Electronic Supplementary Information (ESI)

In_3-cluster-based cationic metal-organic frameworks with nitrogen-rich ligand for highly effective and fast removal of anionic cancerogenic dyes

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S1. Supporting Figures

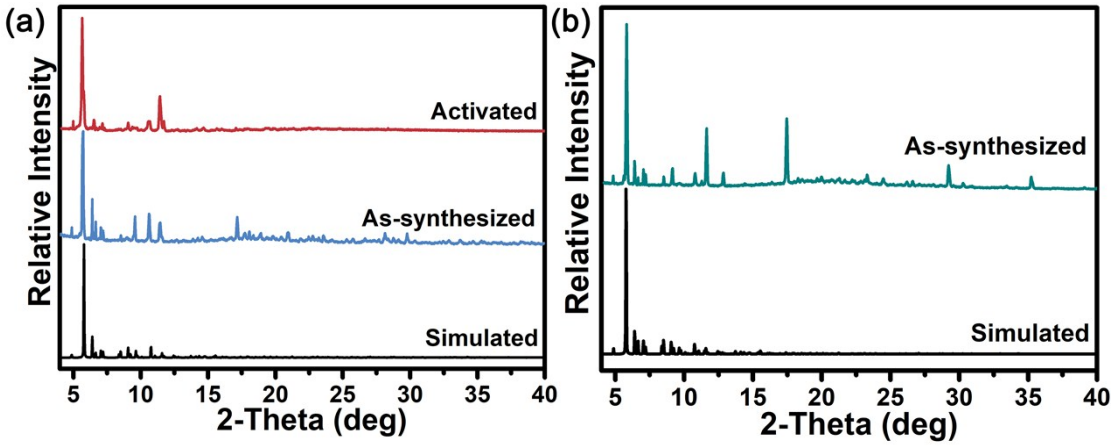

Fig. S1 Powder X-ray diffraction (PXRD) patterns of (a) **In-TATAB** and (b) **Fe-TATAB**.

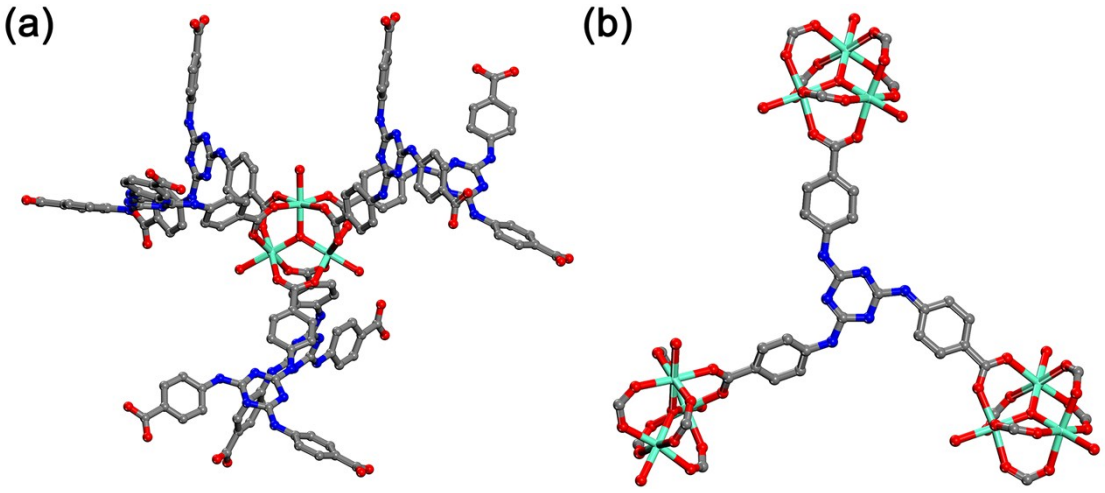

Fig. S2 Connection mode of (a) metal-cluster and (b) organic ligand.

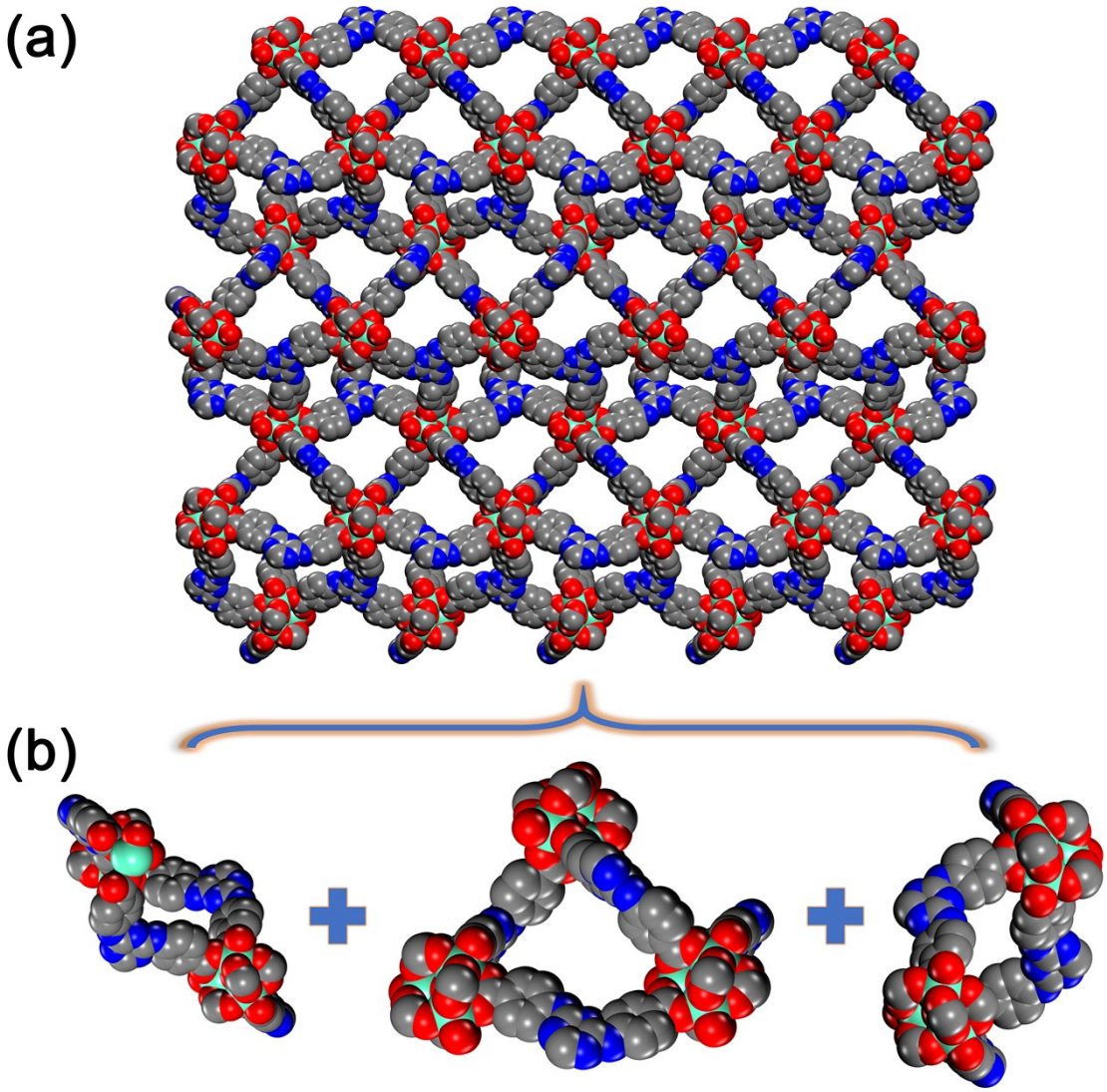

Fig. S3 CPK views of the structure of **In-TATAB**: (a) 3D frameworks of **In-TATAB** and (b) three kinds of channels of **In-TATAB**. Color scheme: In (cyan), C (gray), O (red) and N (blue).

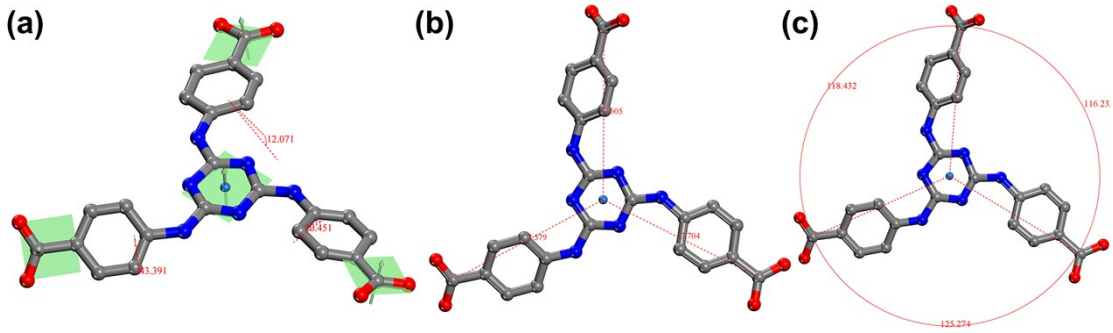

Fig. S4 Analysis of organic ligand TATAB: (a) the angles between the plane of three carboxylic groups and triazine ring, (b) distances and (c) angles between three carboxylic groups and center of triazine ring.

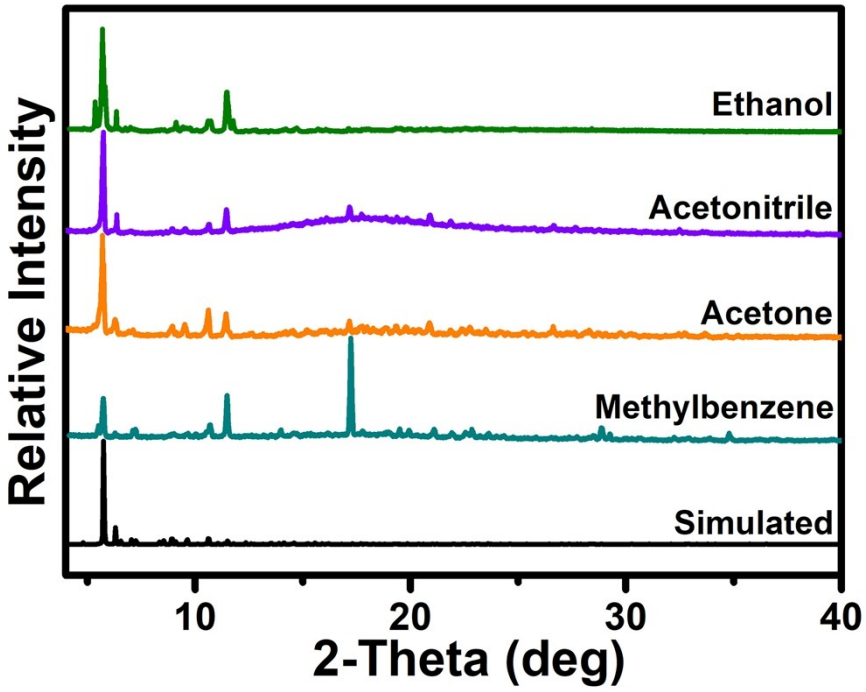

Fig. S5 PXRD patterns of stability test of **In-TATAB** in different solvents.

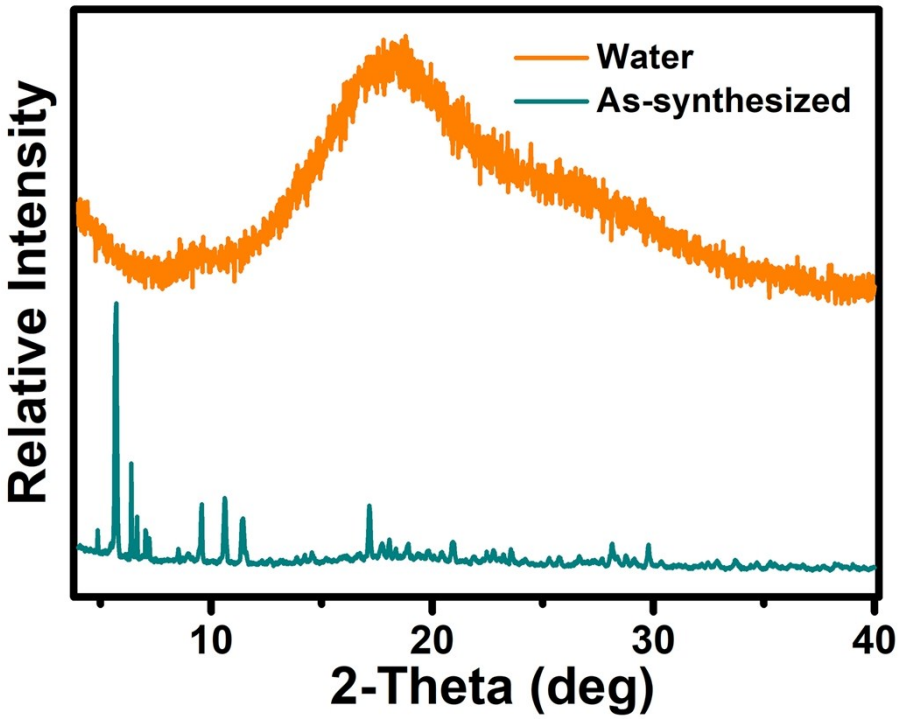

Fig. S6 PXRD patterns of stability test of **In-TATAB** in water.

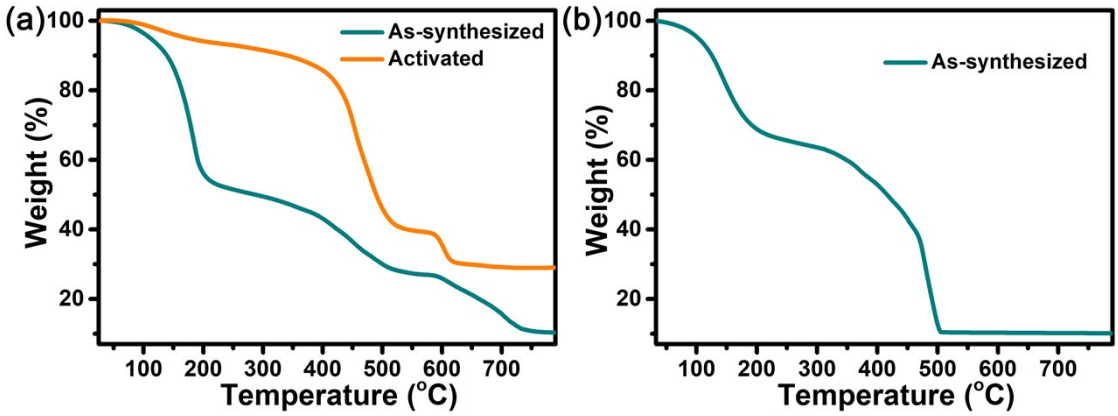

Fig. S7 TGA curves of (a) **In-TATAB** and (b) **Fe-TATAB**.

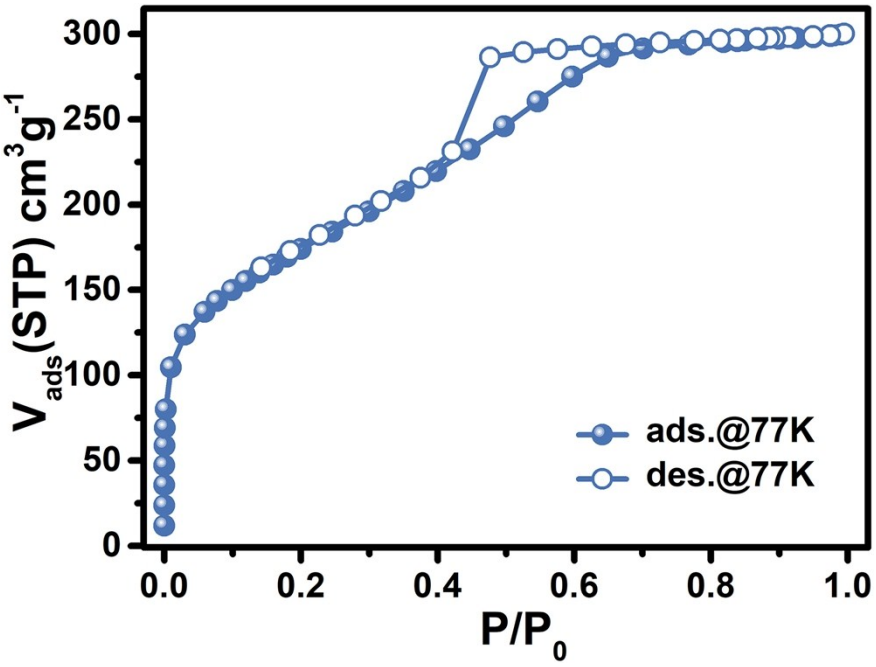

Fig. S8 N_2 isotherm of **In-TATAB**.

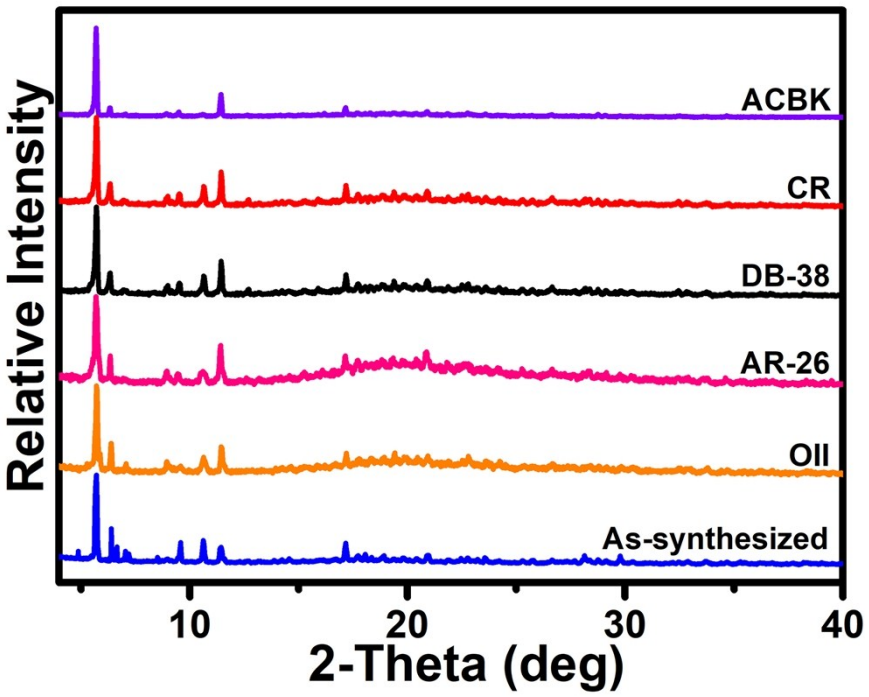

Fig. S9 PXRD patterns of **In-TATAB** after adsorptions of different dye molecules.

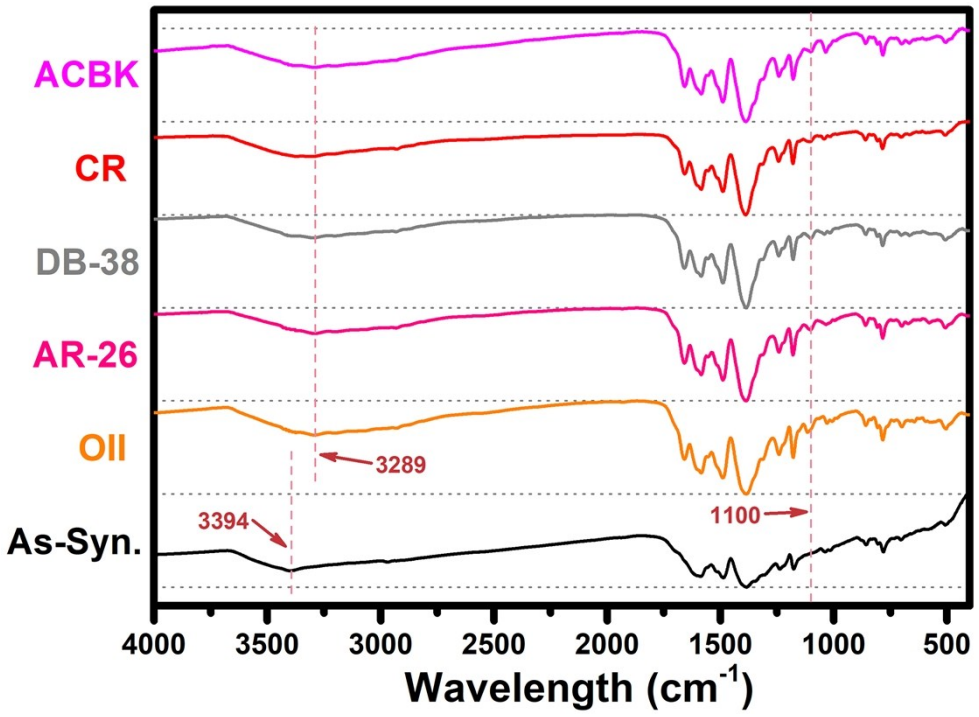

Fig. S10 Infrared patterns of **In-TATAB** samples after adsorptions of different dye molecules.

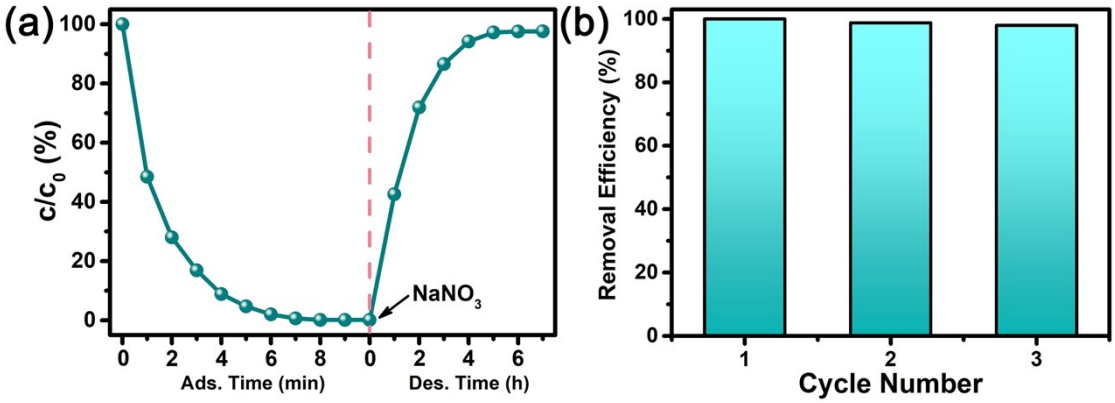

Fig. S11 (a) Adsorption-desorption test of **In-TATAB** using AR-26, (b) cycle-tests of adsorption of AR-26.

S2. Supporting Tables

Table S1. Crystal data and structure refinement for **In-TATAB**

formula	$C_{48}H_{30}O_{16}N_{12}In_3$
formula Weight	1375.3
temperature	296(2) K
wavelength	0.71073 Å
crystal system, space group	Tetragonal, $P4_12_12$
a (Å)	19.519(4)
b (Å)	19.519(4)
c (Å)	49.1068(4)
V (Å^3)	18709.3(9)
Z, D_c (Mg/M^3)	4, 0.488
F (000)	2708
θ range (deg)	1.123~25.507
reflns collected/unique	125326/17411
R_{int}	0.1174
data/restraints/params	17411/930/359
GOF on F^2	0.891
R_1, wR_2 (I>2 σ (I))	R_1 = 0.0359, wR_2 = 0.0683
R_1, wR_2 (all data)	R_1 = 0.0750, wR_2 = 0.0798

Table S2. Crystal data and structure refinement for **Fe-TATAB**

formula	$C_{48}H_{30}O_{16}N_{12}Fe_3$
formula Weight	1198.39
temperature	296(2) K
wavelength	0.71073 Å
crystal system, space group	Tetragonal, $P4_12_12$
a (Å)	19.519(4)
b (Å)	19.519(4)
c (Å)	49.1068(4)
V (Å^3)	18709.3(9)
Z, D_c (Mg/M^3)	4, 0.425
F (000)	2432
θ range (deg)	1.123~25.054
reflns collected/unique	16563/9120
R_{int}	0.1687
data/restraints/params	16563/924/359
GOF on F^2	1.008
R_1, wR_2 (I>2 σ (I))	R_1 = 0.0521, wR_2 = 0.1132
R_1, wR_2 (all data)	R_1 = 0.1287, wR_2 = 0.1337