

Supporting Information

Fe-based MOFs for Photocatalytic CO₂ Reduction: Role of Coordination Unsaturated Sites and Dual Excitation Pathways

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

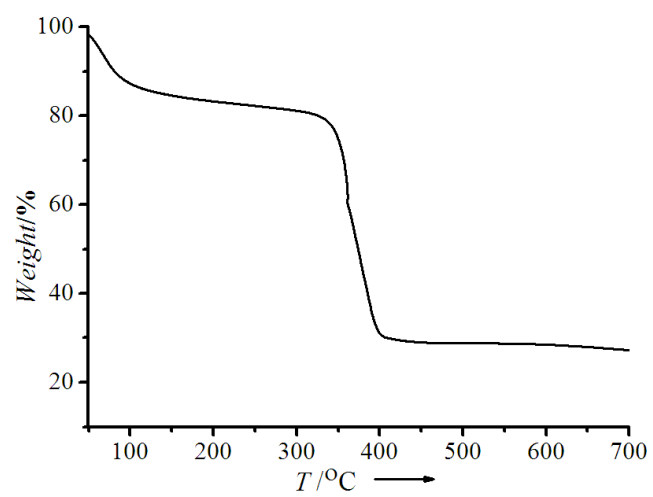


Figure S2 N₂ adsorption/desorption of the as-prepared MIL-101(Fe).

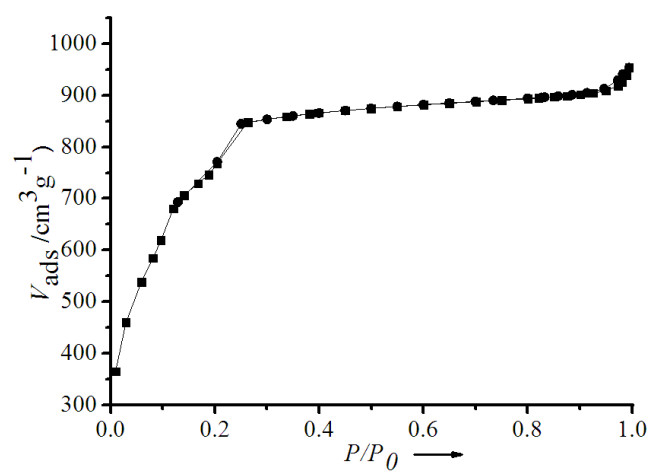


Figure S3 The ^{13}C NMR spectra for the product obtained from the reaction with $^{12}\text{CO}_2$

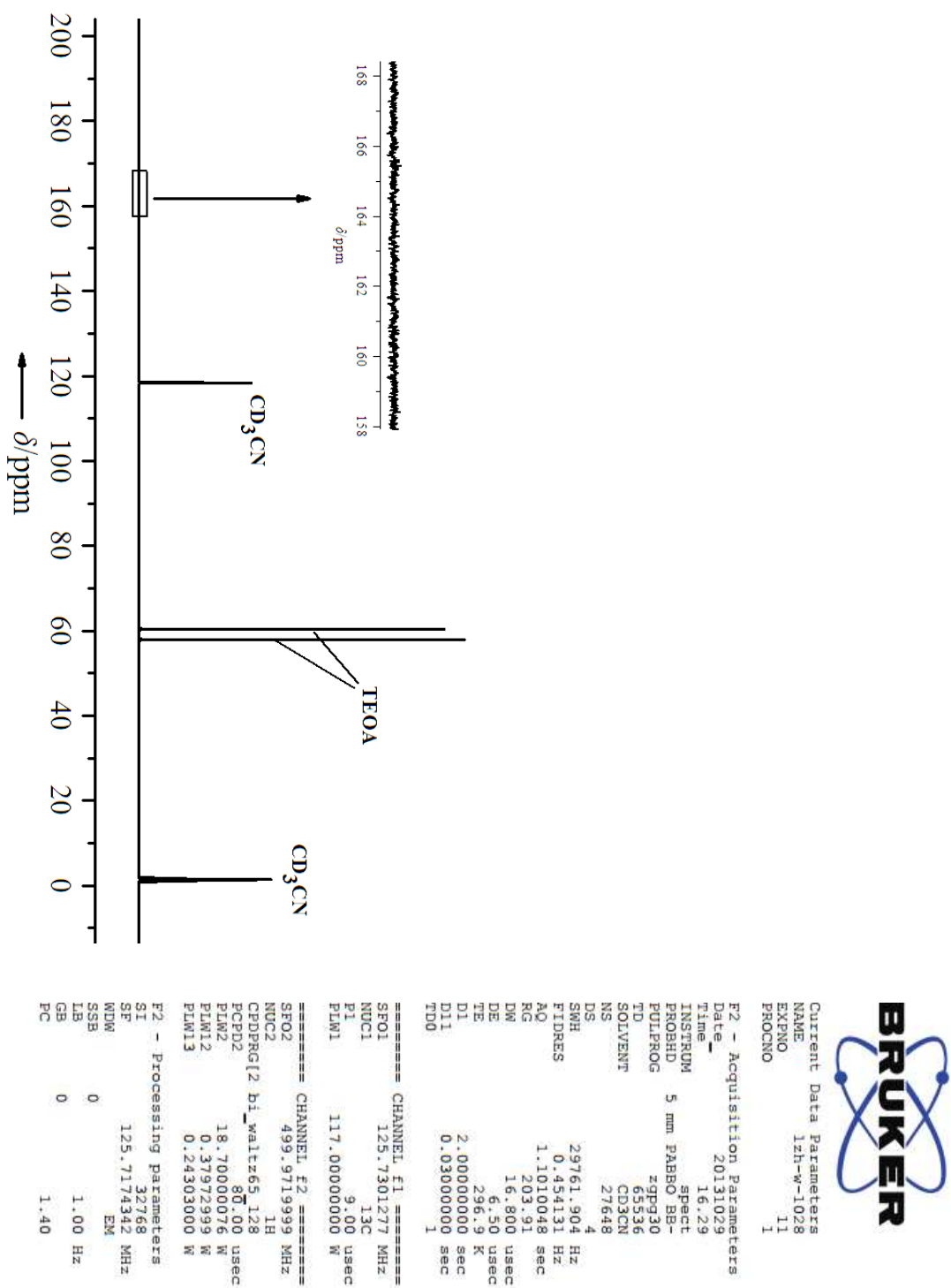
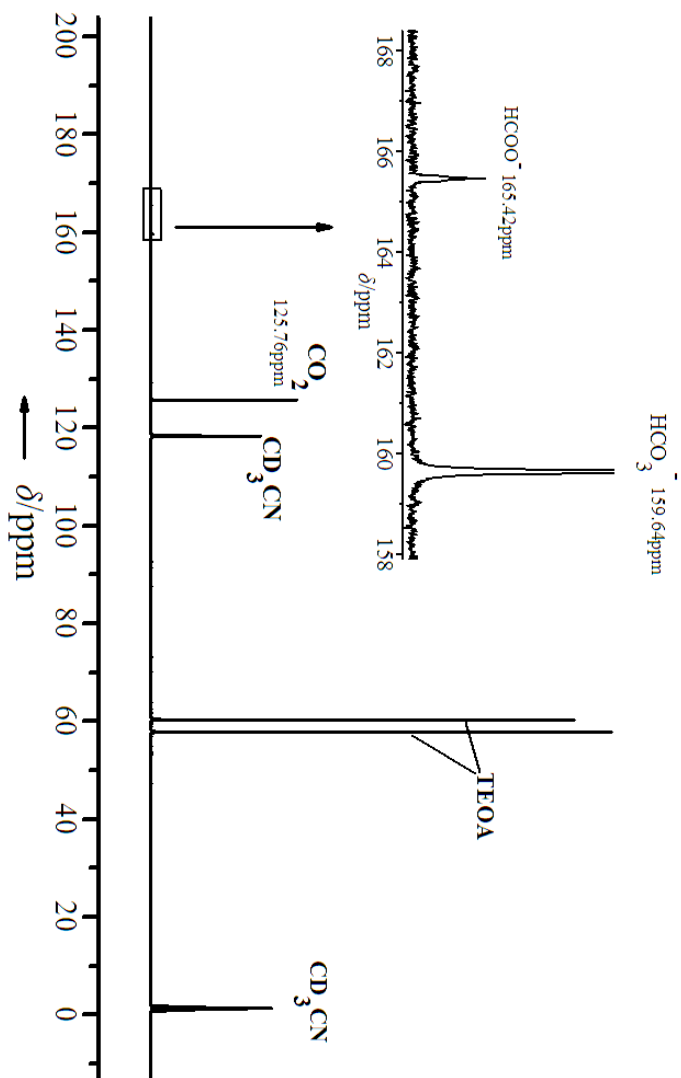


Figure S4 The ^{13}C NMR spectra for the product obtained from the reaction with $^{13}\text{CO}_2$



Current Data Parameters
NAME 1zh-w-1028
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131029
Time 16.29
INSTRUM spect
PROBHD 5 mm PABBO-BB-
PULPROG zgpg30
TD 65536
SOLVENT CD3CN
NS 27648
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 203.91
DW 16.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
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NUC1 13C
P1 9.00 usec
PLW1 117.00000000 W

===== CHANNEL f2 =====
SFO2 499.9719999 MHz
NUC2 1H
CPDPRG2 b1_waltz65_128
PCPD2 80.00 usec
PLW2 18.70000076 W
PLW12 0.37972999 W
PLW13 0.24303000 W

F2 - Processing parameters
SI 32768
SF 125.7174342 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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)

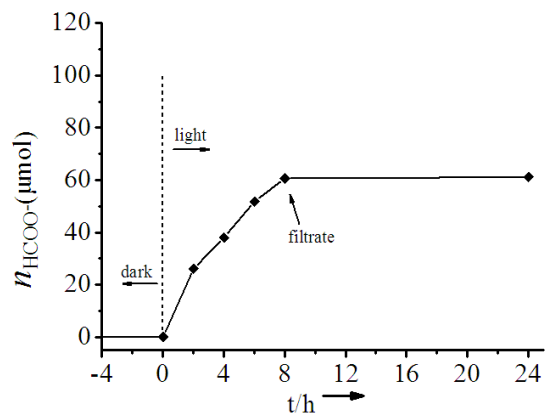


Figure S6 The recycling use of MIL-101(Fe) for photocatalytic CO₂ reduction

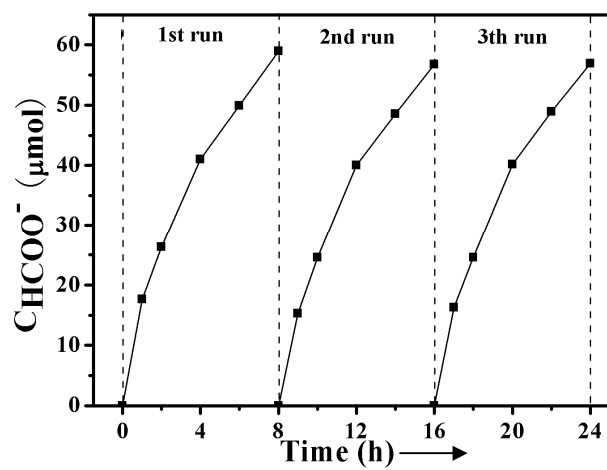


Figure S7 XRD of MIL-101(Fe) (fresh and after the photocatalytic reaction)

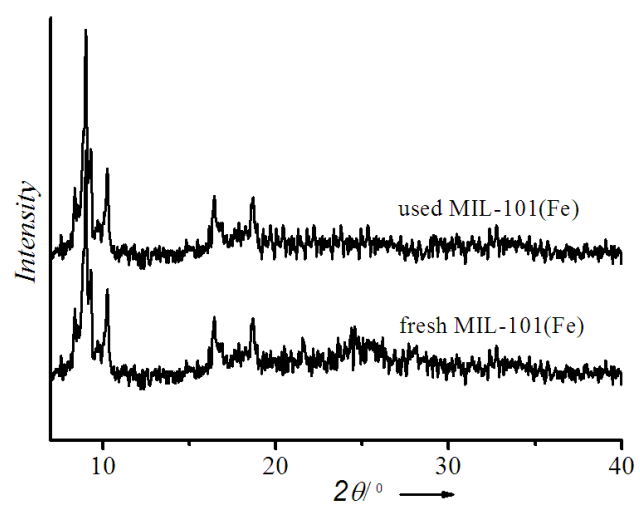


Figure S8 IR of MIL-101(Fe) (fresh and after the photocatalytic reaction)

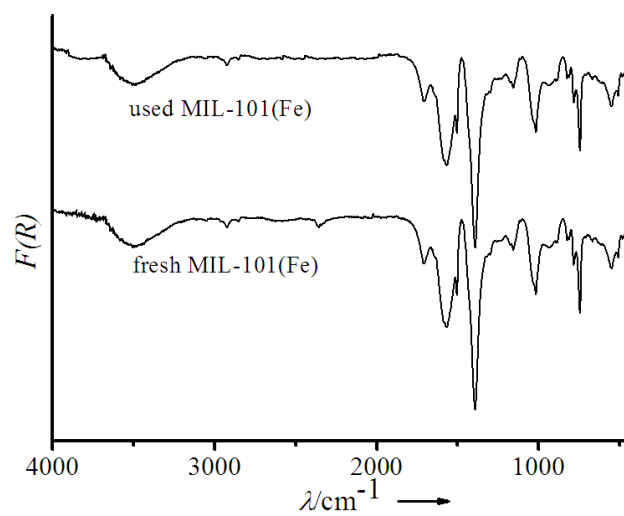


Figure S9 TG of MIL-101(Fe) (fresh and after the photocatalytic reaction)

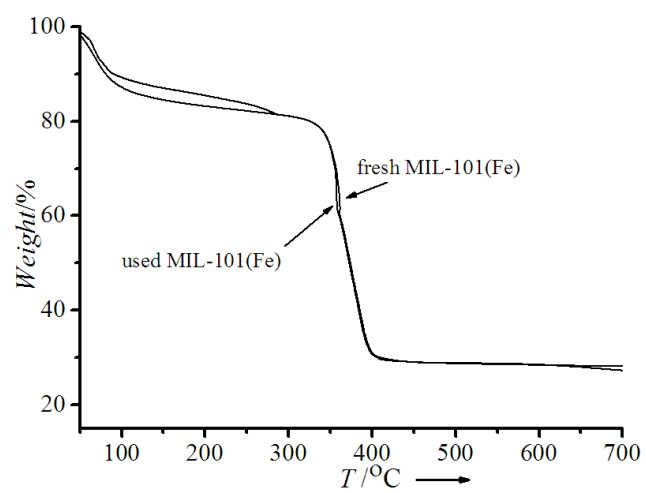


Figure S10 N₂ adsorption/desorption isotherm of MIL-101(Fe) (fresh and after the photocatalytic reaction)

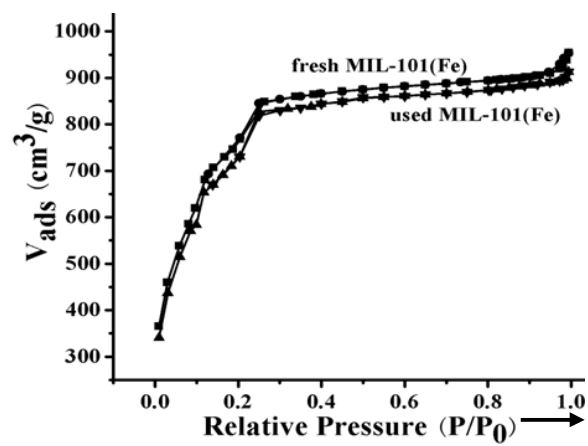


Figure S11 Mott–Schottky plots for MIL-101(Fe). The ac amplitude is 20 mV and the frequency is in the range 0.5–1.5 KHz.

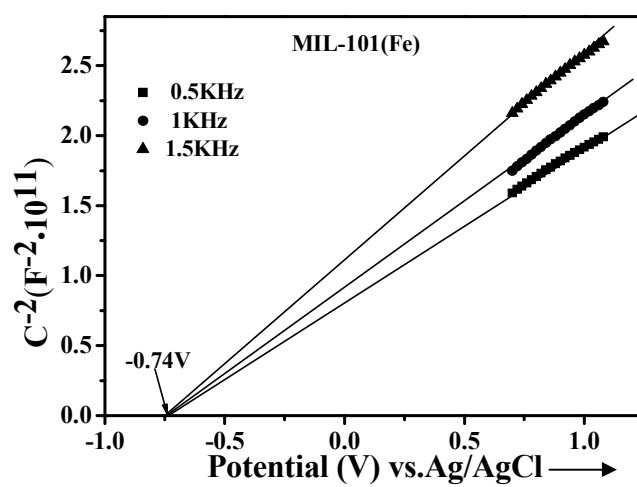


Figure S12 XRD of MIL-53(Fe) (fresh and after the photocatalytic reaction)

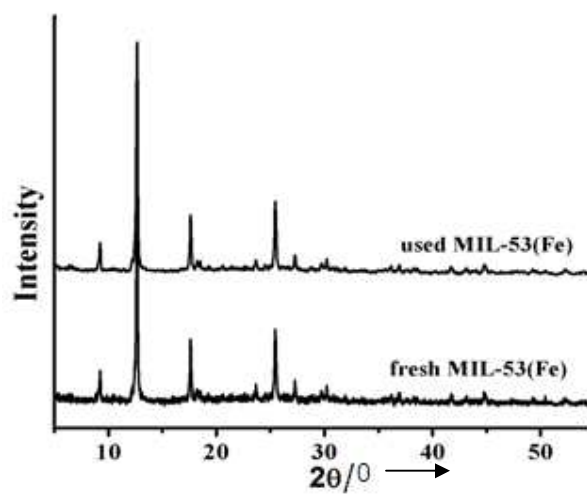


Figure S13 TG of MIL-53(Fe) (fresh and after the photocatalytic reaction)

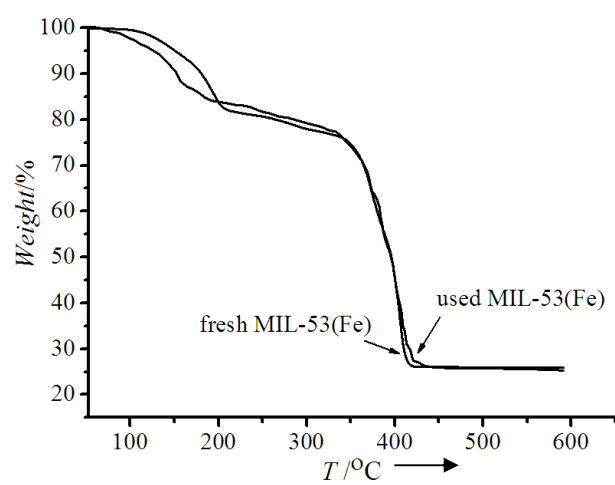


Figure S14 XRD of MIL-88B (Fe) (fresh and after the photocatalytic reaction)

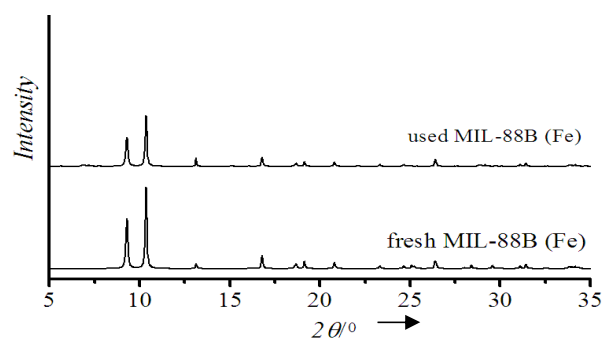


Figure S15 TG of MIL-88B(Fe) (fresh and after the photocatalytic reaction)

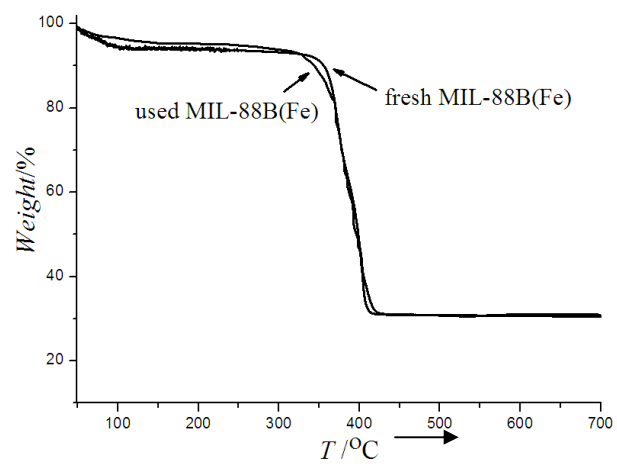


Figure S16 UV-vis spectra of MIL-53(Fe) and NH₂-MIL-53(Fe)

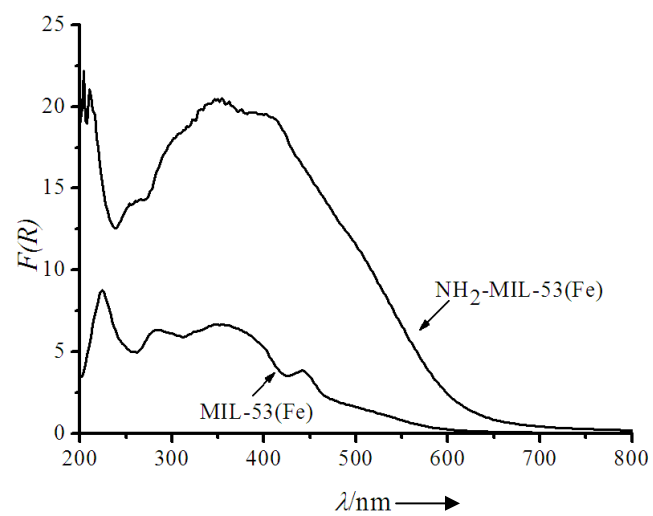


Figure S17 UV-vis spectra of MIL-88B(Fe) and NH₂-MIL-88B(Fe)

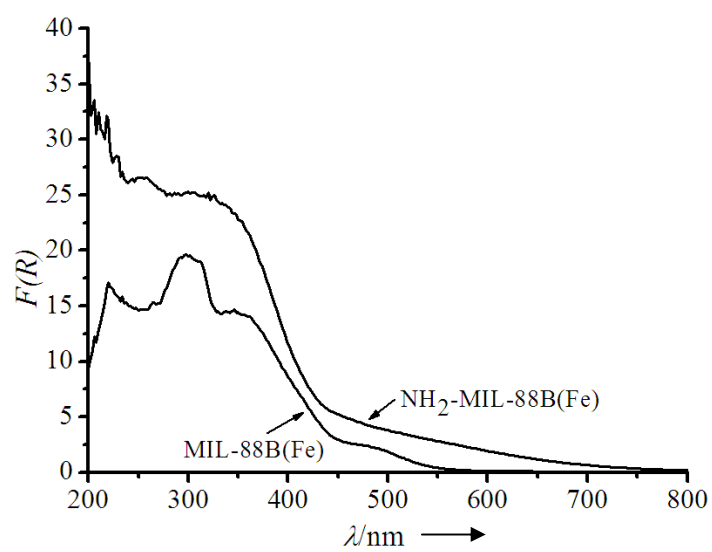


Figure S18 The amount of HCOO^- produced as a function of the irradiation time over MIL-53(Fe).

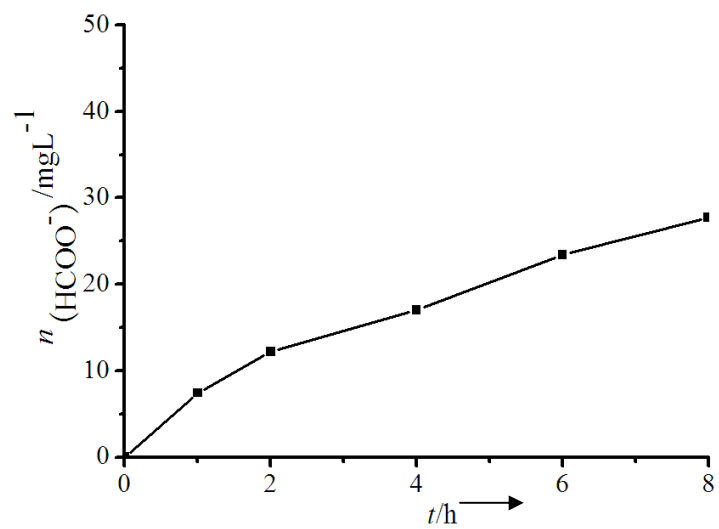


Figure S19 The amount of HCOO^- produced as a function of the irradiation time over MIL-88B(Fe).

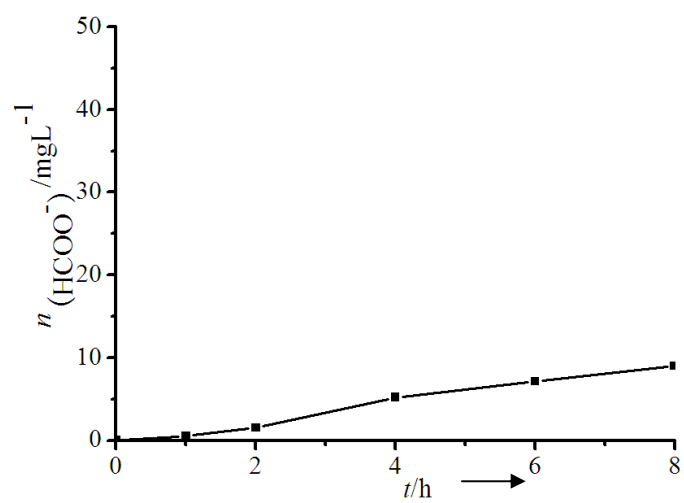


Figure S20 Mott–Schottky plots for MIL-53(Fe). The ac amplitude is 20 mV and the frequency is in the range 0.5–1.5 KHz.

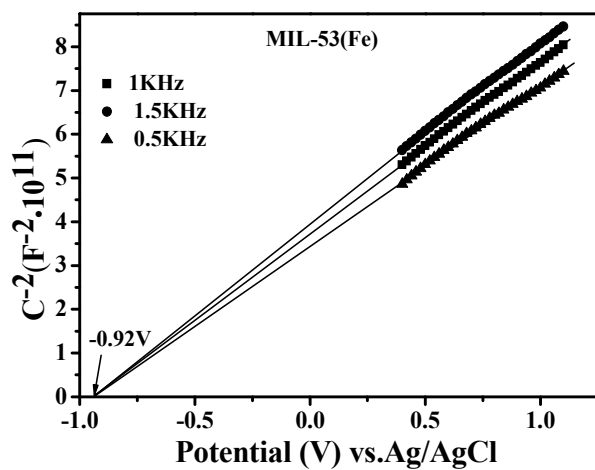


Figure S21 Mott–Schottky plots for MIL-88B(Fe). The ac amplitude is 20 mV and the frequency is in the range 0.5–1.5 KHz.

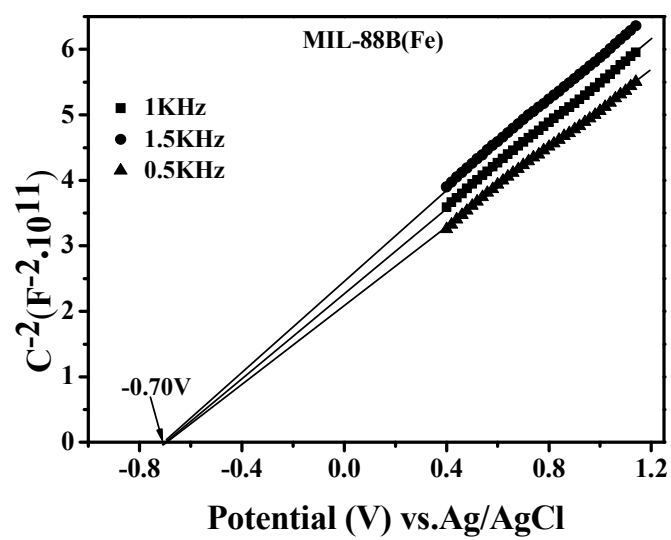


Figure S22 CO₂ adsorption isotherms (1 atm, 273K) of (a) MIL-101(Fe); (b) MIL-53(Fe); (c) MIL-88(Fe).

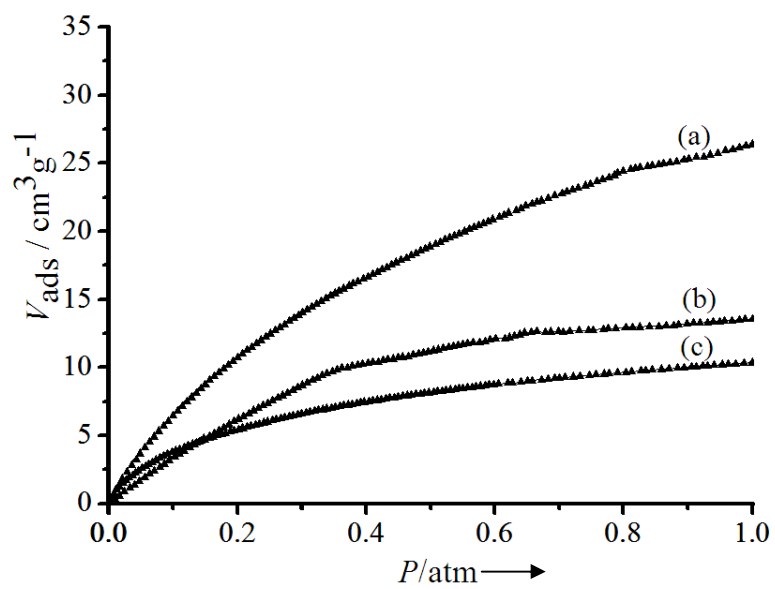


Figure S23 In situ FT-IR analyses of CO₂ adsorption process over pretreated MIL-53(Fe).

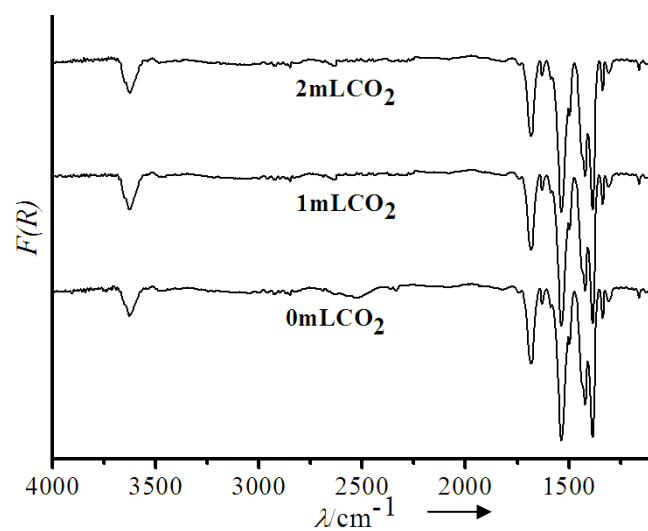


Figure S24 In situ FT-IR analyses of CO₂ adsorption process over pretreated MIL-88B(Fe).

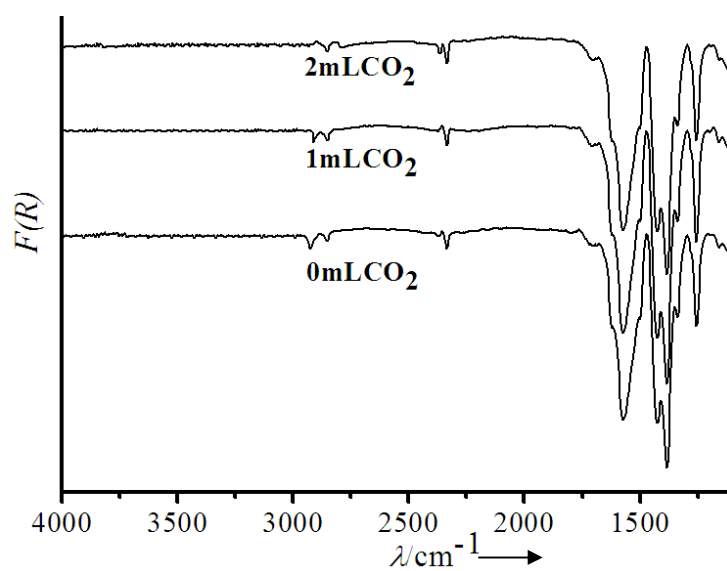


Figure S25 XRD pattern of $\text{NH}_2\text{-MIL-53(Fe)}$.

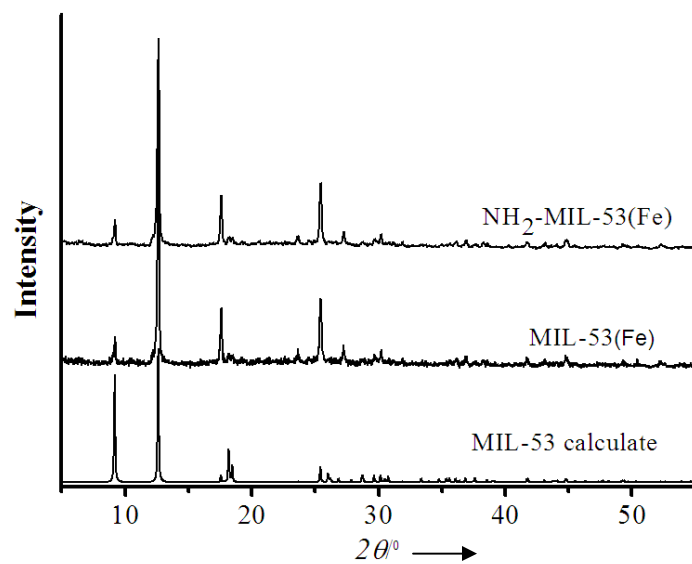


Figure S26 XRD pattern of $\text{NH}_2\text{-MIL-88B(Fe)}$.

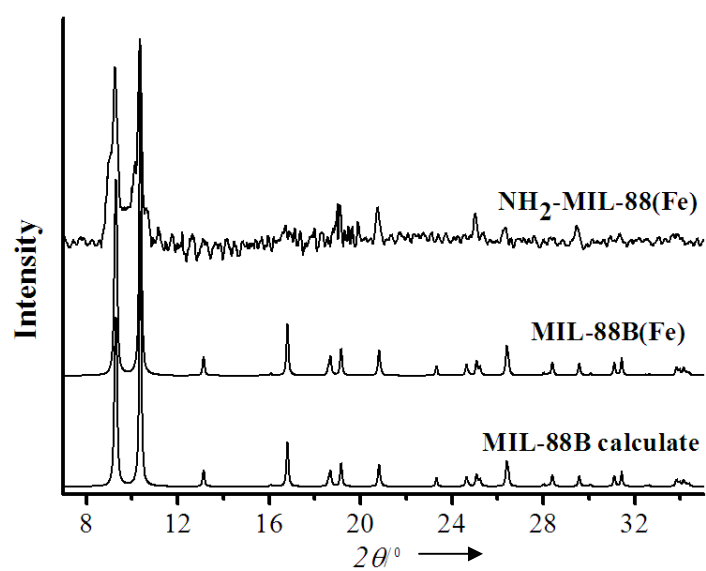


Figure S27 FT-IR spectrum of NH₂-MIL-101(Fe).

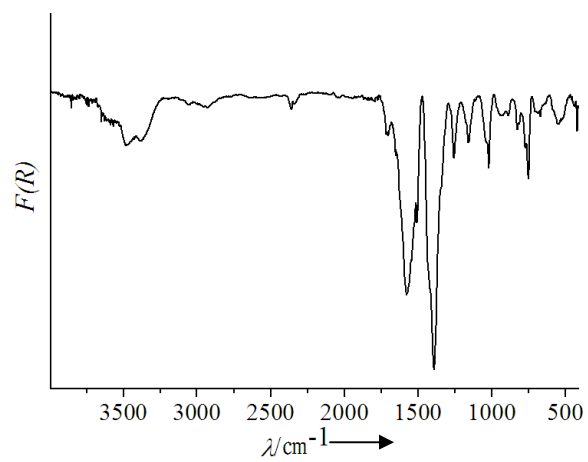


Figure S28 FT-IR spectrum of NH₂-MIL-53 (Fe).

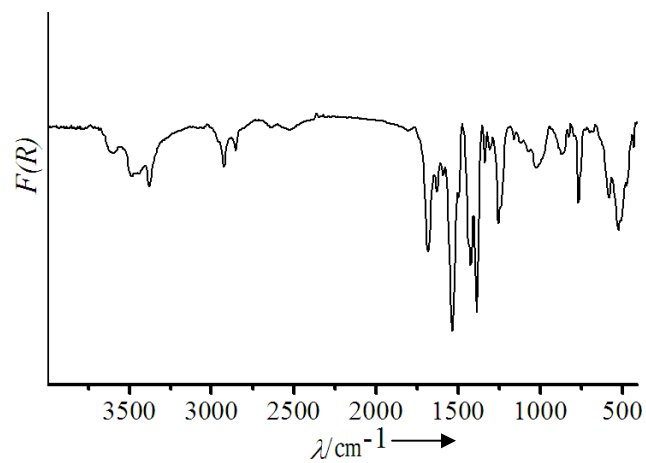


Figure S29 FT-IR spectrum of NH₂-MIL-88B(Fe).

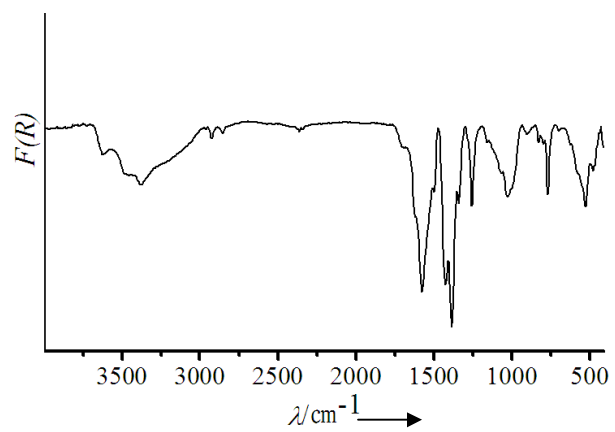


Figure S30 N₂ adsorption/desorption isotherm of NH₂-MIL-101(Fe).

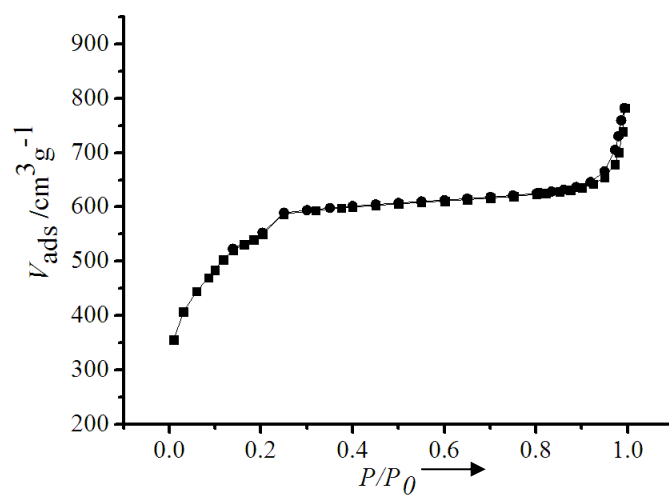


Figure S31 TG of NH₂-MIL-101(Fe).

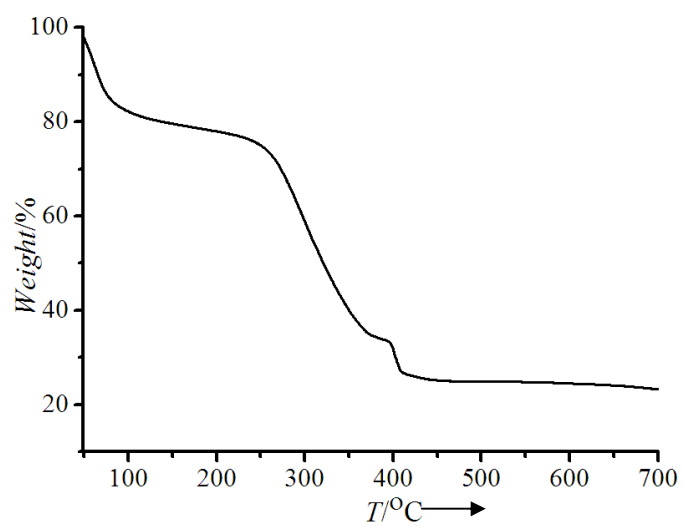


Figure S32 TG of NH₂-MIL-53(Fe).

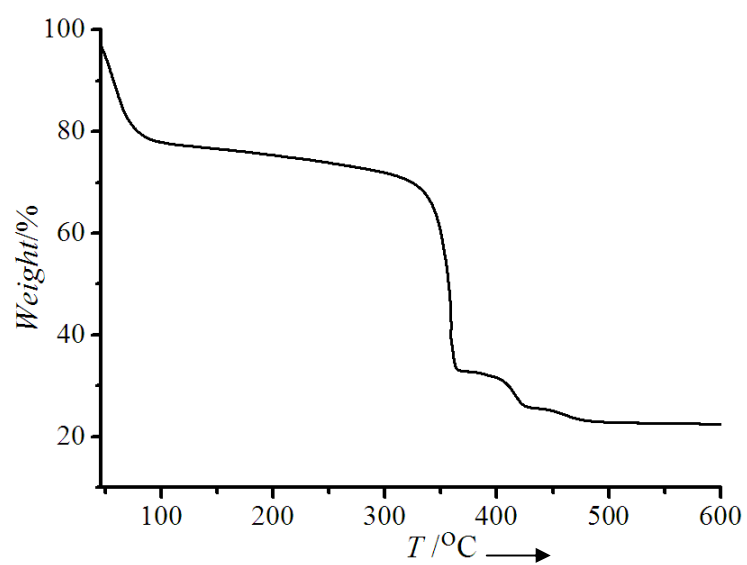


Figure S33 TG of NH₂-MIL-88B(Fe).

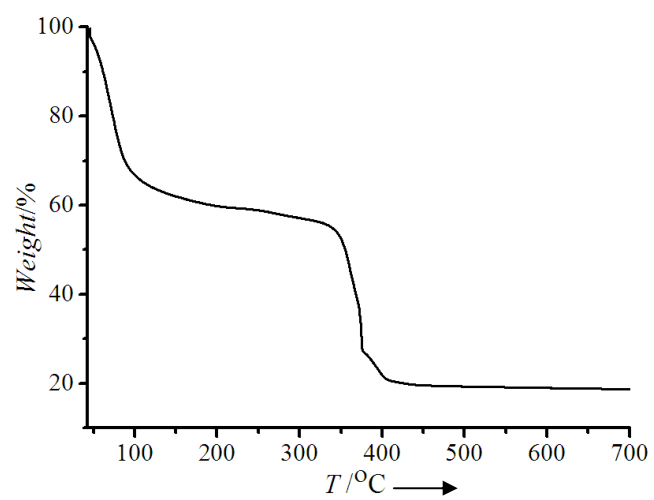


Figure S34 CO₂ adsorption isotherms (1 atm, 273K) of (a) NH₂-MIL-101(Fe); (b) NH₂-MIL-53(Fe); (c) NH₂-MIL-88(Fe).

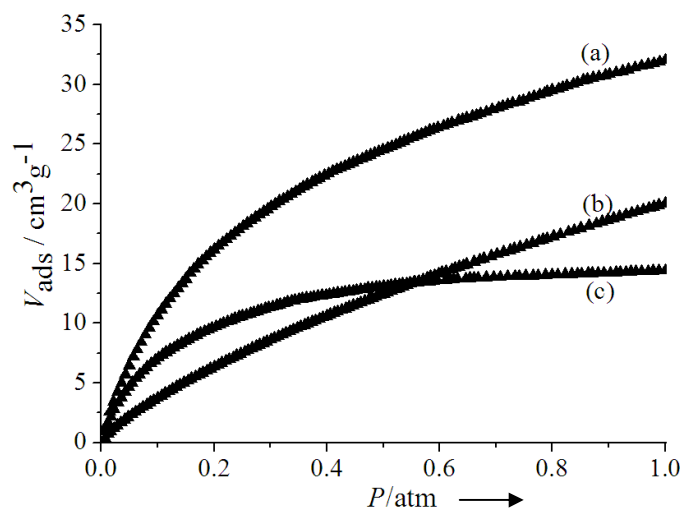


Table S1 QE for photocatalytic CO₂ reduction over NH₂-MIL-101(Fe) and MIL-101(Fe) at different wavelength

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