

## Supporting Information

# Two mesoporous anionic metal-organic frameworks for selective and efficient adsorption of cationic organic dye

Yu Gao,<sup>a#</sup> Yuzhu Li,<sup>a#</sup> Chen Liang,<sup>a</sup> Peipei Cen,<sup>\*b</sup> Jing Xi,<sup>a</sup> Yan Guo,<sup>\*a</sup> Weiming Song<sup>a</sup>  
and Xiangyu Liu<sup>\*ac</sup>

<sup>a</sup> State Key Laboratory of High-efficiency Utilization of Coal and Green Chemical Engineering, National Demonstration Center for Experimental Chemistry Education, College of Chemistry and Chemical Engineering, Ningxia University, Yinchuan 750021, China.

<sup>b</sup> College of Public Health and Management, Ningxia Medical University, Yinchuan 750021, China.

<sup>c</sup> State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing, 210023, China.

**Corresponding author:**

**Dr. Prof. Xiangyu Liu**

**E-mail: xiangyuliu432@126.com**

**Corresponding author:**

**Dr. Yan Guo**

**E-mail: 452785231@qq.com**

**Corresponding author:**

**Dr. Peipei Cen**

**E-mail: 13895400691@163.com**

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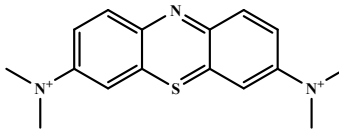
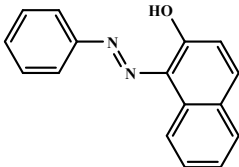
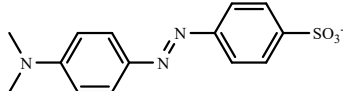
**Table S1.** Selected bond lengths (Å) and bond angles (°) for **1-2**

Compound 1			
Zn(1)-O(3_2)	1.956(3)	O(6_1)-Zn(1)O(2_1)#2	87.53(17)
Zn(1)-O(6_1)	1.960(3)	O(6_3)#1-Zn(1)-O(2_1)#2	147.18(19)
Zn(1)-O(6_2)#1	2.003(4)	O(1_1)#2-Zn(1)-O(2_1)#2	57.3(2)
Zn(1)-O(1_1)#2	2.077(5)	O(3_2)-Zn(1)-C(1_1)#2	108.4(2)
Zn(1)-O(2_1)#2	2.214(5)	O(6_1)-Zn(1)-C(1_1)#2	106.3(2)
Zn(1)-C(1_1)#2	2.492(6)	O(6V3)#1-Zn(1)-C(1_1)#2	119.6(2)
Zn(2)-O(4_2)	1.953(3)	O(1_1)#2-Zn(1)-C(1_1)#2	27.8(2)
Zn(2)-O(5_1)	1,953(3)	O(2_1)-Zn(1)-C(1_1)#2	29.7(2)
Zn(2)-O(1_2)#3	1.956(3)	O(4_2)-Zn(2)-O(5_1)	129.61(15)
Zn(2)-O(5_3)#1	1,989(4)	O(4_2)-Zn(2)-O(1_2)#3	107.86(13)
Zn(3)-O(4_1)#4	1.954(3)	O(5_1)-Zn(2)-O(1_2)#3	112.67(15)
Zn(3)-O(6_2)#2	1.957(3)	O(4_2)-Zn(2)-O(5_3)#1	100.14(14)
Zn(3)-O(2_3)#3	1.959(4)	O(5_1)-Zn(2)-O(5_3)#1	101.46(15)
Zn(3)-O(3_3) #2	1,984(4)	O(1_2)#3-Zn(2)-O(5_3)#1	99.39(15)
O(3_2)-Zn(1)-O(6_1)	123.17(15)	O(4_1)#4-Zn(3)-O(6_2)	119.04(16)
O(32)-Zn(1)-O(63)#1	101.84(14)	O(4_1)#4-Zn(3)-O(2_3)	107.26(15)
O(61)-Zn(1)-O(63)#1	98.30(15)	O(6_2)-Zn(3)-O(2_3)	115.72(15)
O(32)-Zn(1)-O(11)#2	105.93(17)	O(4_1)#4-Zn(3)-O(3_3)#2	93.10(15)
O(61)-Zn(1)-O(11)#2	124.89(18)	O(6_2)-Zn(3)-O(3_3)#2	112.33(15)
O(63)#1-Zn(1)-O(11)#2	94.25(18)	O(2_3)-Zn(3)-O(3_3)#2	106.63(17)
O(3_2)-Zn(1)-O(2_1)#2	101.73(19)	C(1_1)-O(1_1)-Zn(1)#3	96.3(5)
#1 +x,+y,-1+z; #2 1+x,+y,+z; #3 -1+x,+y,+z; #4 1+x,1+y,1+z; #5 -1+x,-1+y,-1+z; #6 +x,+y,1+z			
Compound 2			
Cd(1)-O(2_1)	2.217(5)	O(6_1)#1-Cd(1)-O(5_1)#1	54.88(17)
Cd(1)-O(1_2)	2.294(8)	O(4_1)#2-Cd(1)-O(5_1)#1	88.54(18)
Cd(1)-O(6_1)#1	2.360(5)	O(3_1)#2-Cd(1)-O(5_1)#1	88.70(17)
Cd(1)-O(4_1)#2	2.394(6)	O(2_1)-Cd(1)-O(2_2)	91.7(2)

Cd(1)-O(3_1)#2	2.398(6)	O(1_2)-Cd(1)-O(2_2)	51.7(2)
Cd(1)-O(5_1)#1	2.446(4)	O(6_1)#1-Cd(1)-O(2_2)	81.2(2)
Cd(1)-O(2_2)	2.507(7)	O(4_1)#2-Cd(1)-O(2_2)	172.5(2)
O(2_1)-Cd(1)-O(1_2)	104.1(3)	O(3_1)#2-Cd(1)-O(2_2)	129.7(3)
O(12)-Cd(1)-O(6_1)#1	88.0(2)	O(5_1)#1-Cd(1)-O(2_2)	85.9(2)
O(1_2)-Cd(1)-O(6_1)#1	131.0(2)	O(2_1)-Cd(1)-C(16_1)#2	104.5(2)
O(2_1)-Cd(1)-O(4_1)#2	89.7(2)	O(1_2)-Cd(1)-C(16_1)#2	108.8(3)
O(1_2)-Cd(1)-O(4_1)#2	134.9(2)	O(4_1)#2-Cd(1)-C(16_1)#2	26.7(3)
O(6_1)#1-Cd(1)-O(4_1)#2	91.5(2)	O(5_1)#1-Cd(1)-C(16_1)#2	89.87(19)
O(2_1)-Cd(1)-O(3_1)#2	119.9(2)	O(2_2)-Cd(1)-C(16_1)#2	158.0(3)
O(1_2)-Cd(1)-O(3_1)#2	81.5(2)	O(2_1)-Cd(1)-C(24_1)#1	115.1(3)
O(6_1)#1-Cd(1)-O(3_1)#2	132.8(2)	O(2_1)-Cd(1)-C(7_2)	99.5(3)
O(4_1)#2-Cd(1)-O(3_1)#2	55.1(2)	O(1_2)-Cd(1)-C(7_2)	26.1(2)
O(2_1)-Cd(1)-O(5_1)#1	142.8(2)	O(3_1)#2-Cd(1)-C(7_2)	105.7(3)
O(1_2)-Cd(1)-O(5_1)#1	103.2(2)	O(5_1)#1-Cd(1)-C(7_2)	94.1(3)

#1  $-1/2+x, 3/2-y, -1+z$ ; #2  $+x, +y, -1+z$ ; #3  $+x, +y, 1+z$ ; #4  $1/2+x, 3/2-y, 1+z$ ; #5  $1-x, +y, -z$

**Table S2.** Molecular weight and dimensions of different dyes molecules.

			
Abbr.	MB <sup>+</sup>	SD <sup>0</sup>	MO <sup>-</sup>
M <sub>w</sub>	284.40	248.28	304.33
x(Å)	4.00	3.68	5.31
y(Å)	7.93	9.74	7.25
z(Å)	16.34	13.55	17.39

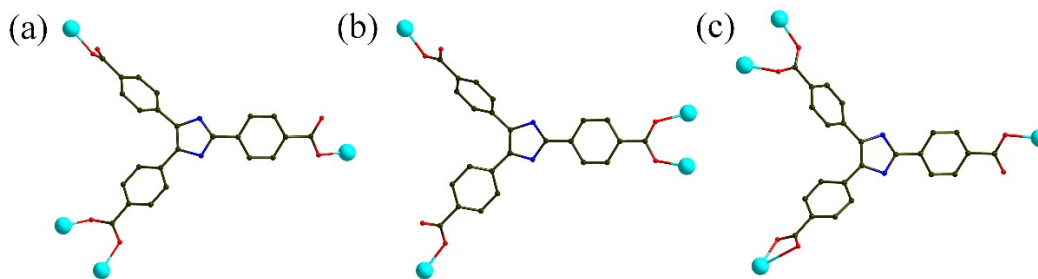


Fig. S1 The coordination modes of ITTC<sup>3-</sup> ligand in 1.

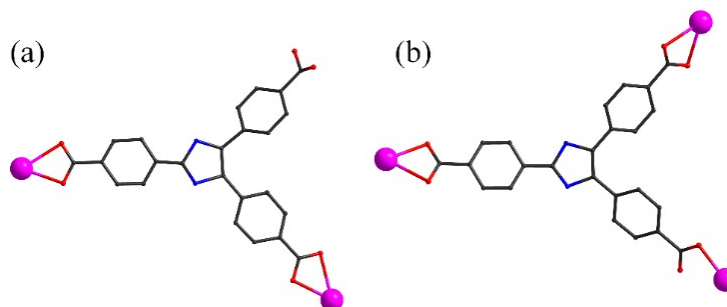


Fig. S2 The coordination modes of ITTC<sup>3-</sup> ligand in 2.

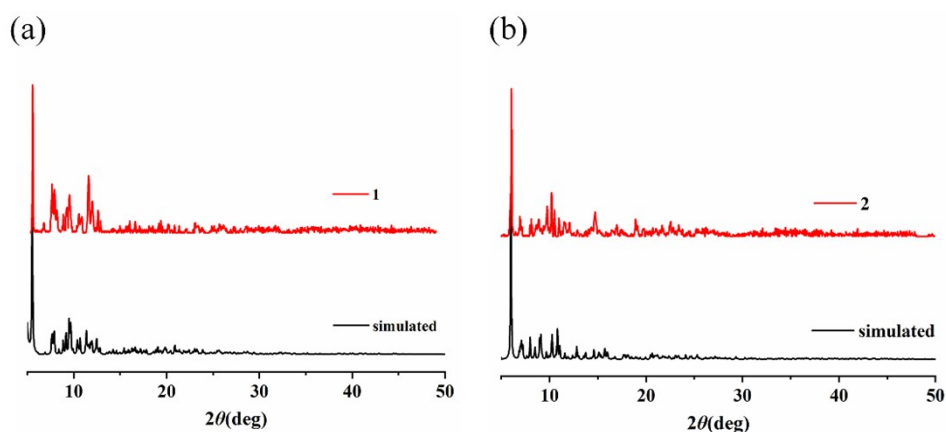


Fig. S3 Powdered X-ray diffraction (PXRD) patterns of 1-2.

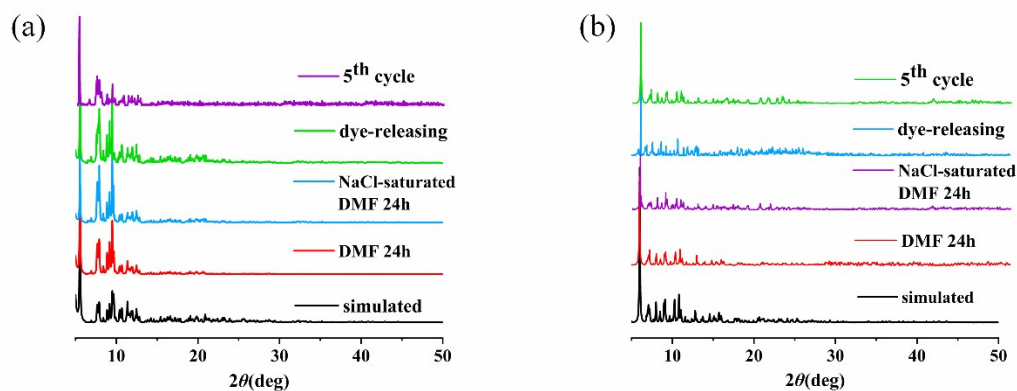


Fig. S4 PXRD patterns of 1(a) and 2(b) after soaking in DMF solutions for 24h, after soaking in NaCl-saturated DMF solution for 24h, after dye-releasing experiment, and after re-usability experiment for MB adsorption.

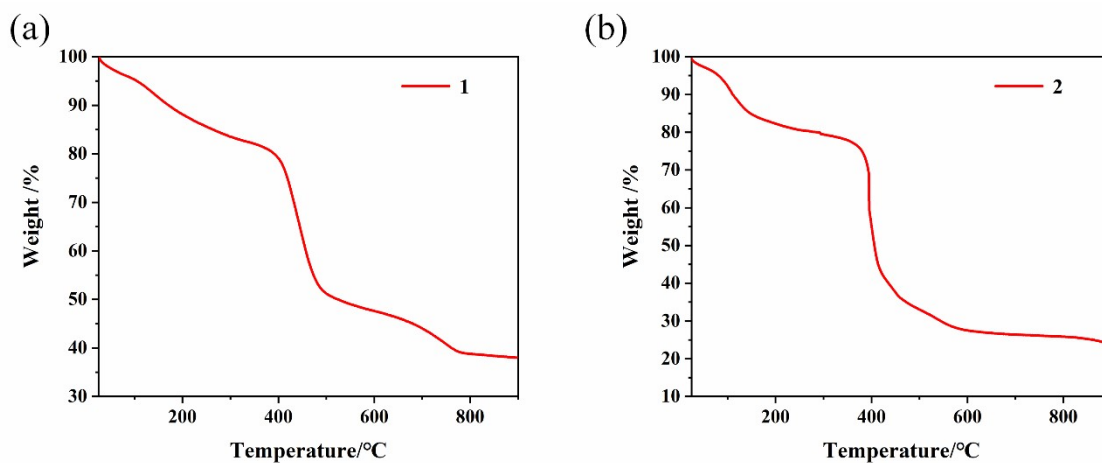


Fig. S5 TG curves of 1-2.

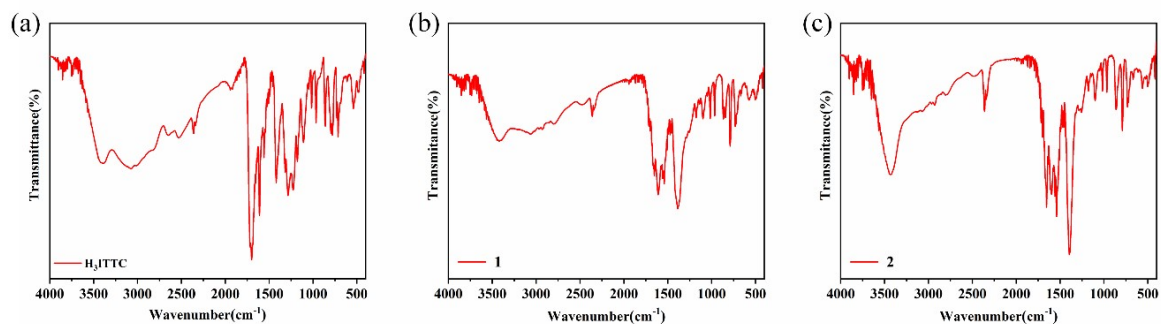


Fig. S6 Infrared Spectra of H<sub>3</sub>ITTC(a), 1(b) and 2(c).

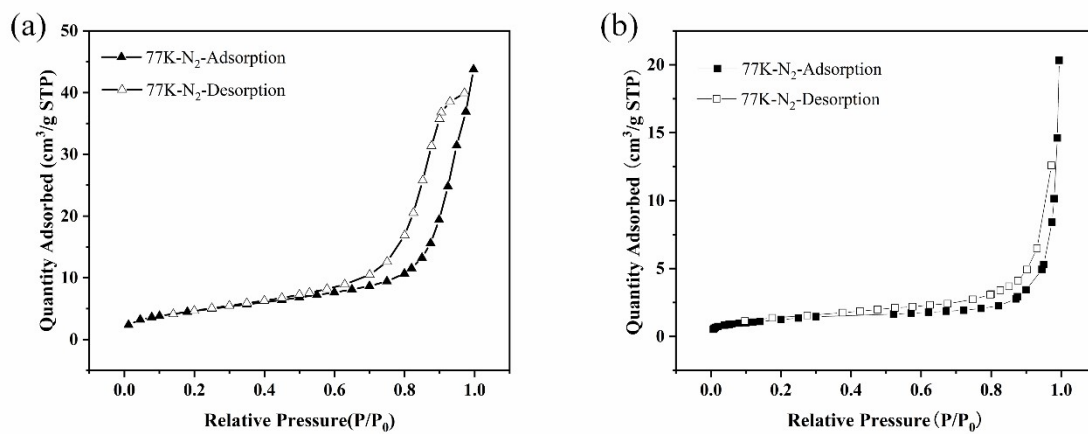


Fig. S7 N<sub>2</sub> adsorption isotherms of 1(a) and 2(b).

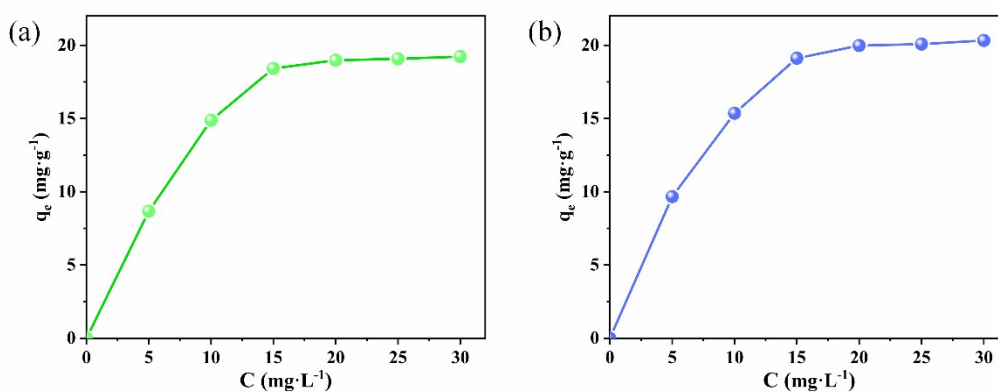


Fig. S8 MB adsorption isotherms of 1(a) and 2(b).

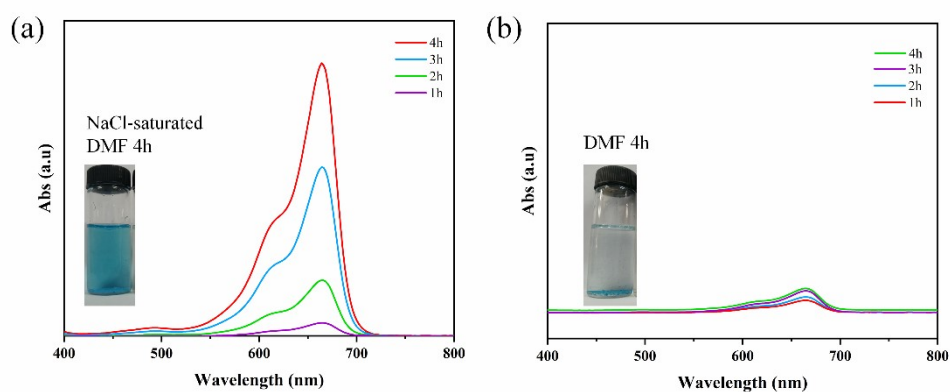


Fig. S9 The dye-releasing process of MB@1 in NaCl-saturated DMF solution(a) and in pure DMF(b).

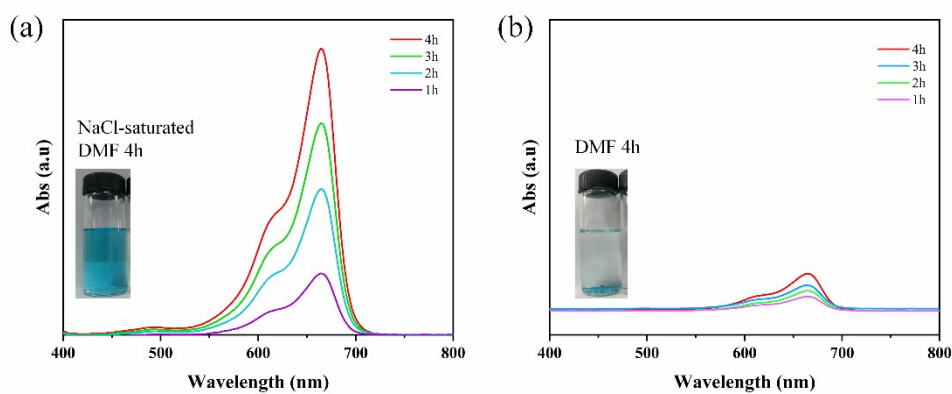
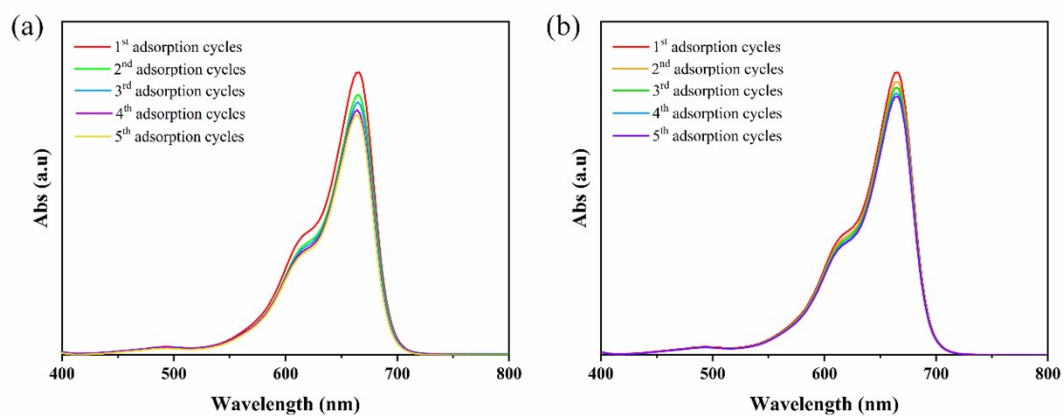


Fig. S10 The dye-releasing process of MB@2 in NaCl-saturated DMF solution(a) and in pure DMF(b).



**Figure S11.** UV-vis spectra of five adsorption and desorption cycles of 1(a) and 2(b) for MB dye molecules.