Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

A Multifunctional Microporous Metal–Organic Framework: Efficient Adsorption of Iodine and Column-chromatographic Dye Separation

Chan Yao,[a] Wei Wang,[a] Shu-Ran Zhang,[a] Hui-Ying Li,[a] Yan-Hong Xu,*[a,b] Zhong-Min Su[c] and Guang-Bo Che*[a]

[a] Key Laboratory of Preparation and Applications of Environmental Friendly Materials (Jilin Normal University), Ministry of Education, Changchun 130103, Jilin, People's Republic of China

[b] Key Laboratory of Functional Materials Physics and Chemistry of the Ministry of Education, Jilin Normal University, Siping 136000, Jilin, People's Republic of China

[c] Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun, 130024, Jilin, People's Republic of China

Table S1 Crystal data and structure refinements for **JLNU-4**.

Identification code	**JLNU-4**
Formula	$C_{36}H_{51}N_7O_{15}Cd_2$
Formula weight	1046.65
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	14.3590(9)
b (Å)	14.4350(10)
c (Å)	22.6110(14)
α (°)	90
β (°)	98.6970(11)
γ (°)	90
V (Å^3)	4632.7(5)
Z	4
D_{calcd}.[g cm^{-3}]	1.001
F(000)	1360
Reflections collected	25012 / 9129
R(int)	0.0463
Goodness-of-fit on F^2	1.097
R_1[a] [$I>2\sigma(I)$]	0.0781
wR_2[b]	0.2803

$^{a}R_1 = \sum\left\|F_o\right|-\left|F_c\right\| / \sum\left|F_o\right|$. $^{b}wR_2 = \left|\sum w(\left|F_o\right|^2-\left|F_c\right|^2)\right| / \sum\left|w(F_o^2)^2\right|^{1/2}$.

Table S2 The selected bond lengths for **JLNU-4**.

JLNU-4			
O(1)-Cd(1)	2.301(6)	O(6)-Cd(2)	2.244(7)
O(1)-Cd(2)	2.307(6)	O(7)-Cd(1)	2.276(7)
O(2)-Cd(1)	2.570(7)	O(8)-Cd(2)	2.308(9)
O(3)-Cd(1)	2.415(6)	O(9)-Cd(2)	2.235(12)
O(4)-Cd(1)	2.276(6)	O(10)-Cd(2)	2.235(8)
O(5)-Cd(1)	2.213(6)	O(11)-Cd(2)	2.269(13)

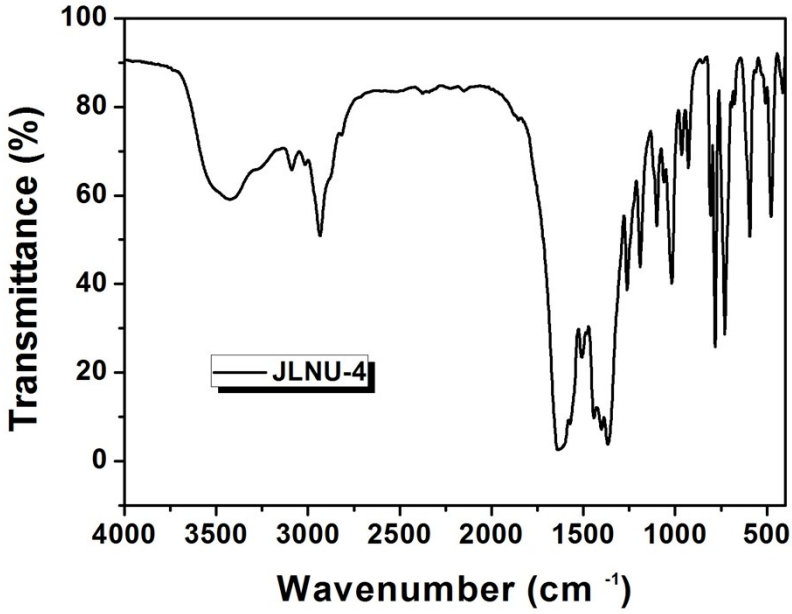

Fig. S1 The IR spectrum of **JLNU-4** in KBr pellets from 4000 cm^{-1} to 400 cm^{-1}.

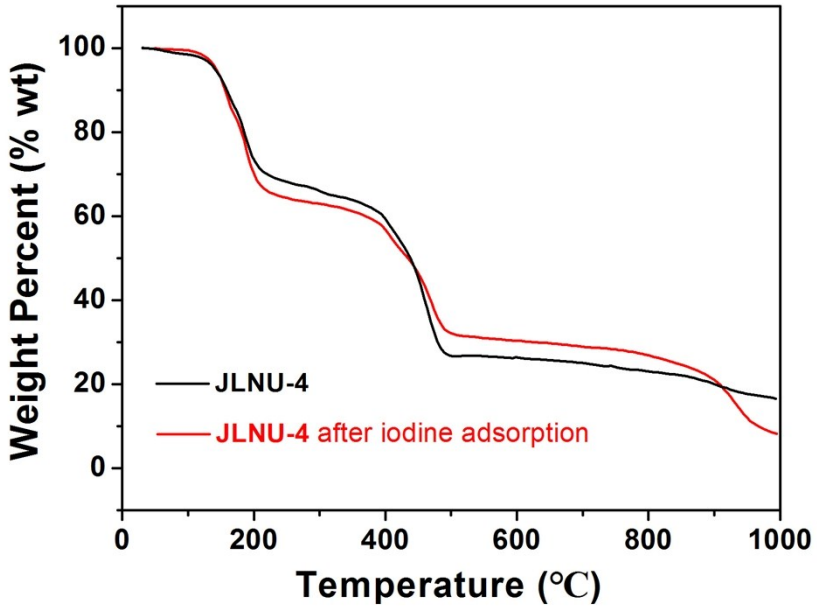

Fig. S2 The TGA curve of (a) **JLNU-4** and (b) **JLNU-4** after iodine adsorption measured under N_2 atmosphere from 40 to 1000 °C at the heating rate of 10 °C·min^{-1}.

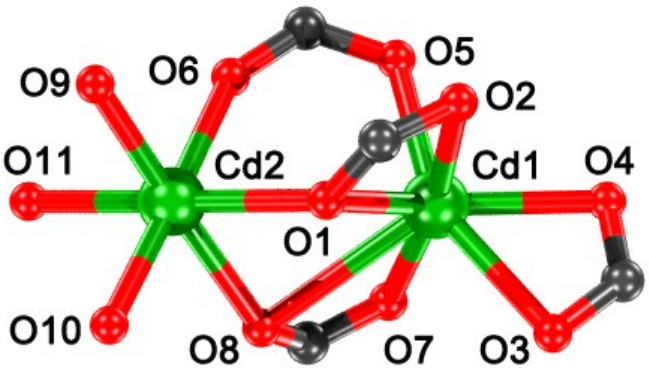

Fig. S3 Ball-and-stick representation of a binuclear $[Cd_2(CO)_4(H_2O)_2(DMA)]$ cluster in **JLNU-4**.

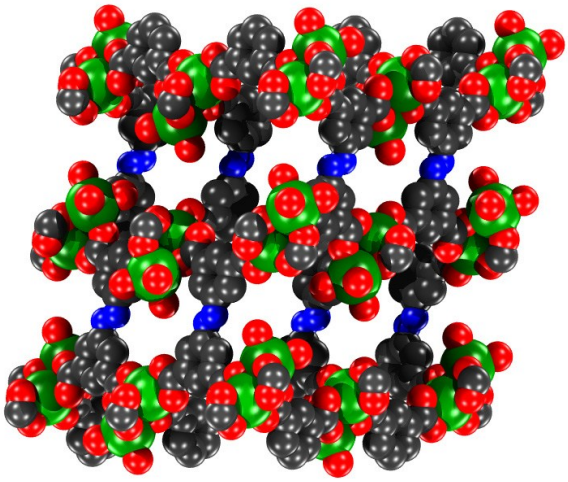

Fig. S4 Space-filling representation of the packing arrangement for the 3D structure in **JLNU-4**.

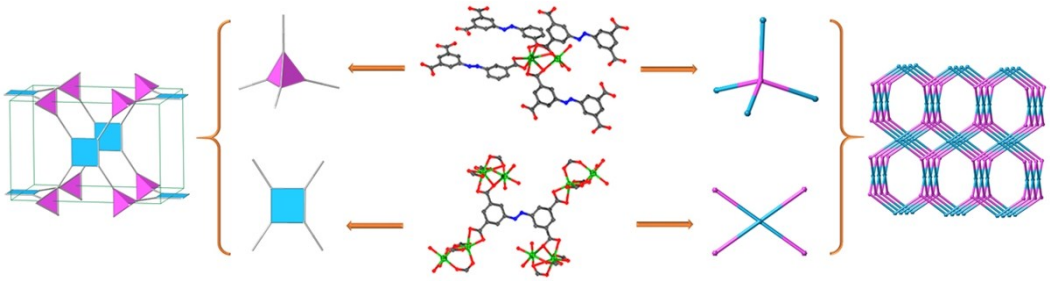

Fig. S5 Polyhedral and ball-and-stick view of the (4,4)-connected topology network in **JLNU-4**.

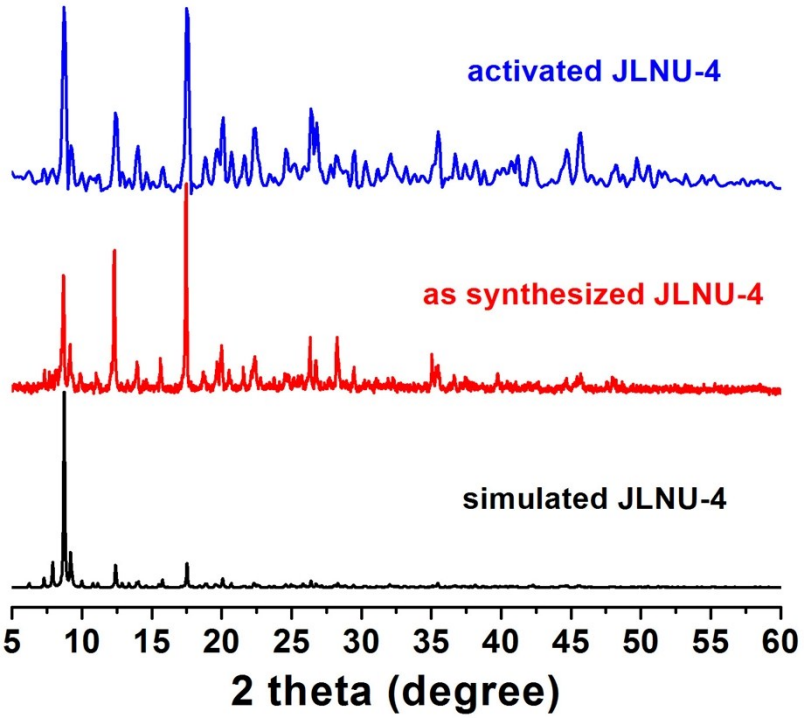

Fig. S6 PXRD patterns of simulated **JLNU-4** (black), as-synthesized **JLNU-4** (red) and activated **JLNU-4** (blue).

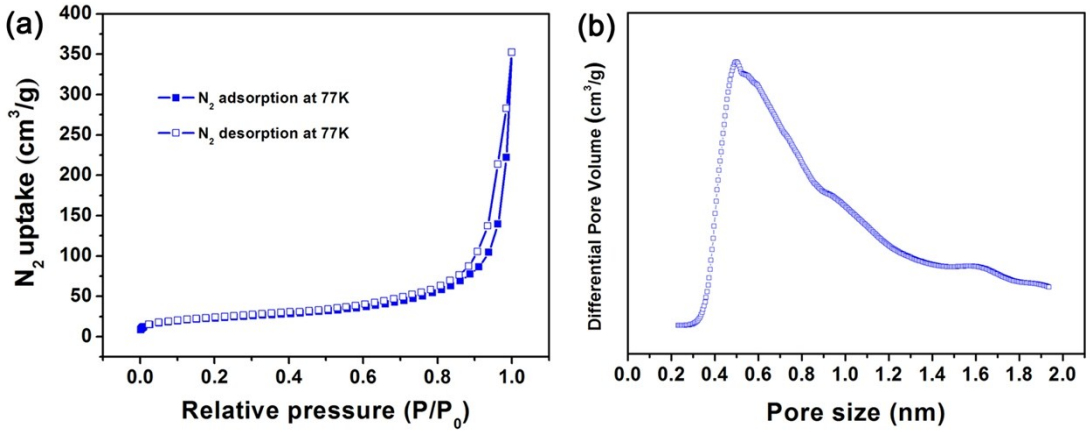

Fig. S7 (a) The N_2 gas-sorption isotherms of **JLNU-4** measured at 77 K, 1 atm. (b) The pore size distribution of **JLNU-4** calculated using density functional theory (DFT) method.

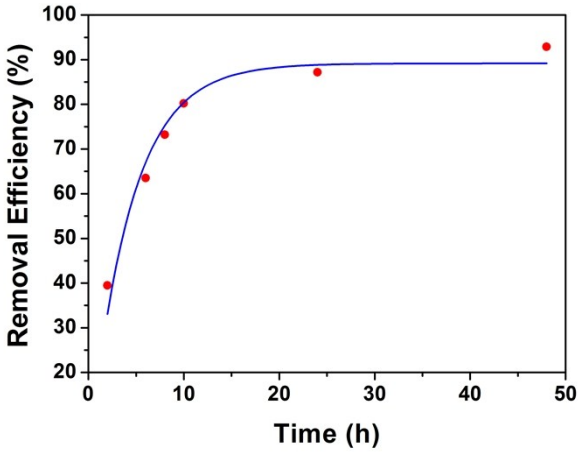

Fig. S8 The iodine adsorption kinetic was analyzed by the pseudo-first-order kinetic model. The initial concentration of iodine solution is 4 mg·mL^{-1}.

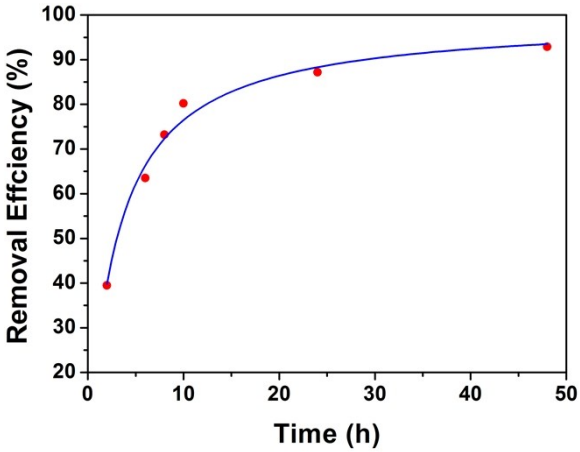

Fig. S9 The iodine adsorption kinetic was analyzed by the pseudo-second-order kinetic model. The initial concentration of iodine solution is 4 mg·mL^{-1}.

Table S3 Parameters of the iodine adsorption kinetic analyzed by the pseudo-first-order model and pseudo-second-order model for **JLNU-4**.

Pseudo-first-order			Pseudo-second-order		
k_1 (h^{-1})	Q_e (%)	R^2	k_2 (h^{-1})	Q_e (%)	R^2
0.2318	89.166	0.95034	0.00337	99.3008	0.9837

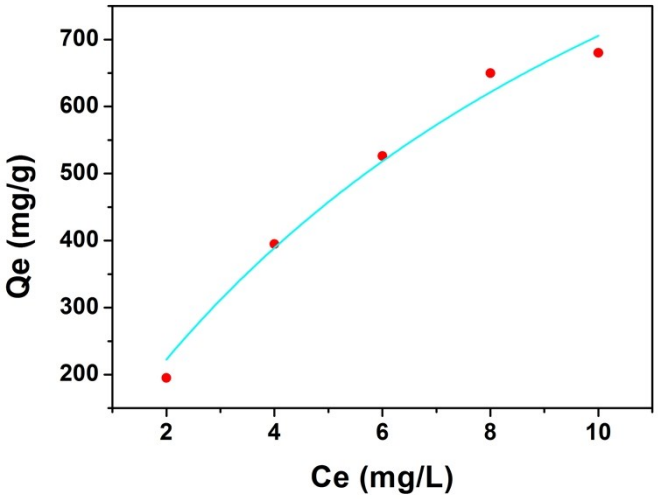

Fig. S10 The Langmuir adsorption isotherm of the iodine adsorption for **JLNU-4**.

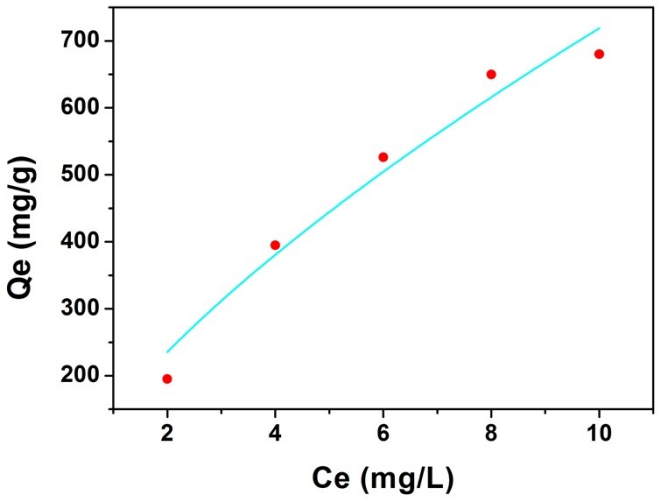

Fig. S11 The Freündlich adsorption isotherm of the iodine adsorption for **JLNU-4**.

Table S4 Parameters of two different simulation models extracted from experimental adsorption isotherms data for **JLNU-4**.

Langmuir adsorption isotherm			Freündlich adsorption isotherm		
Q_m (mg·g^{-1})	k_L (mg^{-1})	R^2	k_F (mg^{-1})	n	R^2
1540.464	0.08449	0.98043	145.484	1.44124	0.95821

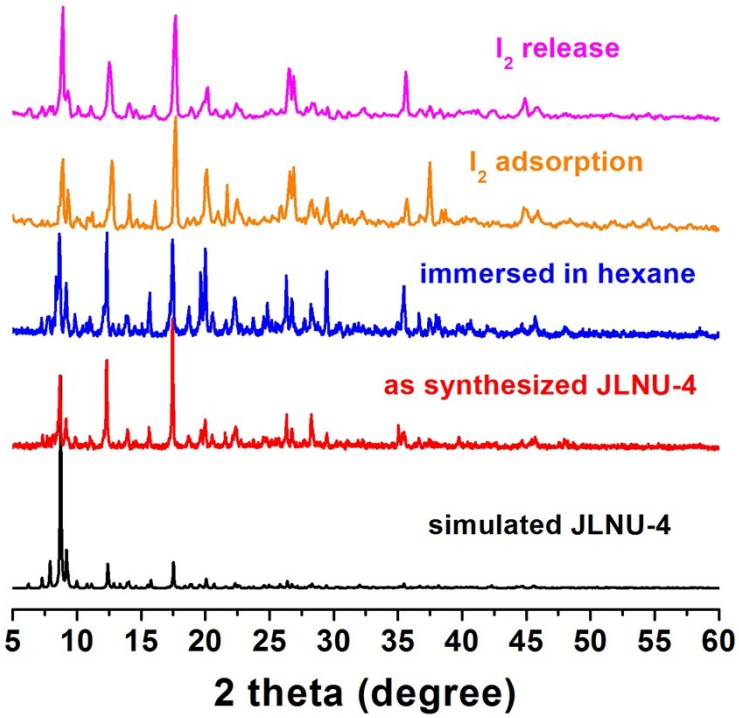

Fig. S12 PXRD patterns of simulated **JLNU-4** (black), as-synthesized **JLNU-4** (red), immersed in hexane solution (blue), as-synthesized **JLNU-4** after iodine adsorption and release.

Table S5 The gravimetric measurement of **JLNU-4** during the iodine adsorption in vapor phase at a time interval.[a]

Time interval	Weight (g)
0	5.8156
2	5.8266
4	5.8301
6	5.8330
8	5.8339
10	5.8347
12	5.8347
14	5.8348

[a]The weight measured at a time interval was the total mass of **JLNU-4** and the vessel, in which the initial weight of **JLNU-4** was 30 mg.

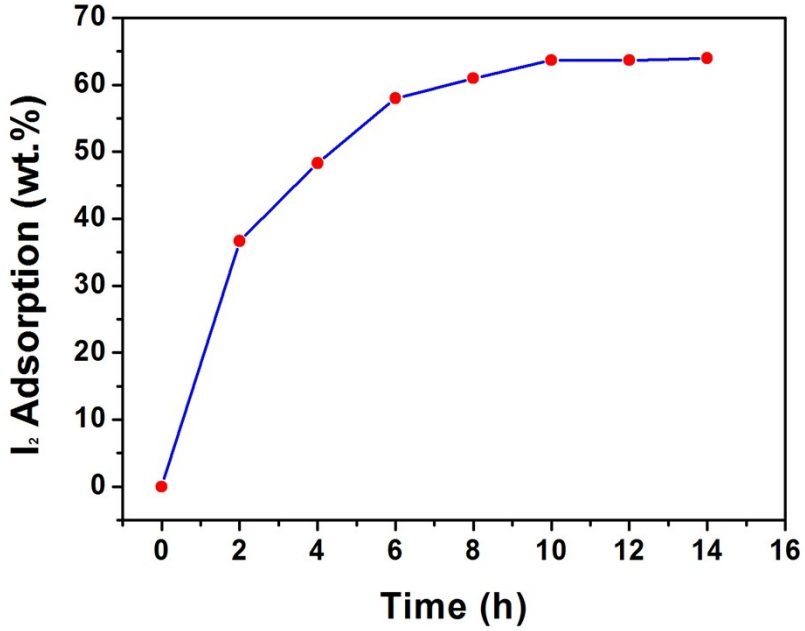

Fig. S13 Gravimatric uptake of iodine for **JLNU-4** as a function of time at 350 K.

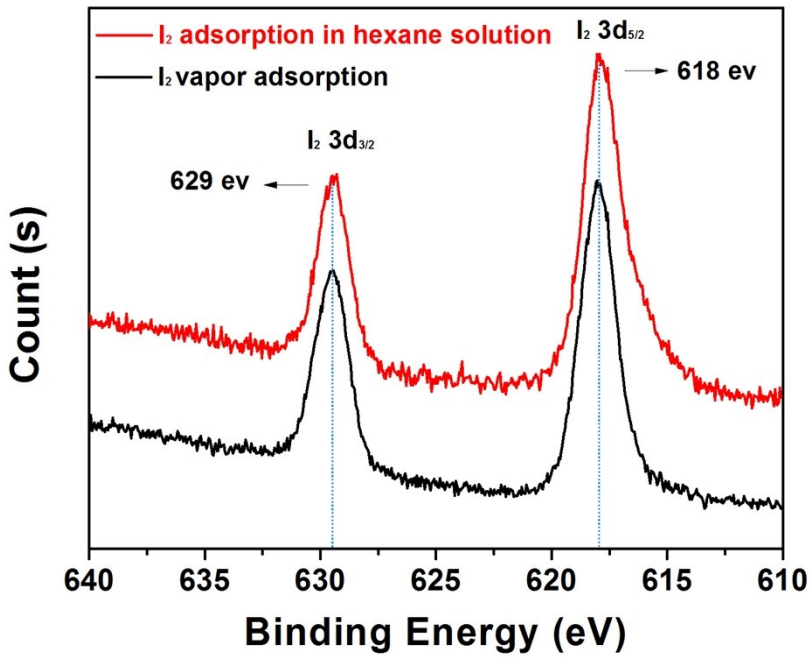

Fig. S14 XPS spectrum of **JLNU-4** after iodine adsorption in hexane solution and iodine vapor adsorption, respectively.

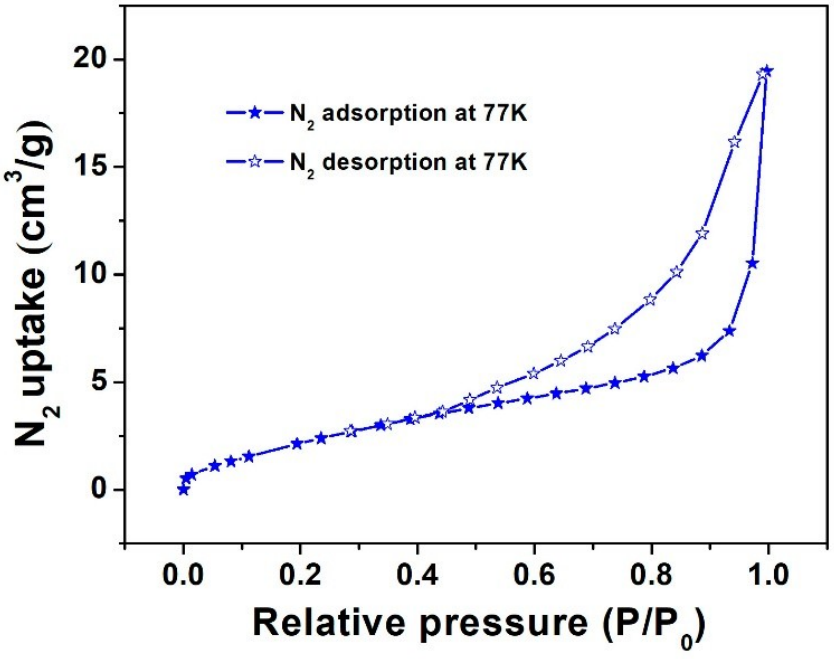

Fig. S15 The N_2 gas-sorption isotherms of MB loaded **JLNU-4** measured at 77 K, 1 atm.

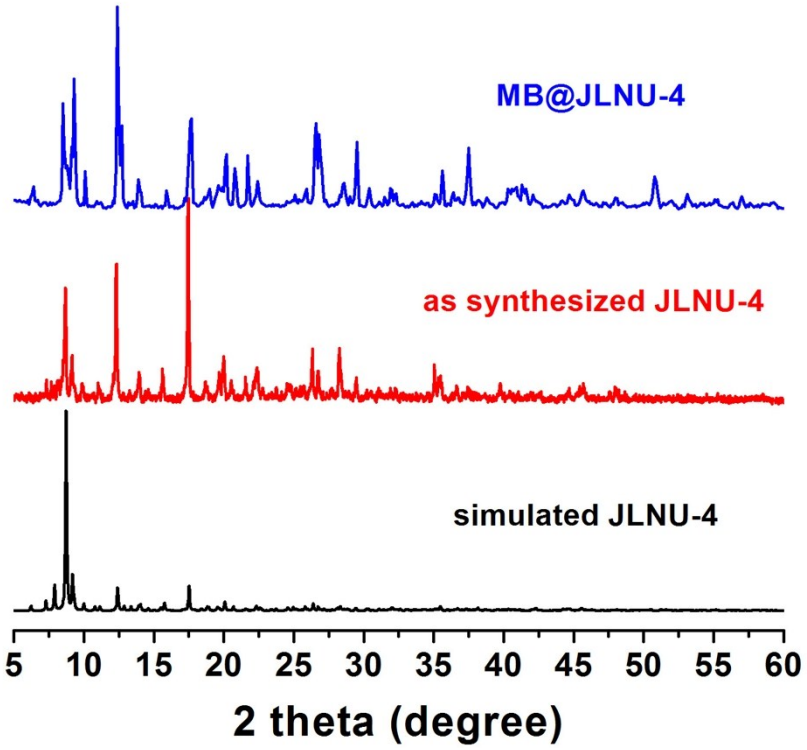

Fig. S16 XRPD patterns of simulated **JLNU-4** (black), as-synthesized **JLNU-4** (red) and after the absorption of MB (blue), respectively.

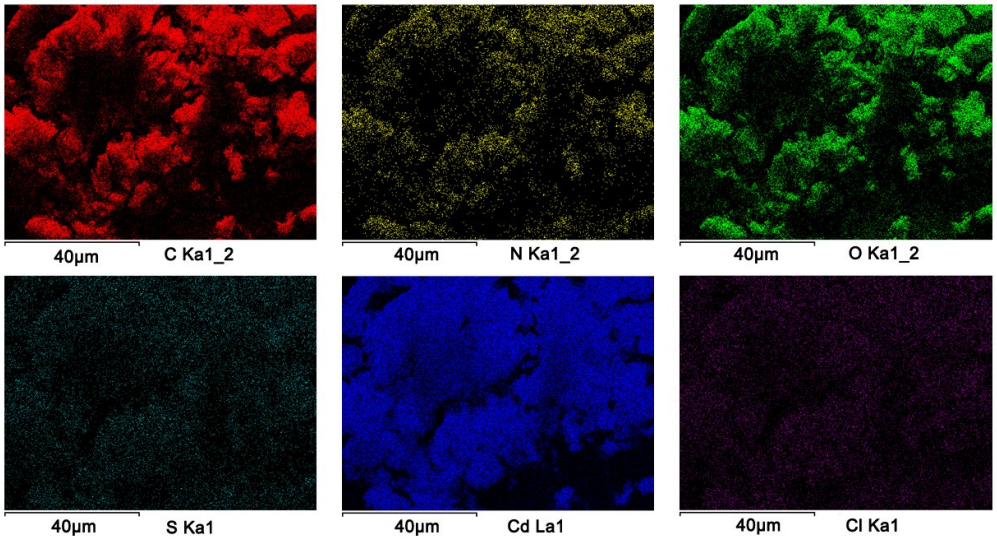

Fig. S17 EDS images of MB loaded **JLNU-4**.

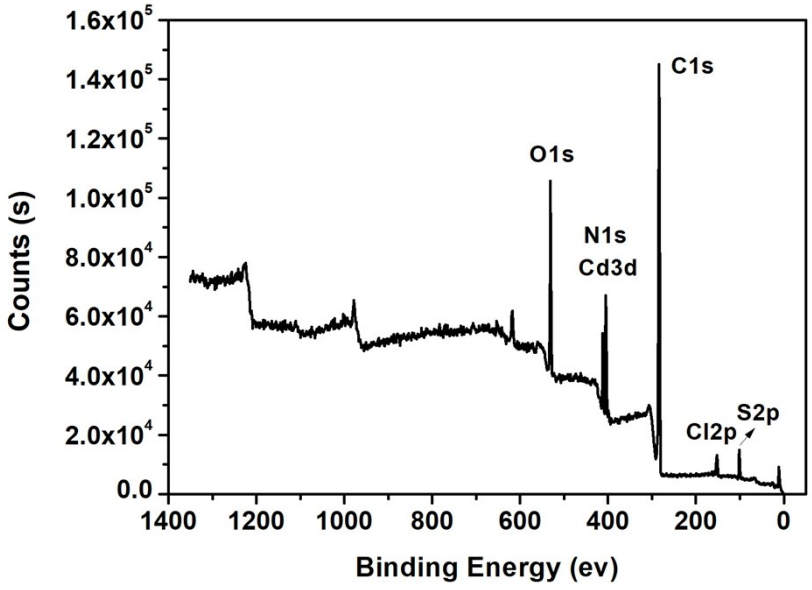

Fig. S18 XPS spectrum of contained elements for MB loaded **JLNU-4**.

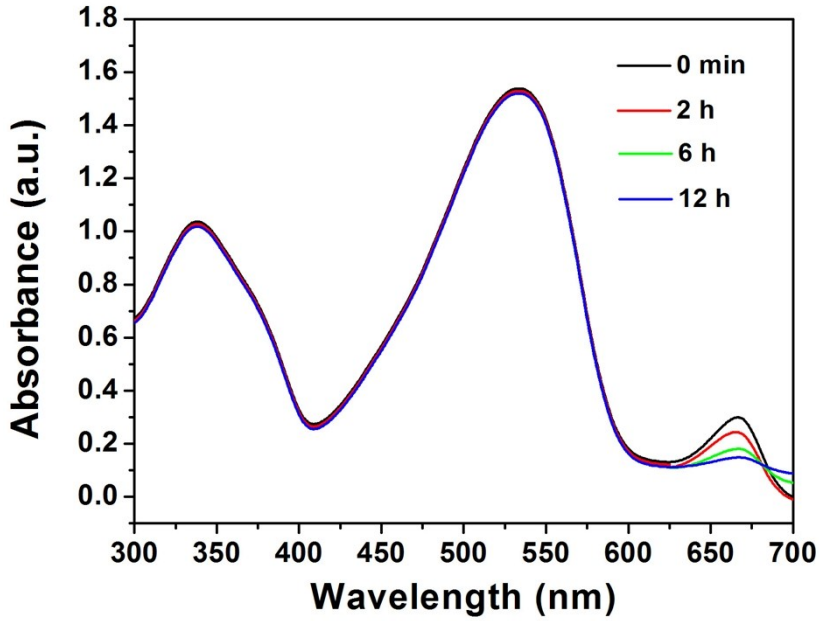

Fig. S19 UV/vis spectra of the effluent during the dye mixture of MB and CR passing through the MOF-filled chromatographic column.