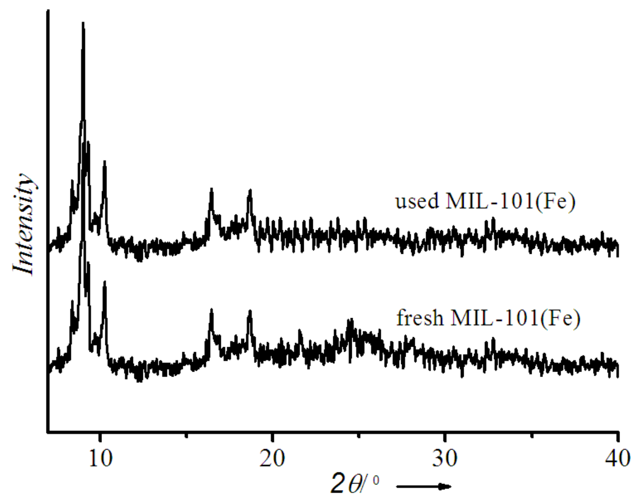

Figure S8 IR of MIL-101(Fe) (fresh and after the photocatalytic reaction)

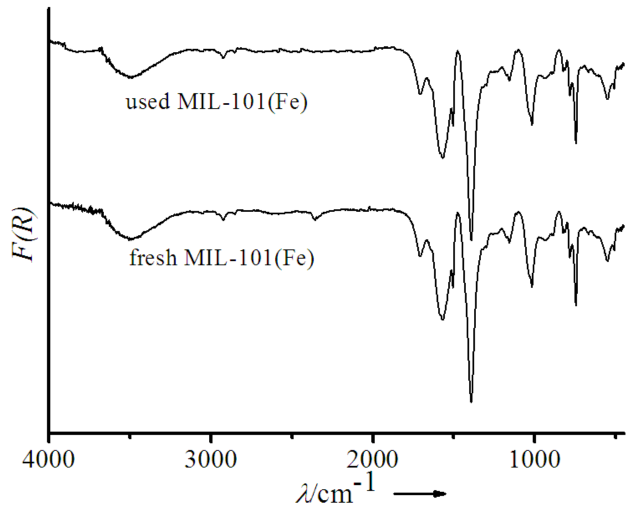

Figure S9 TG of MIL-101(Fe) (fresh and after the photocatalytic reaction)

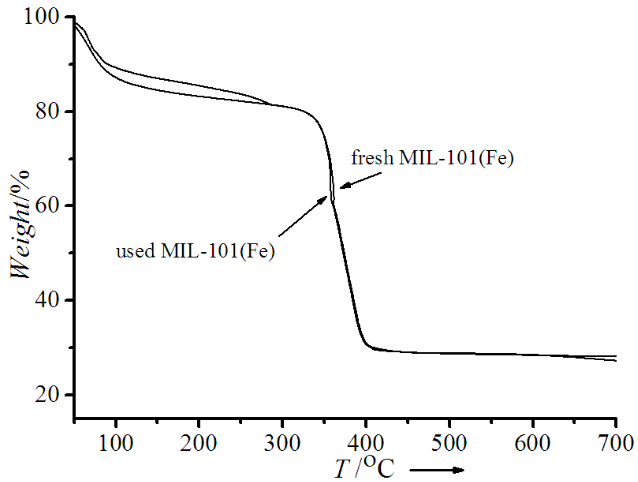

Figure S10 N_2 adsorption/desorption isotherm of MIL-101(Fe) (fresh and after the photocatalytic reaction)

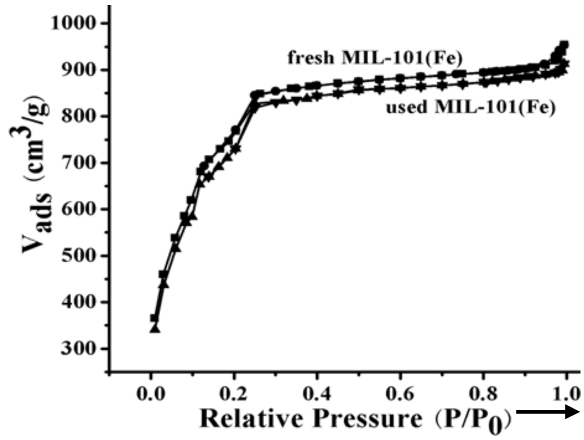

Figure S11 Mott−Schottky plots for MIL-101(Fe). The ac amplitude is 20 mV and the frequency is in the range 0.5−1.5 KHz.

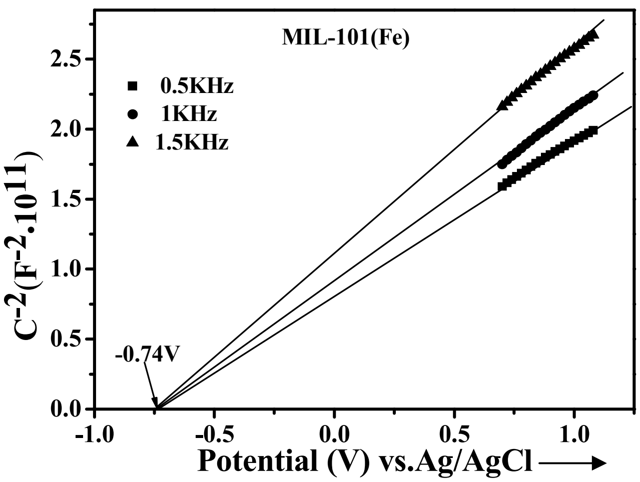

Figure S12 XRD of MIL-53(Fe) (fresh and after the photocatalytic reaction)

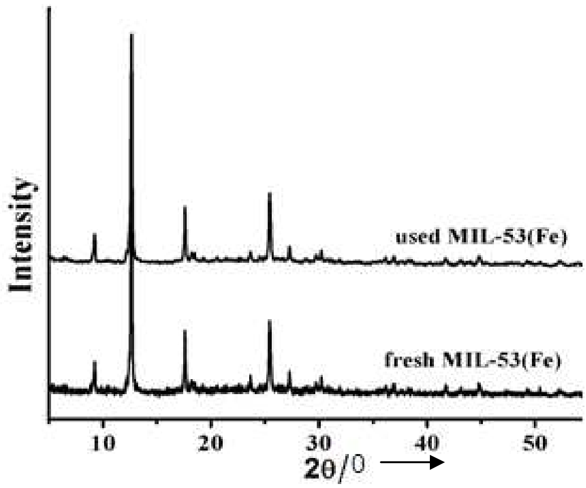

Figure S13 TG of MIL-53(Fe) (fresh and after the photocatalytic reaction)

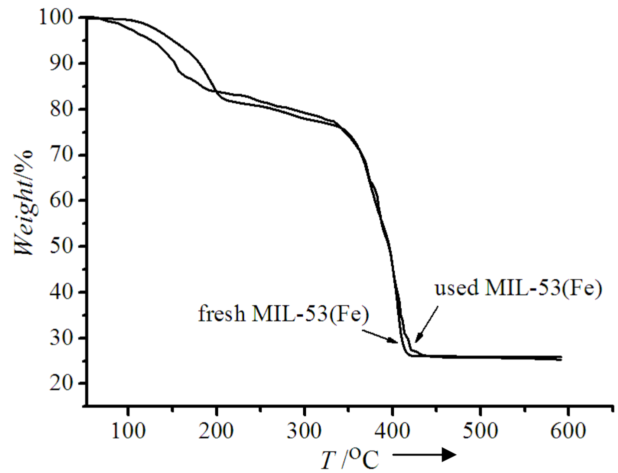

Figure S14 XRD of MIL-88B (Fe) (fresh and after the photocatalytic reaction)

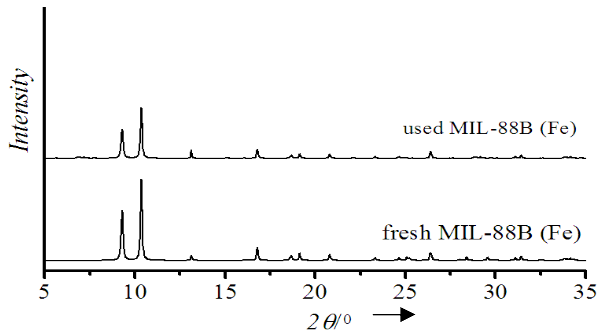

Figure S15 TG of MIL-88B(Fe) (fresh and after the photocatalytic reaction)

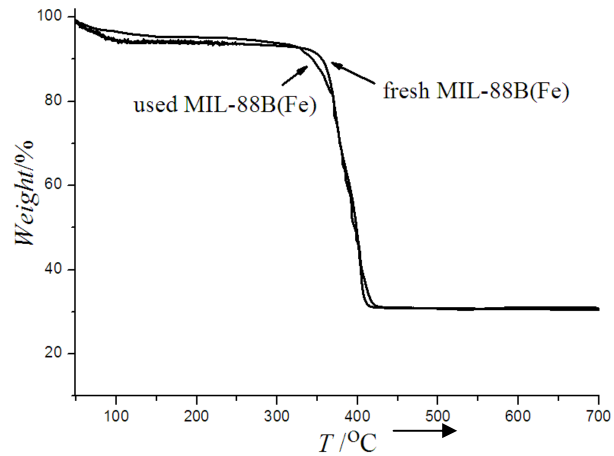

Figure S16 UV-vis spectra of MIL-53(Fe) and NH_2-MIL-53(Fe)

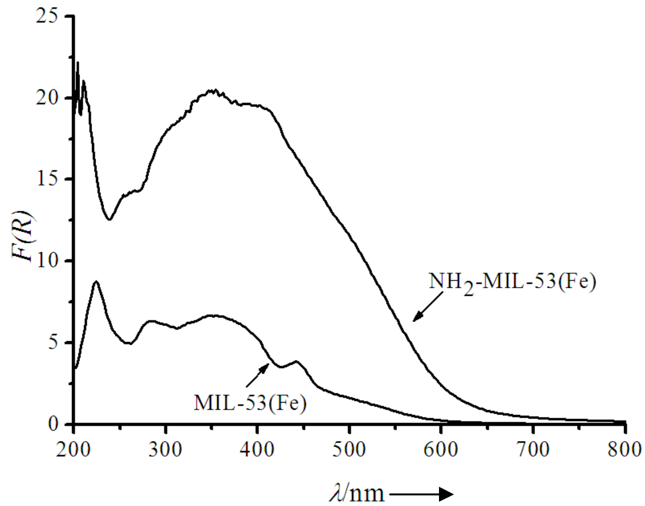

Figure S17 UV-vis spectra of MIL-88B(Fe) and NH_2-MIL-88B(Fe)

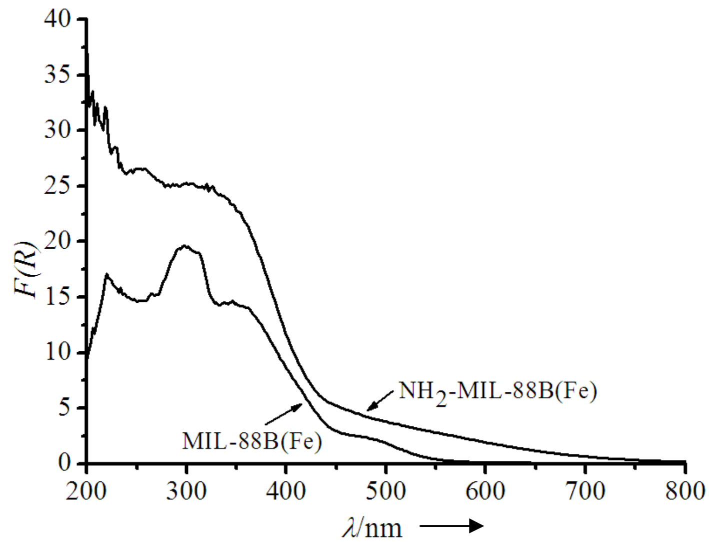

Figure S18 The amount of $HCOO^-$ produced as a function of the irradiation time over MIL-53(Fe).

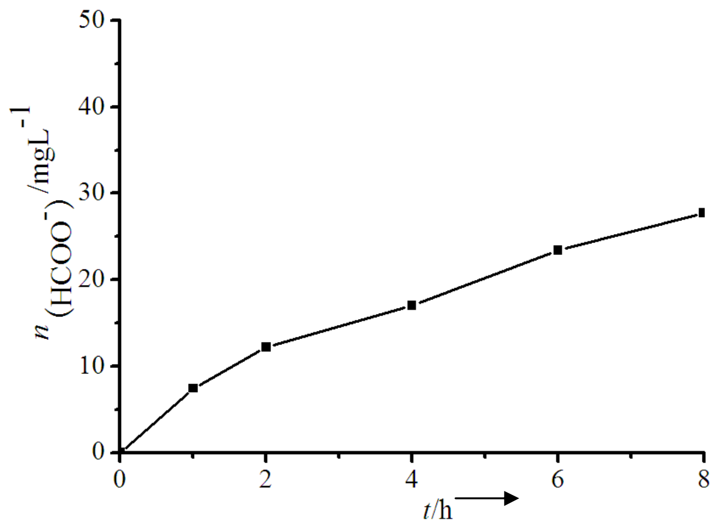

Figure S19 The amount of $HCOO^-$ produced as a function of the irradiation time over MIL-88B(Fe).

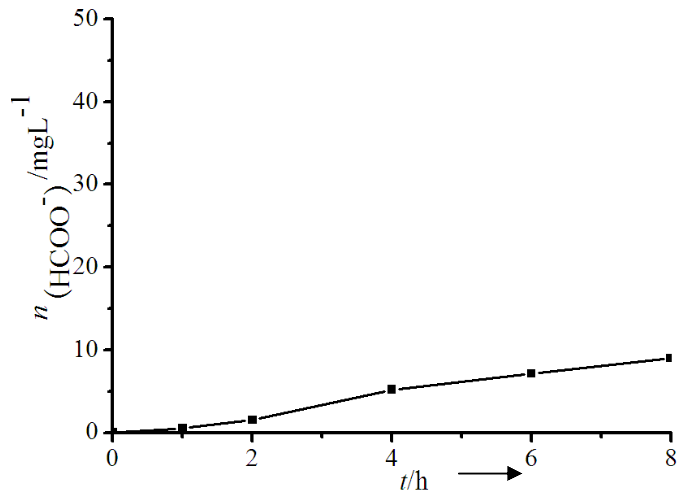

Figure S20 Mott−Schottky plots for MIL-53(Fe). The ac amplitude is 20 mV and the frequency is in the range 0.5−1.5 KHz.

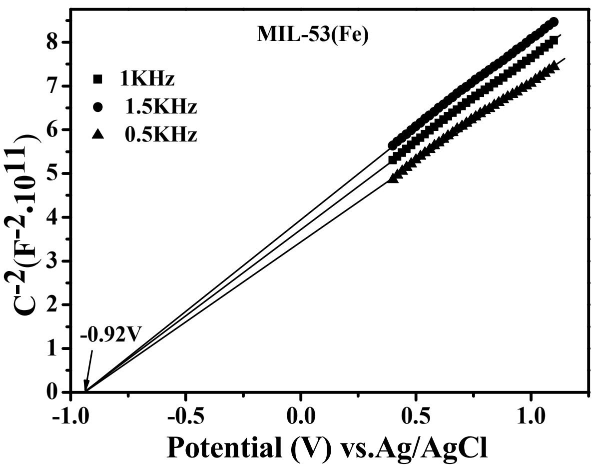

Figure S21 Mott−Schottky plots for MIL-88B(Fe). The ac amplitude is 20 mV and the frequency is in the range 0.5−1.5 KHz.

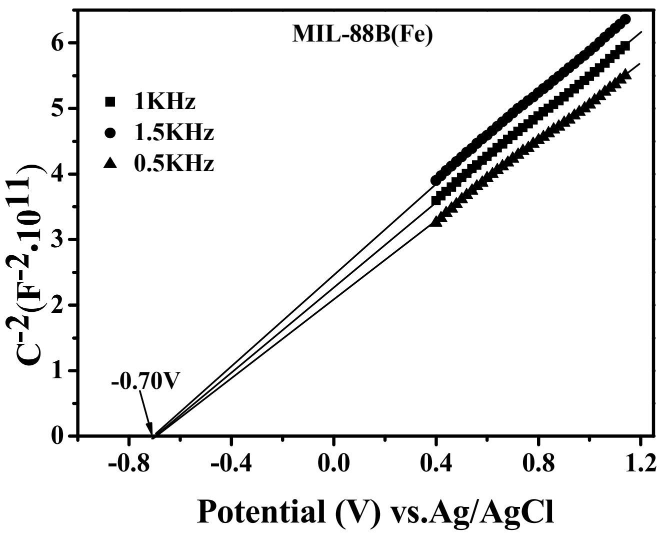

Figure S22 CO_2 adsorption isotherms (1 atm, 273K) of (a) MIL-101(Fe); (b) MIL-53(Fe); (c) MIL-88(Fe).

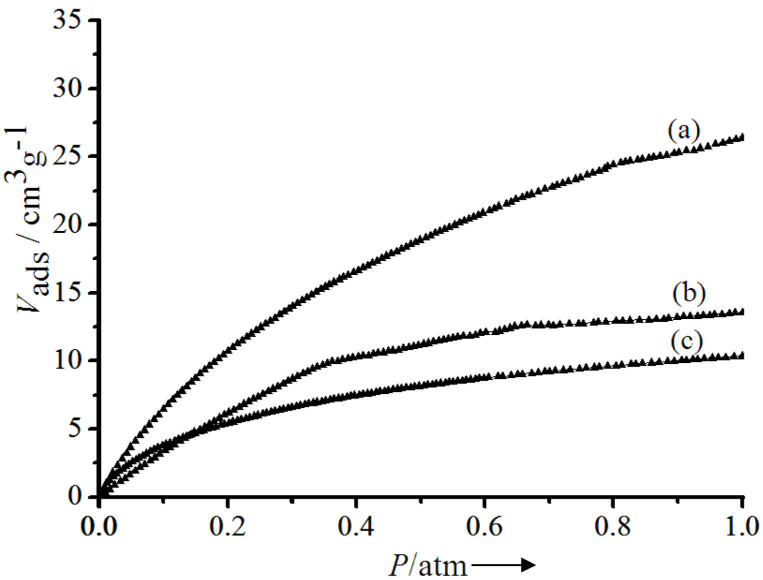

Figure S23 In situ FT-IR analyses of CO_2 adsorption process over pretreated MIL-53(Fe).

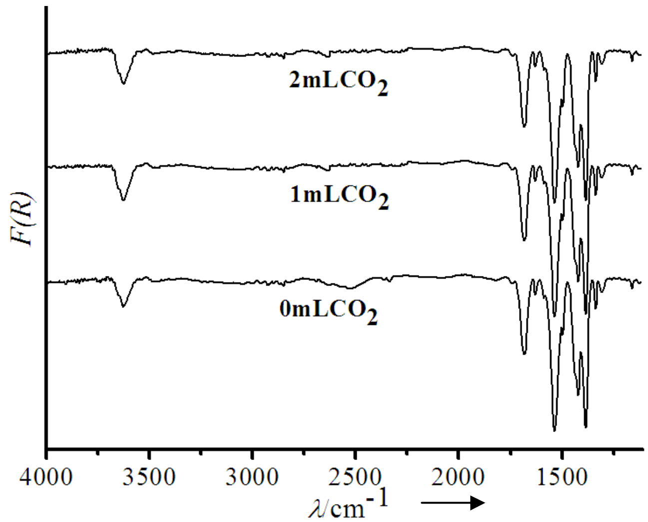

Figure S24 In situ FT-IR analyses of CO_2 adsorption process over pretreated MIL-88B(Fe).

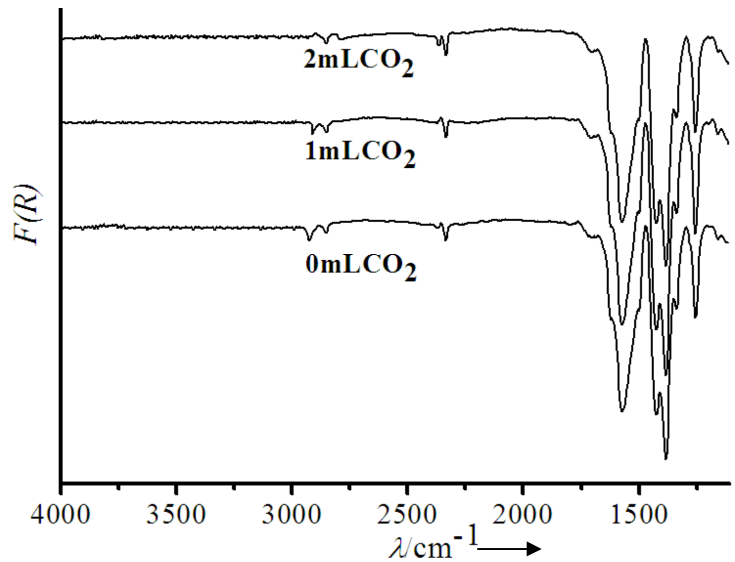

Figure S25 XRD pattern of NH_2-MIL-53(Fe).

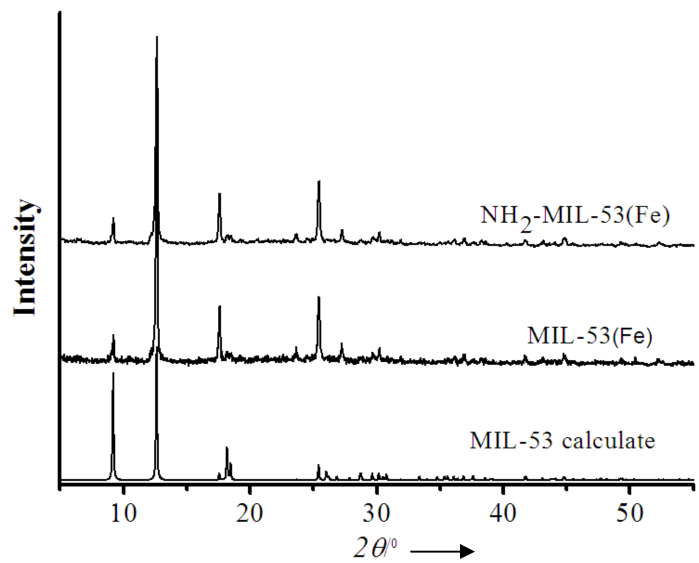

Figure S26 XRD pattern of NH_2-MIL-88B(Fe).

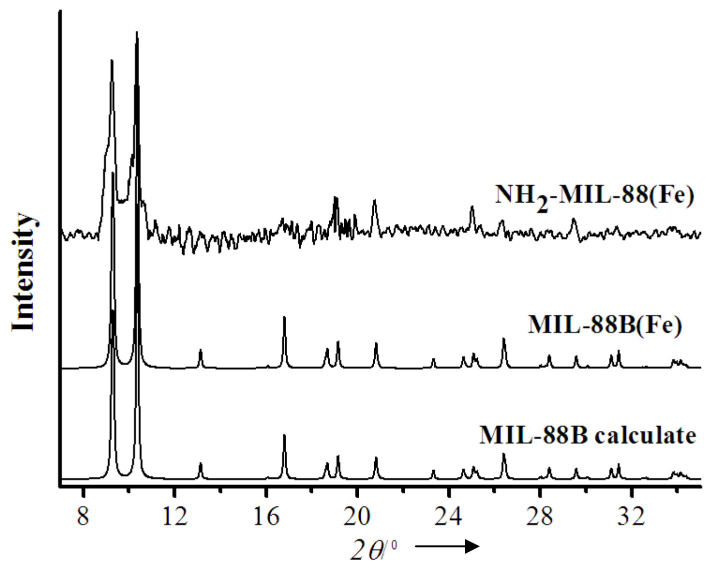

Figure S27 FT-IR spectrum of NH_2-MIL-101(Fe).

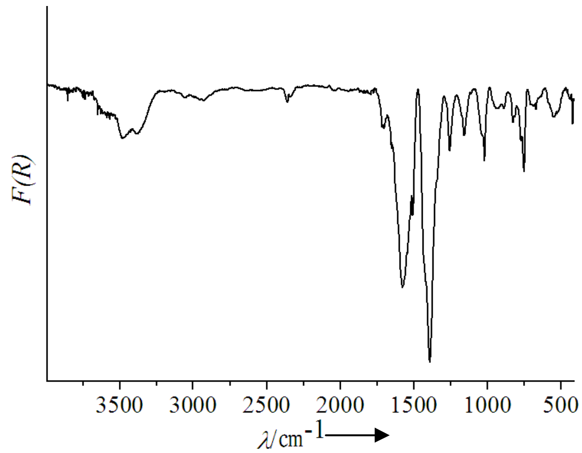

Figure S28 FT-IR spectrum of NH_2-MIL-53 (Fe).

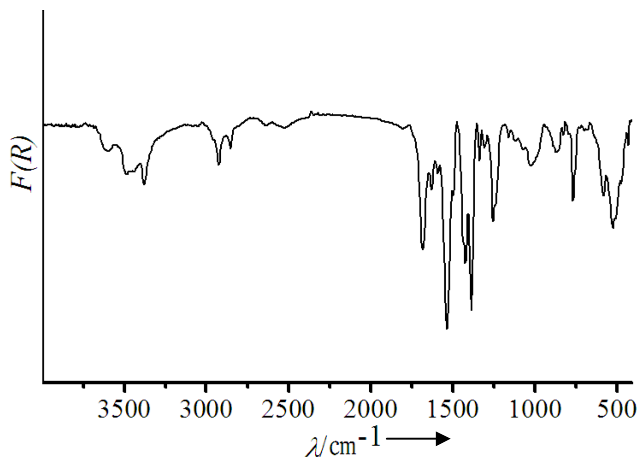

Figure S29 FT-IR spectrum of NH_2-MIL-88B(Fe).

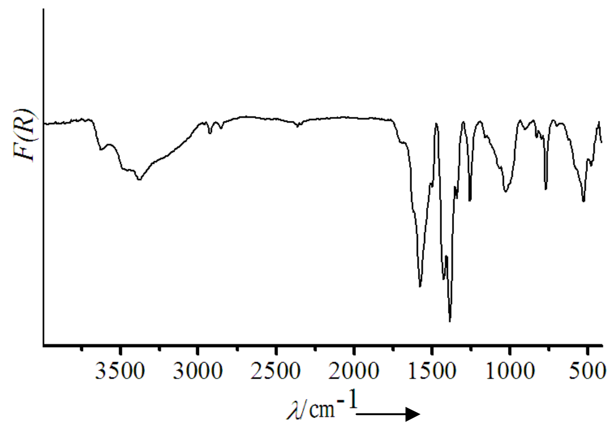

Figure S30 N_2 adsorption/desorption isotherm of NH_2-MIL-101(Fe).

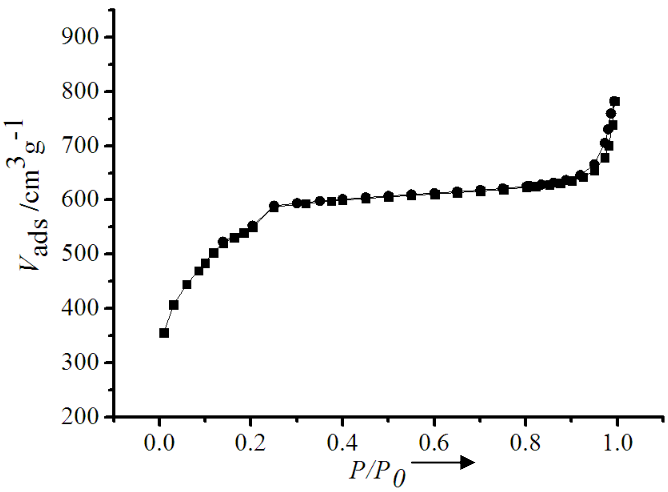

Figure S31 TG of NH_2-MIL-101(Fe).

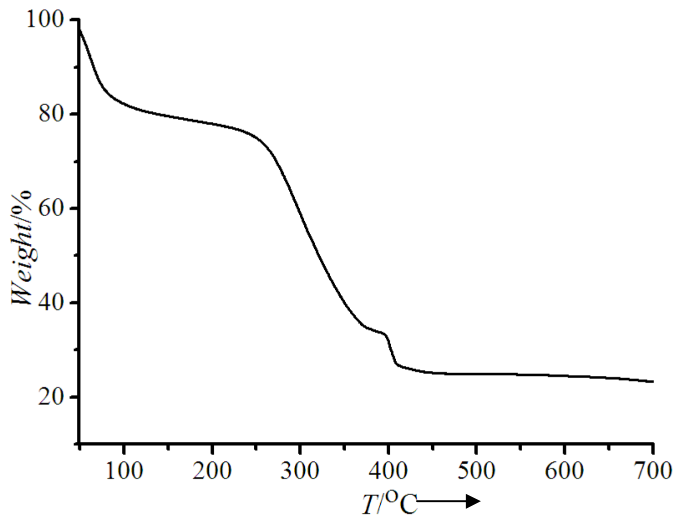

Figure S32 TG of NH_2-MIL-53(Fe).

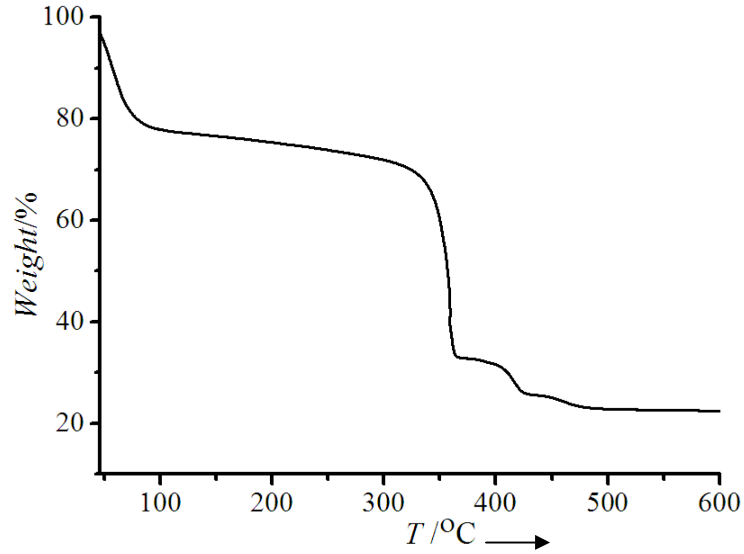

Figure S33 TG of NH_2-MIL-88B(Fe).

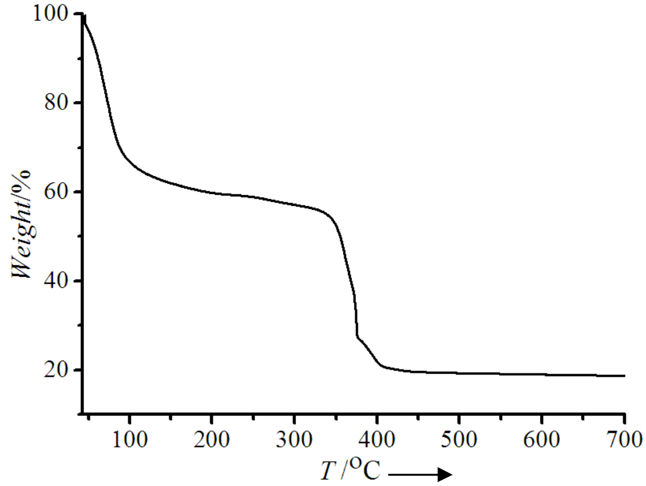

Figure S34 CO_2 adsorption isotherms (1 atm, 273K) of (a) NH_2-MIL-101(Fe); (b) NH_2-MIL-53(Fe); (c) NH_2-MIL-88(Fe).

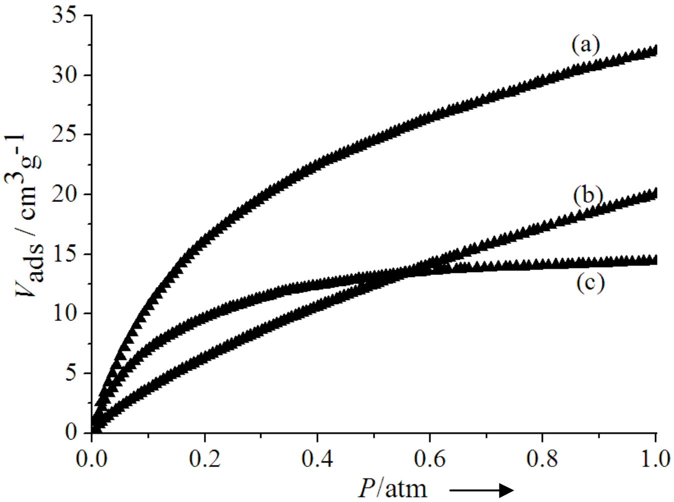

Table S1 QE for photocatalytic CO_2 reduction over NH_2-MIL-101(Fe) and MIL-101(Fe) at different wavelength

Sample	wavelength/nm	QE ($\times 10^{-4}$)
NH_2-MIL-101(Fe)	450	1.3
	500	0.7
	550	0.6
MIL-101(Fe)	450	0.8
	500	0.3
	550	0.2