Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

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Metal-Organic Framework MIL-100(Fe) for the Adsorption of Malachite Green from Aqueous Solution

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Preparation and Characterization of Adsorbents. MIL-53 was synthesized according to Férey G. et al.[S1] Typically, 1300 mg of $Al(NO_3)_3 \cdot 9H_2O$ and 288 mg of terephthalic acid were mixed with 5 mL of ultrapure water. The obtained mixture was transferred to a Teflon-lined bomb. Then, the Teflon-lined bomb was sealed, placed in an oven, and left at 220 °C for 3 days. The white crystalline solid was thus obtained. After washing with water, the solid was purified and activated upon heating in air at 330 °C for 3 days.

MIL-101 was synthesized according to Férey et al.[S2] Typically, $Cr(NO_3)_3 \cdot 9H_2O$ (800 mg, 2.0 mmol), terephthalicacid (332 mg, 2.0 mmol) and HF (0.4 mL, 2.0 mmol) were mixed with ultrapure water (9.5 mL). The obtained mixture was transferred to a Teflon-lined bomb. Then, the Teflon-lined bomb was sealed, placed in an oven, and left at 200 °C for 8 h. The green crystalline solid was thus obtained. After thorough washing with DMF, the solid was emerged in ethanol in 1 h, and collected by centrifugation at 10000 rpm for 5 min. The procedure was repeated 3 times to eliminate the unreacted terephthalic acid from MIL-101. The solid was obtained by centrifugation at 10000 rpm for 5 min and then evacuated in vacuum under 150 ^{o}C for 12 h.

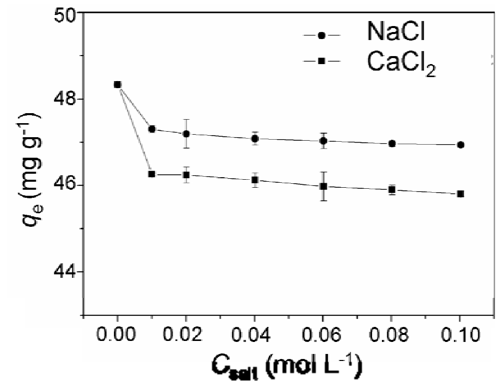

Figure S1. Effect of the concentration of NaCl and $CaCl_2$ on the adsorption of MG (100 mg L^{-1}) on MIL-100 (10 mg L^{-1}). Other conditions: temperature, 30 ^{o}C; pH 5.

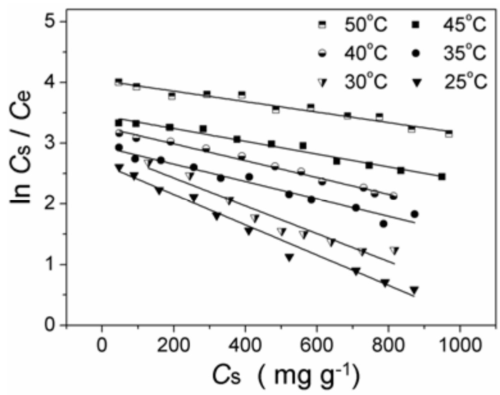

Figure S2. Plots of ln (C_s/C_e) vs. C_s at various temperatures.

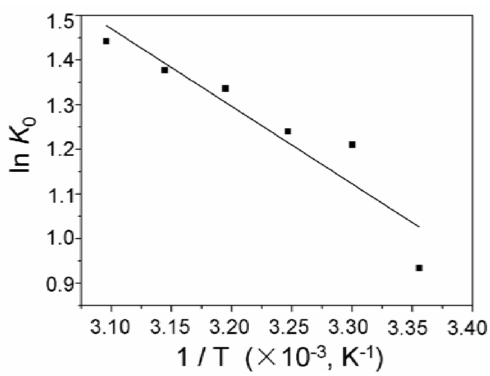

Figure S3. Plots lnK_0 against 1/T for the adsorption of MG on MIL-100.

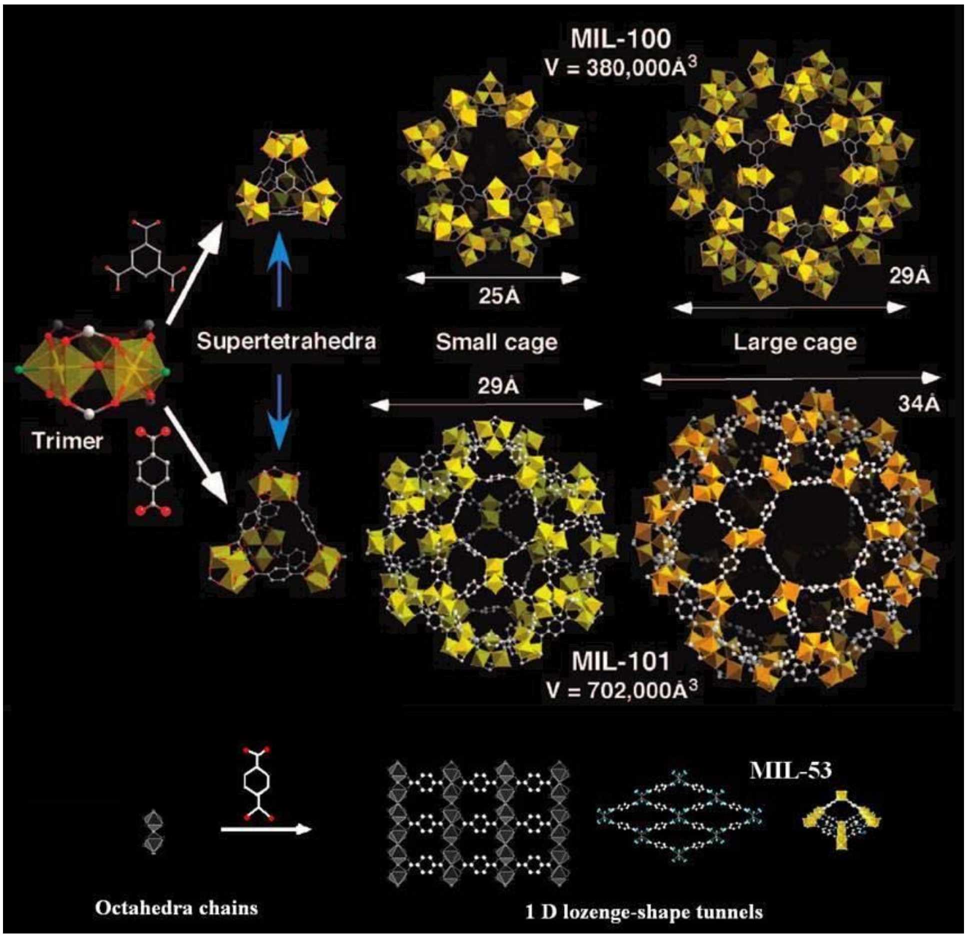

Figure S4. Structures of MIL-100, MIL-101 and MIL-53. This figure is a combination of Figure 1 in Ref.S3 with little modification. Copyright 2008 American Chemical Society and with permission.

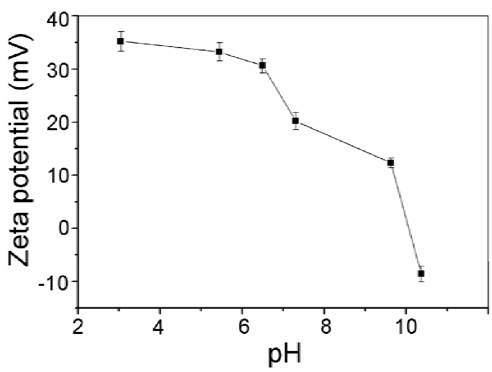

Figure S5. Effect of zeta potentials of MIL-101(Cr) (0.4 mg L^{-1}) with different pH.

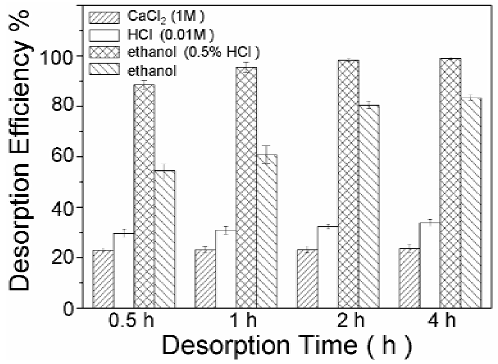

Figure S6. Effects of desorption solution and desorption time on desorption efficiency under ultrasonication.

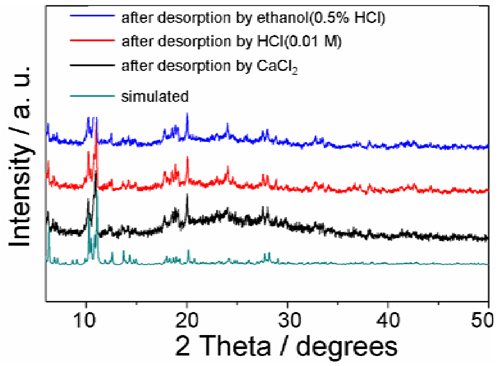

Figure S7. XRD patterns of MIL-100(Fe) after desorption used different solutions.

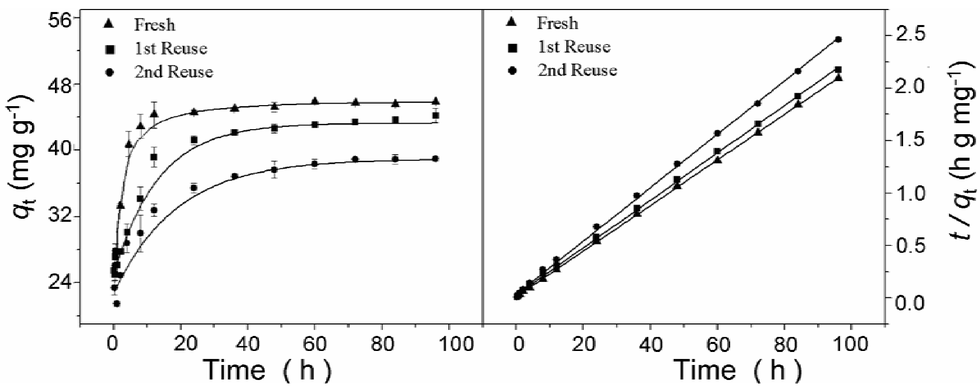

Figure S8. (a) Effect of contact time on the MG adsorption and (b) Pseudo-second-order plots to show the re-usability of a spent MIL-100.

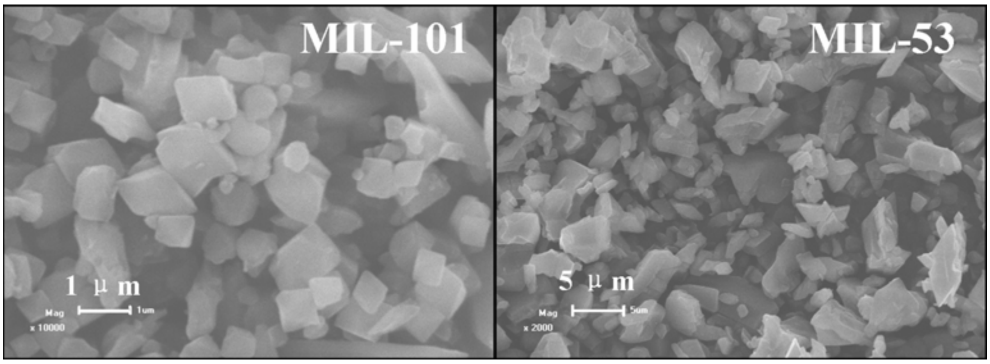

Figure S9. SEM images of the prepared MIL-101 and MIL-53.

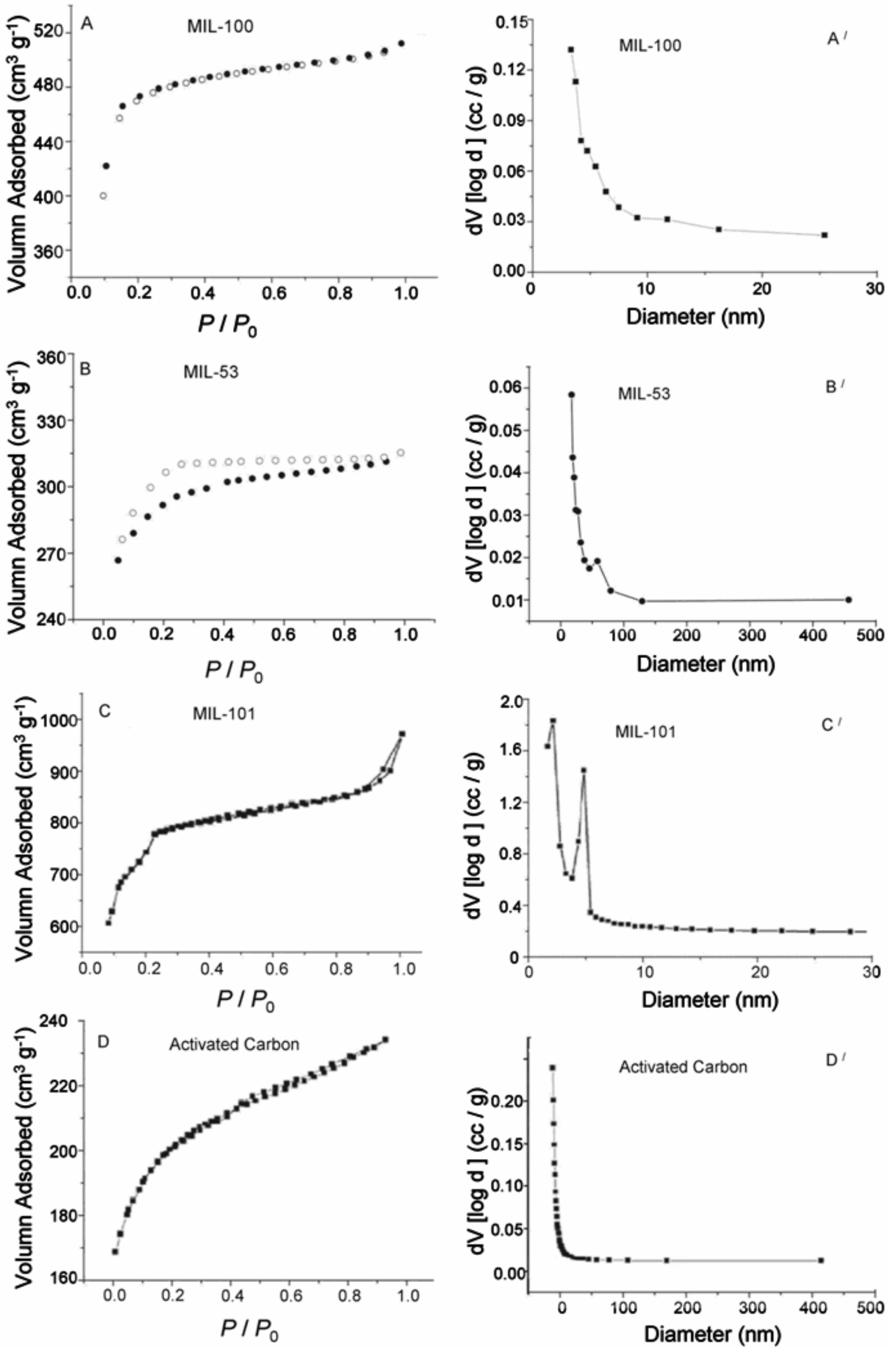

Figure S10. Adsorption-desorption isotherms (left) and N_2 the pore size distribution (right) of MIL-100 (A) MIL-53 (B), MIL-101 (C) and activated carbon (D).

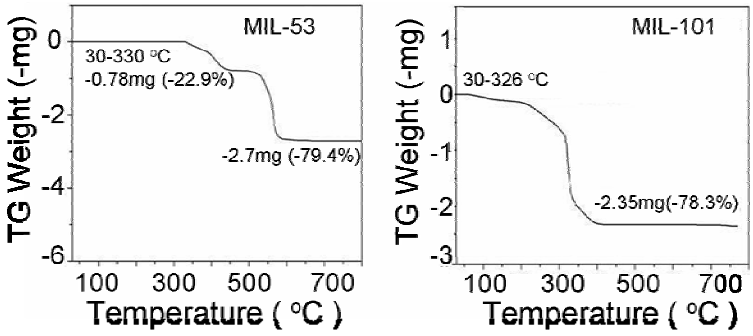

Figure S11. TGA curves of MIL-53 and MIL-101.

Table S1 Molecular Properties and parameter for the MG

dye	planarity	molecular size (Å×Å ×Å)	MW(g mol^{-1})	solubility (g L^{-1})	pKa [S4,S5]	λ_{UVmax} (nm)
Malachite green oxalate	planar	13.8×9.9×4.2	927.03	60 (20℃)	10.3	617nm

Table S2. Characteristic of the Adsorbents

adsorbents	formula	BET surface area (m^2 g^{-1})	pore volume (cm^3 g^{-1})	pore/channel diameter (Å)	open metal sites
MIL-100(Fe)	$Fe_3O(H_2O)_2F(BTC)_2$	1626	0.79	25, 29 [S6]	Yes
MIL-101(Cr)	$Cr_3O(H_2O)_2F(BDC)_3$	2907	1.50	29, 34 [S2]	Yes
MIL-53(Al)	$Al^{III}(OH)(BDC)$	1002	0.03	8.5 [S7]	No
AC	C	600	0.36	-	No

Table S3. Comparison of Adsorption Capacities of Various Adsorbents for MG

adsorbent	q_m (mg g^{-1})	temperature (°C)	ref
MIL-100	485	50	this work
MIL-100	266	30	this work
MIL-53	34.9	30	this work
commercial powder activated carbon	149	30	this work
bamboo-based activated carbon	264	30	S8
cyclodextrin-based material	91.9	25	S4
oil palm trunk fiber	149	30	S9
natural zeolite	24.5	25	S10
chitosan bead	93.6	30	S11
chitosan bead	82.2	50	S11

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