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Supporting information

Trifunctional Metal-Organic Platform for Environmental Remediation: Structural Features With Peripheral Hydroxyl Groups Facilitate Adsorption, Degradation and Reduction

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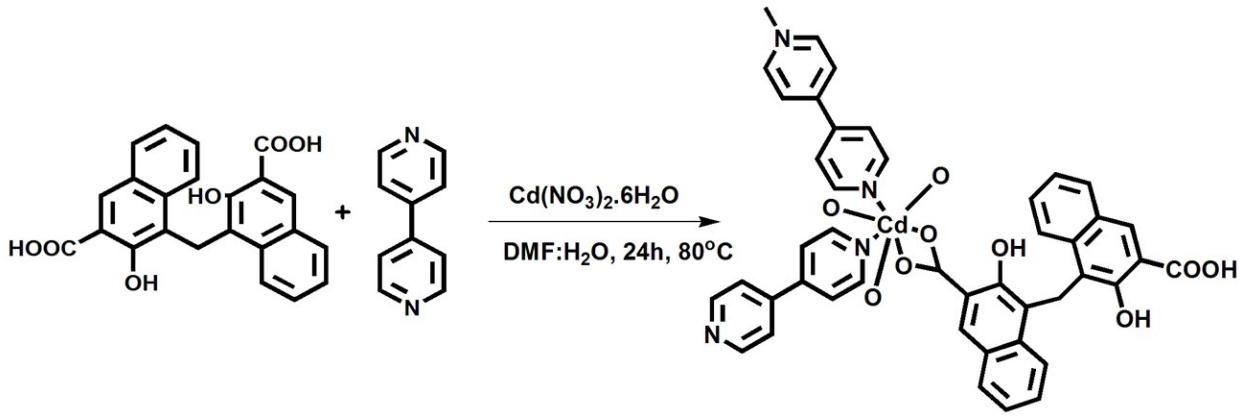

Figure S1. Synthesis scheme of Cd-MOF.

Table S1. Crystal data and structure refinement for Cd-MOF.

1.	Identification code	Cd-MOF
2.	Emperical Formula	$C_{43}H_{30}CdN_4O_6$
3.	Formula weight	811.11
4.	Temperature/K	293 (2)
5.	Crystal System	monoclinic
6.	Space group	$P2_1/c$
7.	Unit Cell dimensions	a/Å = 13.6269 (3), b/Å = 16.8816 (4), c/Å = 19.4131 (5) α/°= 90.00, β/°= 107.141(3), γ/°= 90.00
8.	Volume/ $Å^3$	4267.52 (19)

9.	Z	4
10.	P_{calc} g/cm^3	1.262
11.	μ mm^{-1}	4.490
12.	F(000)	1648.0
13.	Crystal size/mm^3	0.247 × 0.147 × 0.111
14.	2θ range for data collection/°	7.08 to 133.86
15.	Index ranges	$-16 \leq h \leq 15$, $-19 \leq k \leq 13$, $-23 \leq l \leq 22$
16.	Reflection collected	15192
17.	Independent reflections	7484 [R_{int} = 0.0279, R_{sigma} = 0.0350]
18.	Goodness-of-fiton F^2	1.078
19.	Final R indexes[I>2σ(1)]	R1 = 0.0331, wR2 = 0.0889
20.	Final R indexes(all data)	R1 = 0.0384, wR2 = 0.0945
21.	Largest diff. peak/ hole/e Å^3	0.80/ -0.49

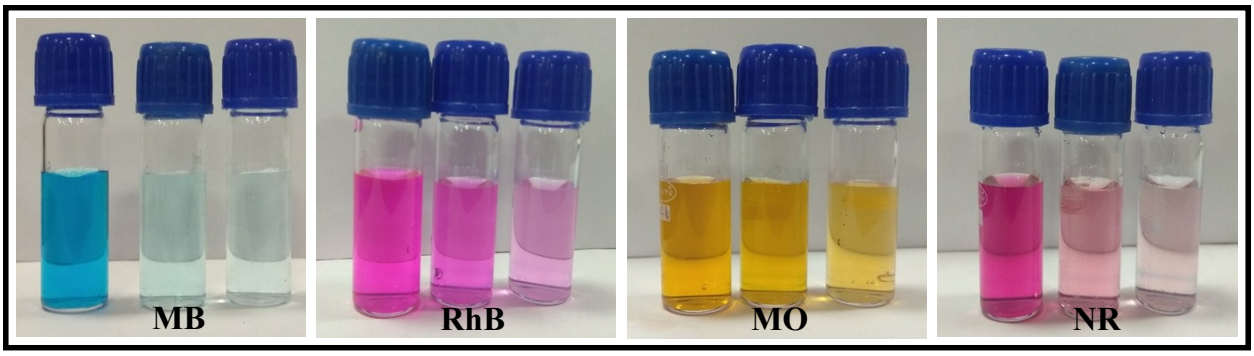

Figure S2. (a) Photographs showing a color change of different dyes during adsorption study using Cd-MOF.

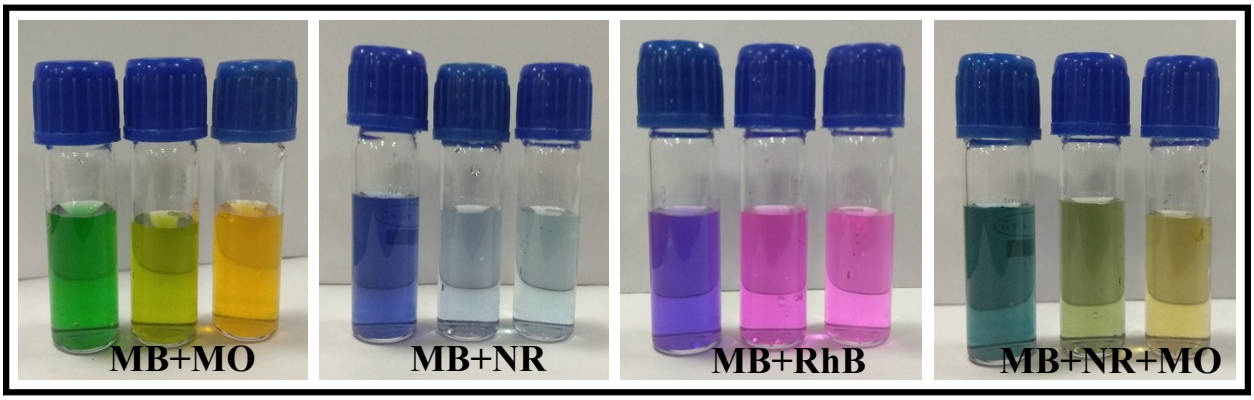

Figure S2. (b) Photographs showing color change during separation study of a mixture of two dyes (a: MB+MO, b: MB+NR, c: MB+RhB.) and three dyes (d: MB+NR+MO) using Cd-MOF.

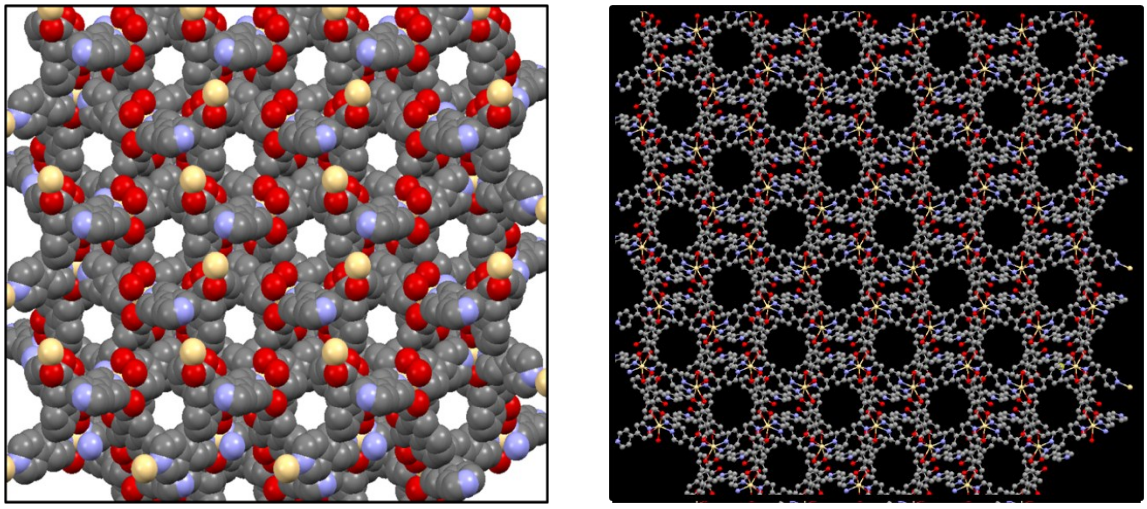

Figure S3. Packing diagram of Cd complex along a-axis.

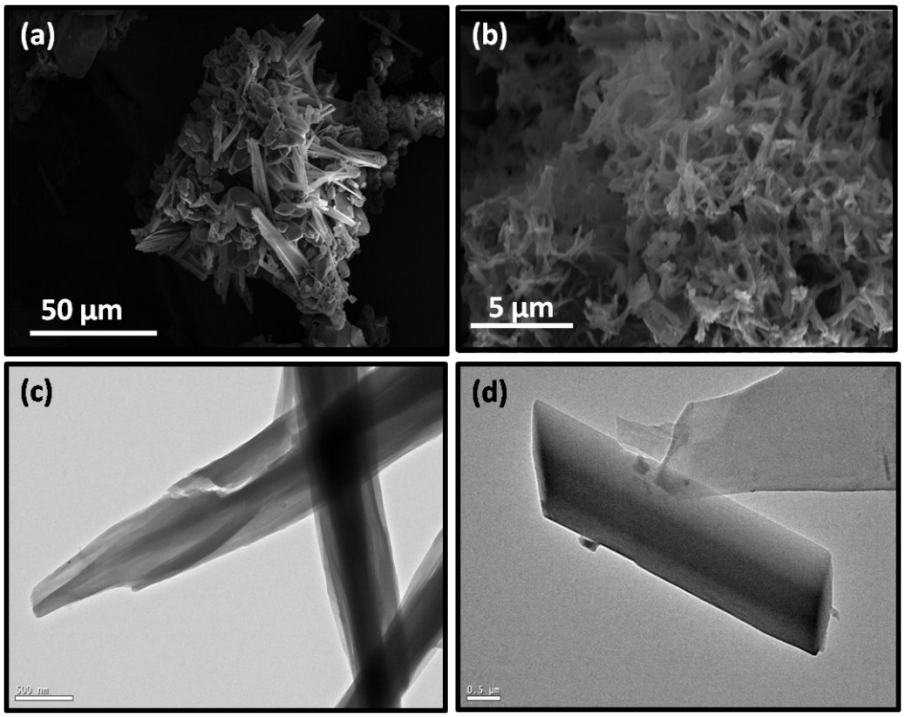

Figure S4. SEM images (a, b) and TEM images (c, d) of Cd-MOF.

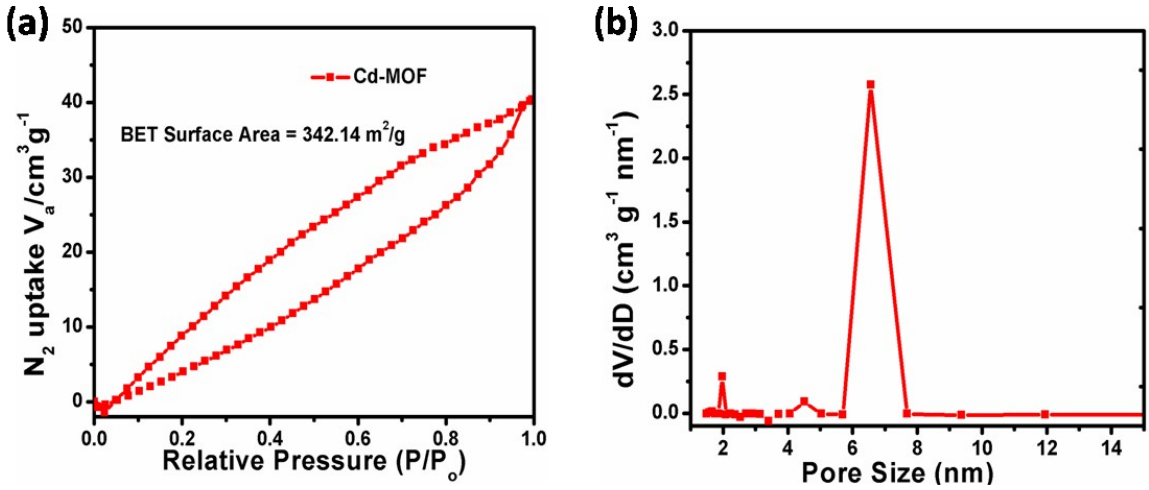

Figure S5. (a) N_2 adsorption isotherms of Cd-MOF. (b) Pore size distribution graph. On the basis of N_2 adsorption studies, BET surface area for Cd-MOF at 77K was found to be 342.14 m^2 g^{-1} and pore radius = 17.585 Å.

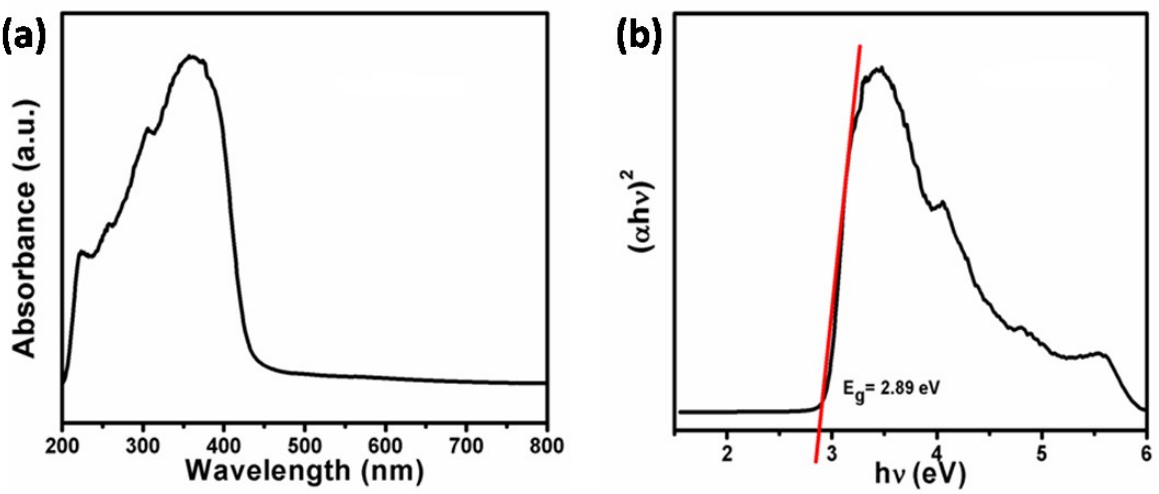

Figure S6. (a) Absorption spectra of Cd-MOF. (b) Plot showing transformed Kubelka–Munk function vs. energy of light for the band gap.

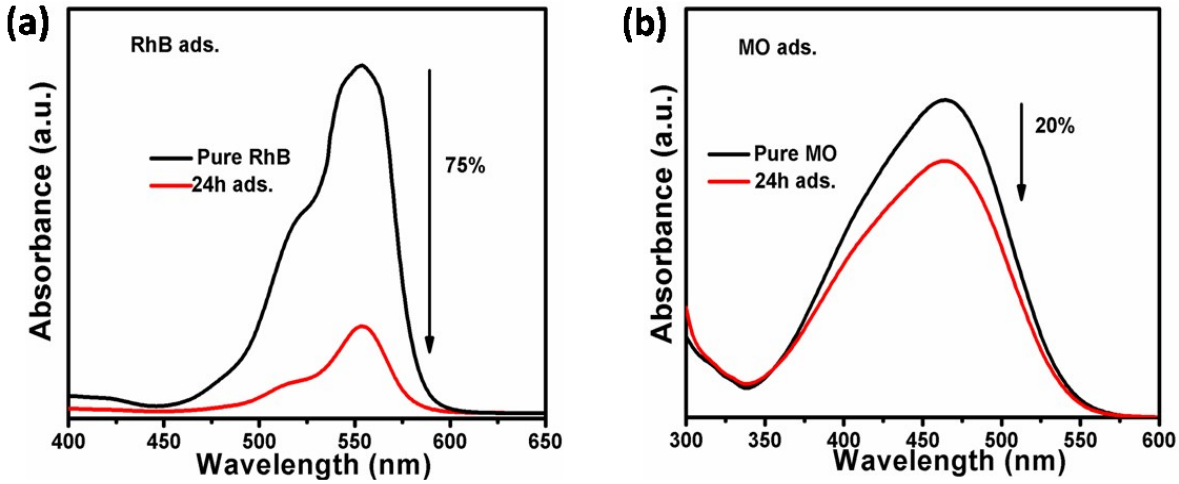

Figure S7. UV-vis spectra for the adsorption study of (a) RhB and (b) MO dye using Cd-MOF upto 24 h.

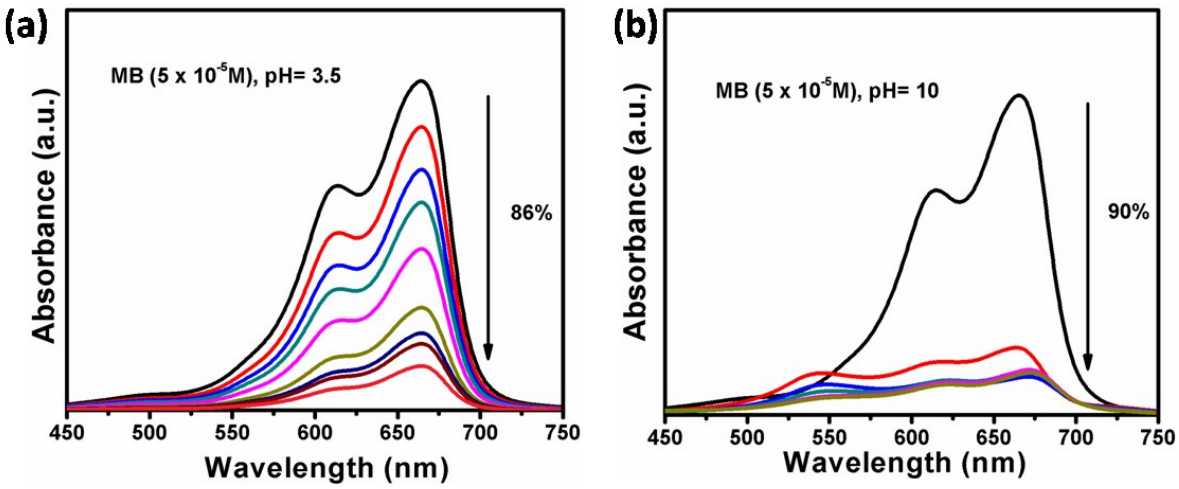

Figure S8. UV-vis spectra of pH dependent adsorption study of MB dye using Cd-MOF.

Table S2. Comparison of MB adsorption capacity with various other reported MOF materials.

Material	%Adsorption/ Adsorption Capacity	Time	Ref.
$[Cd_3(tib)_2(BTB)_2]$. 3DEF. $4.5H_2O$	69%	24 h	Y.-L. Li, Y. Zhao, P. Wang, Y.-S. Kang, Q. Liu, X.-D. Zhang and W.-Y. Sun, Inorg. Chem., 2016, 55, 11821-11830.
$[Cd_3(tib)_2(BTB)_2(DMA)_2(H_2O)_2]$. 2 DMA. $8H_2O$	55%		
{$[Cd_2(BPTC)(DMA)_2(DMPU)_{.5}(H2O)_{.5}](DMPU)_{.5}$}n	25mg/g	24 h	W.-J. Ji, R.-Q. Hao, W.-W. Pei, L. Feng and Q.-G. Zhai, Dalton Trans.,2018, 47, 700-707.
$[Co_3(tib)_2(BPT)_2(H_2O)_2]\cdot DMA\cdot 2.5H_2O$	0.6×10^{-3} mg/g	24 h	Y.-L. Li, Y. Zhao, Y.-S. Kang, X.-H. Liu and W.-Y. Sun, Cryst. Growth Des., 2016, 16, 7112-7123.
$[Co_3(tib)_2(BTB)_2]$.2DMF.$6H_2O$	6.4×10^{-3} mg/g		
$[Cu_{24}(5\text{-hip})_{24}(bpy)_6(H_2O)_{12}]$	0.546 mmol/g	48 h	H.-N. Wang, F.-H. Liu, X.-L. Wang, K.-Z. Shao and Z.-M. Su, J. Mater. Chem. A, 2013, 1, 13060-13063

$[(CH_3)_2NH_2]_2[ZnNa_2(\mu\text{-}H_2O)_2(H_2O)_2(TATAT)].2DMF$	0.75 mg/g	-	C. Y. Sun, X. L. Wang, C. Qin, J. L. Jin, Z. M. Su, P. Huang and K. Z. Shao, Chem. Eur. J.,2013, 19, 3639-3645
$[Cd_6(L)_2(bib)_2(DMA)_4]$	30 mg/g	72 h	F. Y. Yi, J. P. Li, D. Wu and Z. M. Sun, Chem. Eur. J., 2015, 21, 11475-11482.
$[(C_2H_5)_2NH_2]_2[Mn_6(L)(OH)_2(H_2O)_6].4DEF$	67.5%	96 h	Y.-C. He, J. Yang, W.-Q. Kan, H.-M. Zhang, Y.-Y. Liu and J.-F. Ma, J. Mater. Chem. A, 2015, 3, 1675-1681.
$\{[Cd(PA)(4,4'\text{-}bpy)_2](H2O)\}_n$	29.60 mg/g	2 h	Present work

Table S3. Pseudo-second- order kinetics parameters for MB dye adsorbed into Cd-MOF.

Adsorbent	**q_e (mg g^{-1})**	**K_2 (h g mg^{-1})**	**R^2**
	6.66	0.085	0.997
	9.99	0.068	0.995
Cd-MOF	13.33	0.031	0.994
	16.66	0.200	0.997
	33.33	0.137	0.999

Table S4. Langmuir model for MB dye adsorption into Cd-MOF.

Adsorbent	**Dye**	**K_L (L mg^{-1})**	**q_m (mg g^{-1})**	**R^2**
Cd-MOF	MB	0.51	47.05	0.997

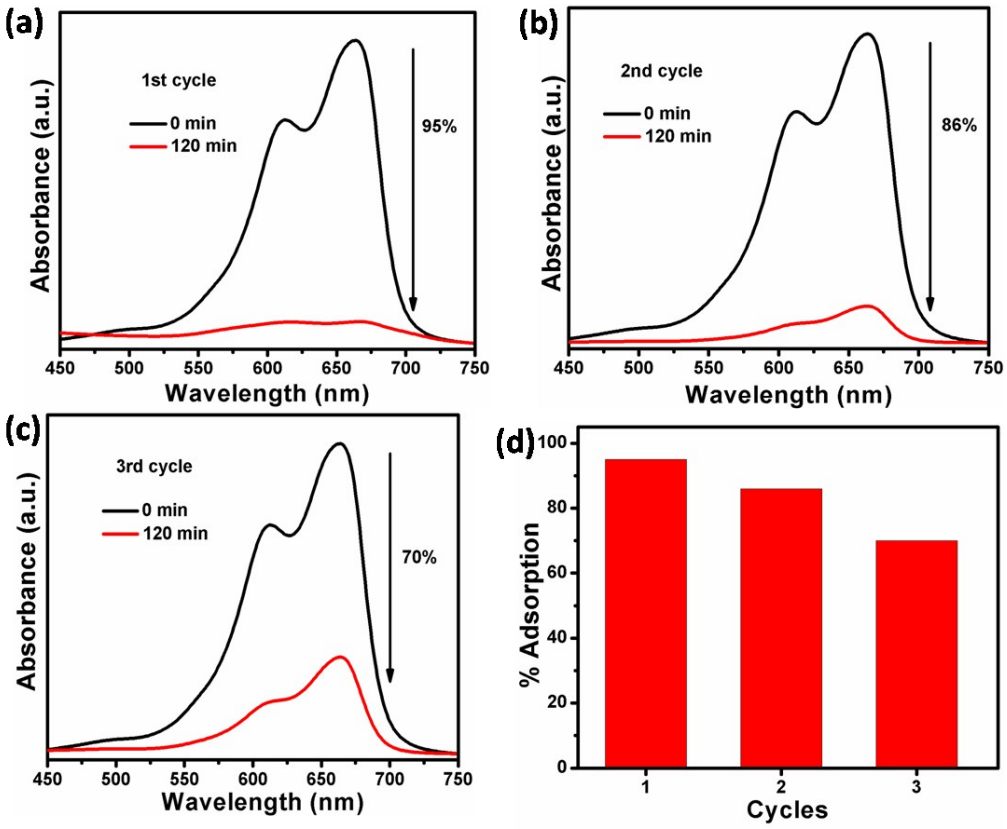

Figure S9. Adsorption caacity (%) of MB dye using Cd-MOF in three successive cycles of adsorption-desorption experiment (a to c). (d) Histogram for adsorption (%) of MB dye in adsorption-desorption experiment using Cd-MOF.

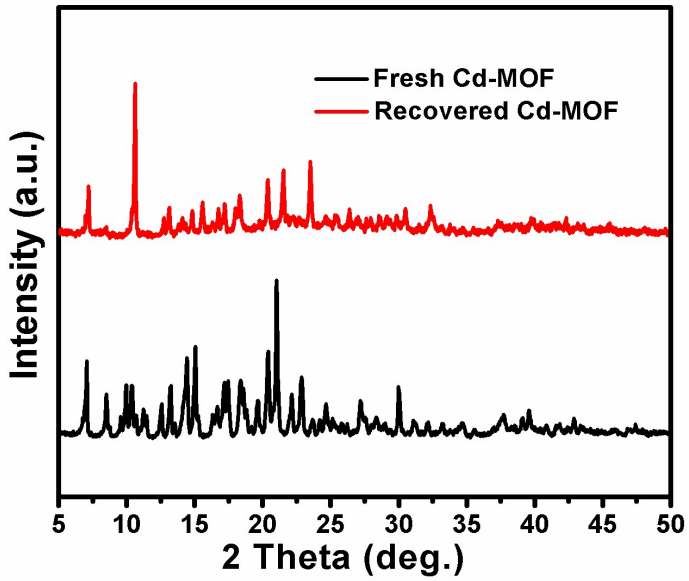

Figure S10. XRD patterns of Cd-MOF before and after MB dye adsorption.

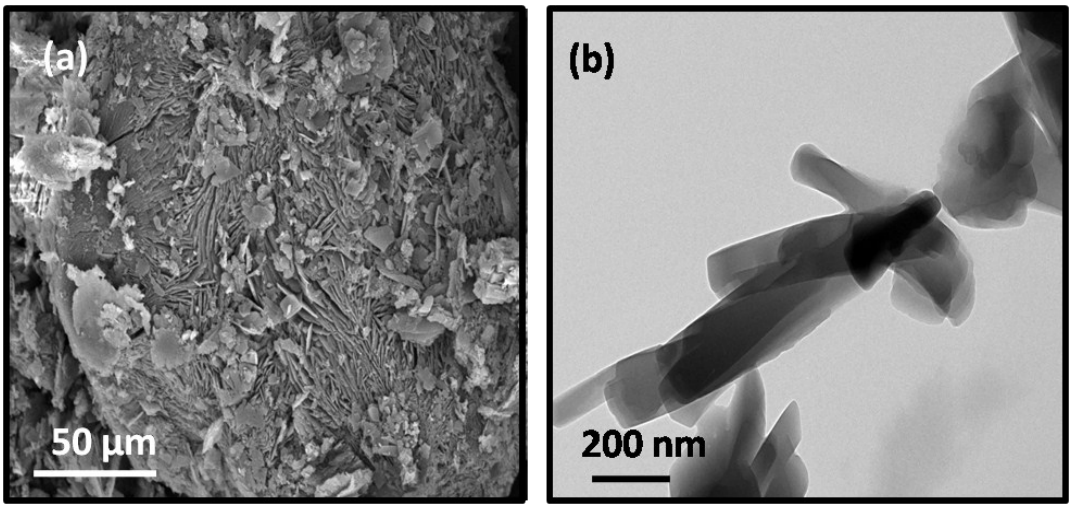

Figure S11. (a) SEM and (b) TEM images of recovered Cd-MOF after MB dye adsorption.

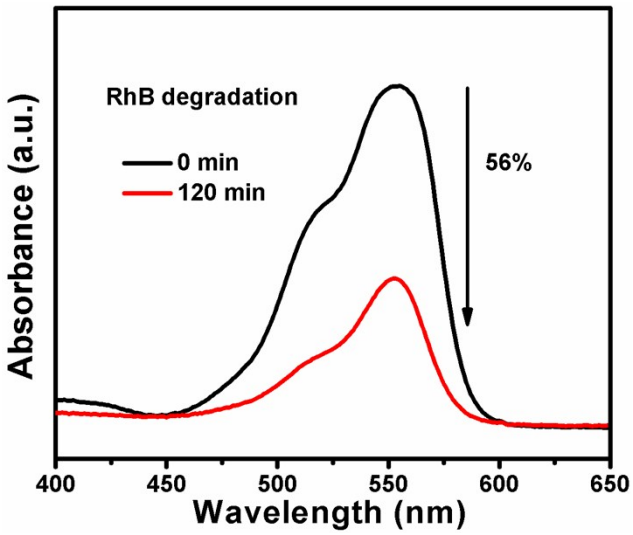

Figure S12. UV-Vis spectra of RhB dye degradation using recovered Cd-MOF.

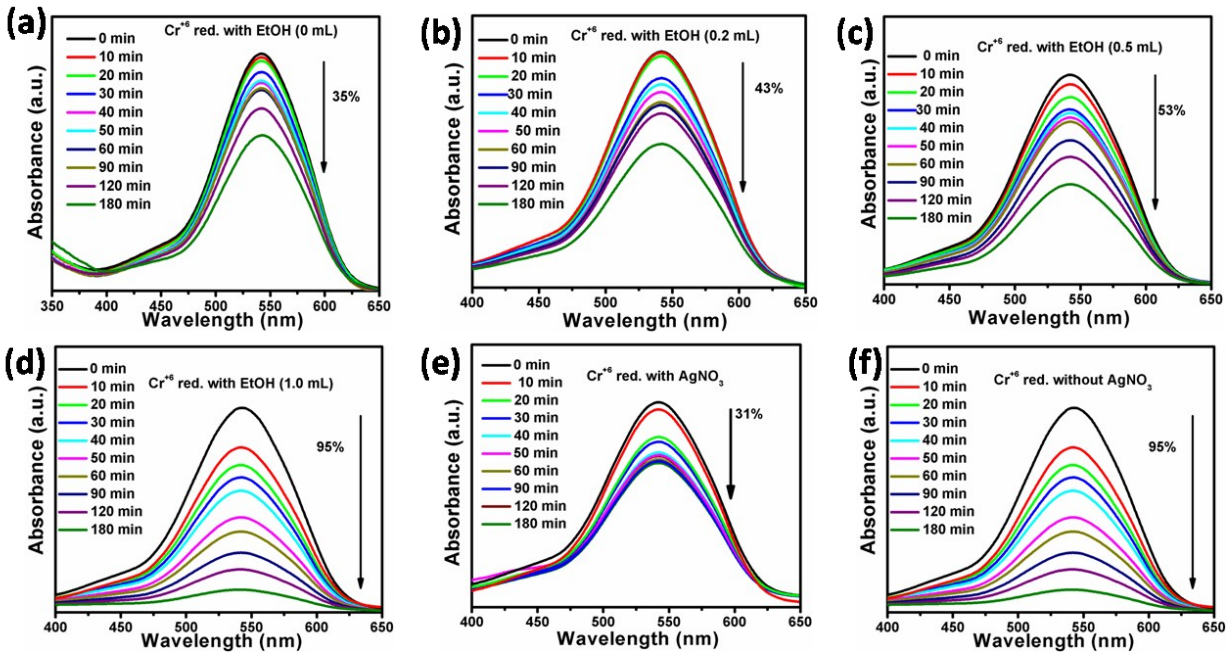

Figure S13. UV-vis spectra for photocatalytic reduction of Cr(VI) during different amount of EtOH (a to d). UV-vis spectra of photocatalytic Cr(VI) reduction. (e) with addition of $AgNO_3$. (f) without addition of $AgNO_3$.

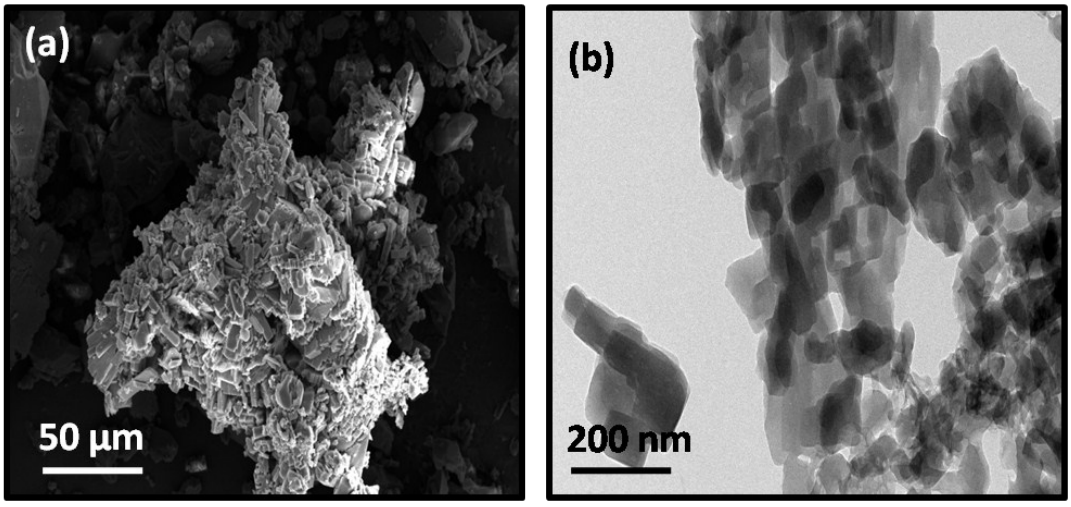

Figure S14. (a) SEM and (b) TEM images of recovered Cd-MOF after photocatalytic Cr(VI) reduction.