Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supporting Information

Amide-functionalized ionic indium-organic frameworks for efficient separation of organic dyes based on diverse adsorption interactions

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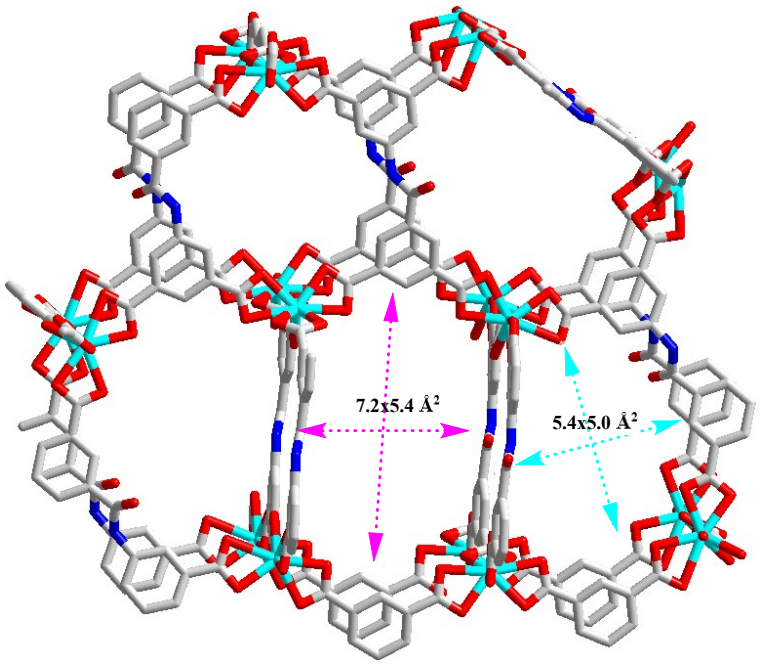


Fig. S1 Ball-and-stick representation of 3D framework of **1** showing two types of channels along the [100] direction.

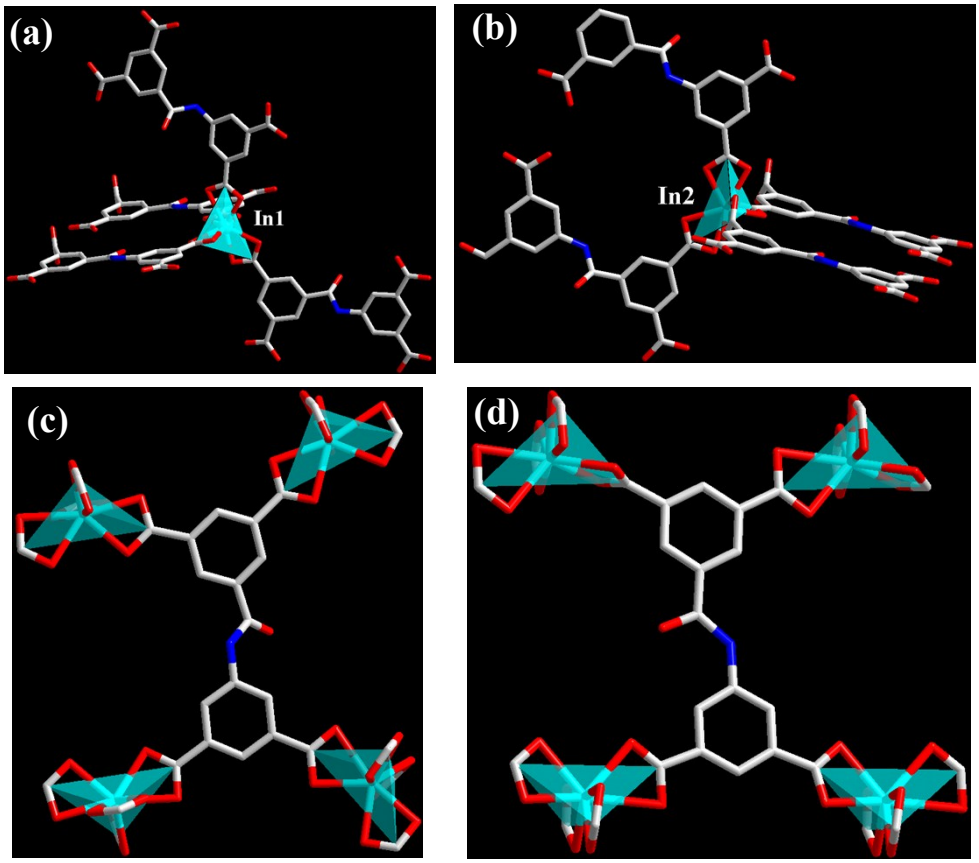


Fig. S2 Two types of indium center (a, b) and ligands (c, d) in **1**.

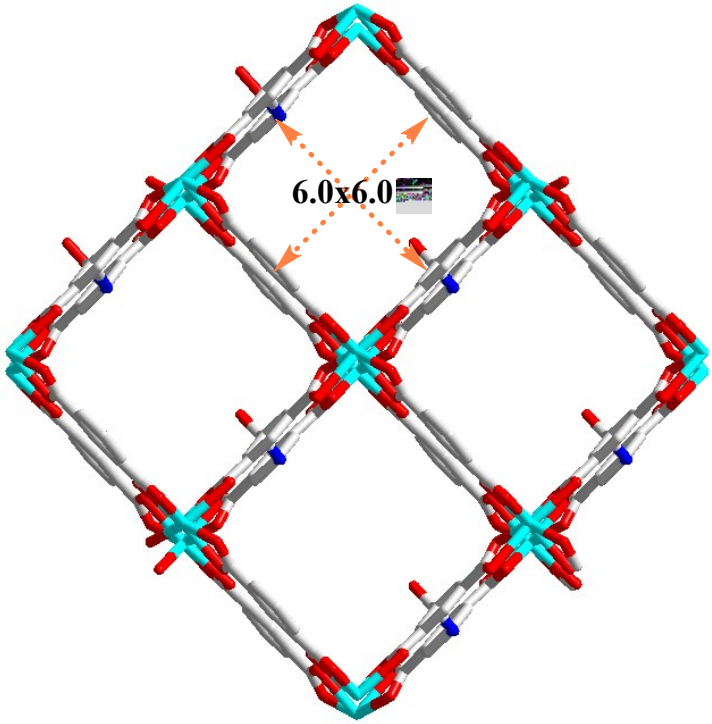


Fig. S3 Ball-and-stick representation of the cuboidal cage of **1** with an internal diameter of about 9.6 Å, which is indicated by the yellow sphere (excluding van der Waals radii).

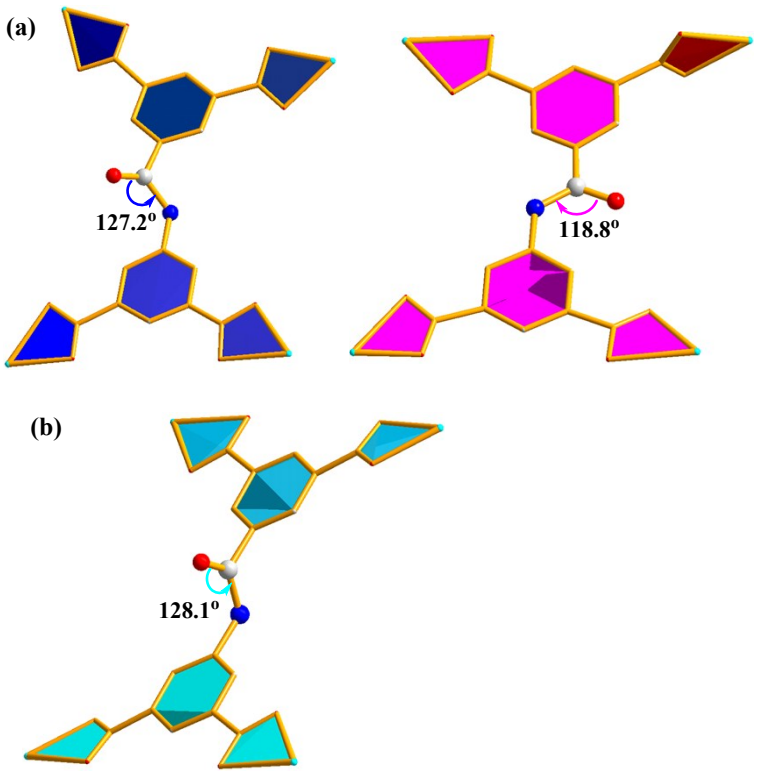


Fig. S4 View of L^- ligands in **1** (a) and **2** (b) with different angles of amide group.

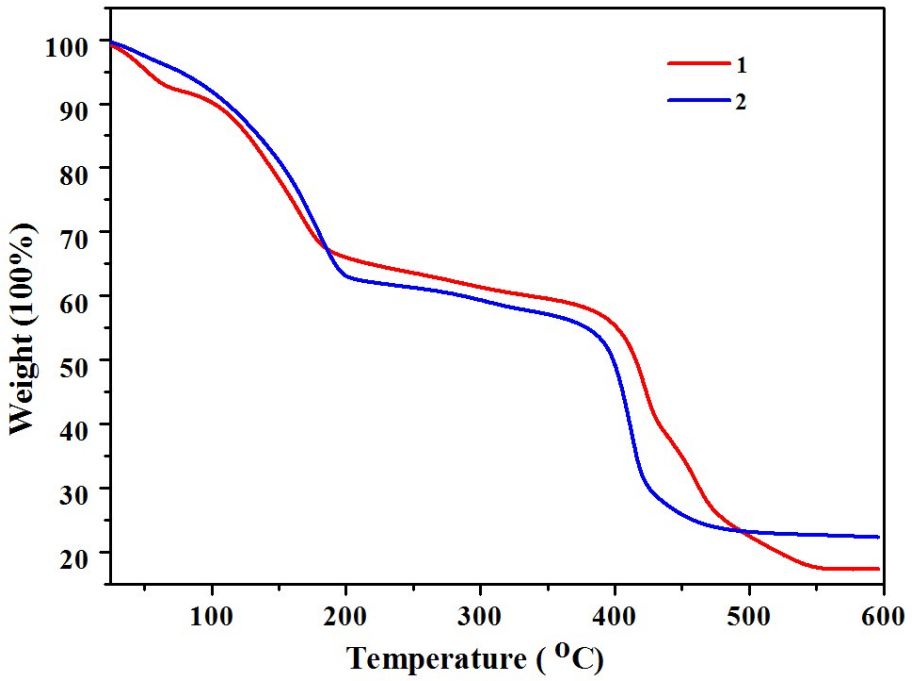


Fig. S5 TGA data of **1** and **2**.

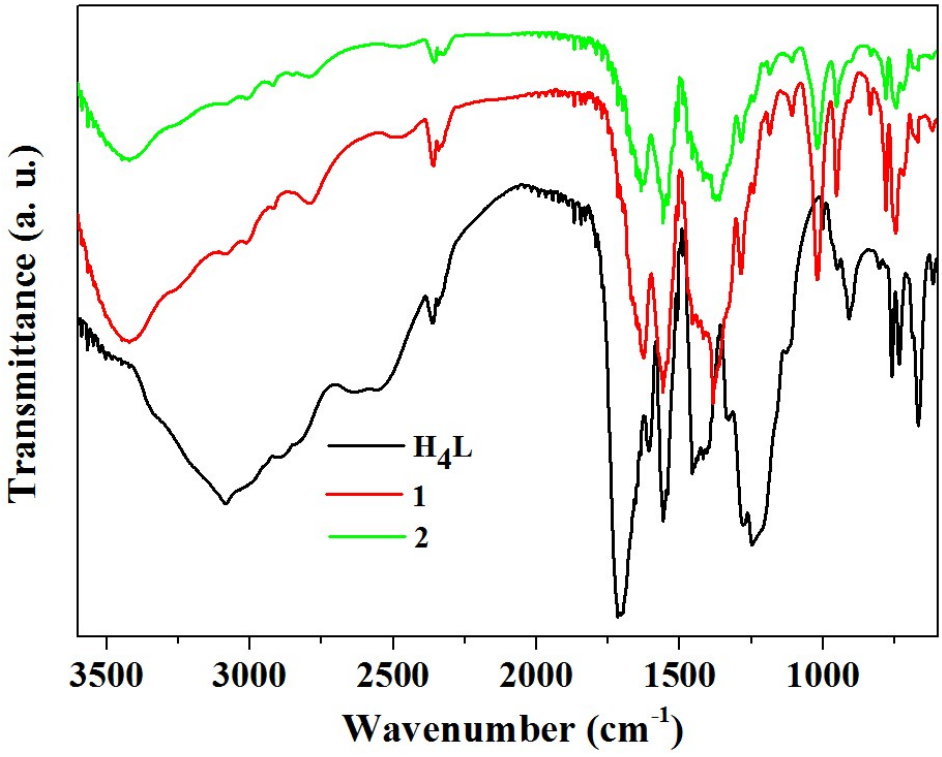


Fig. S6 The infrared spectra of H_4L, **1** and **2**.

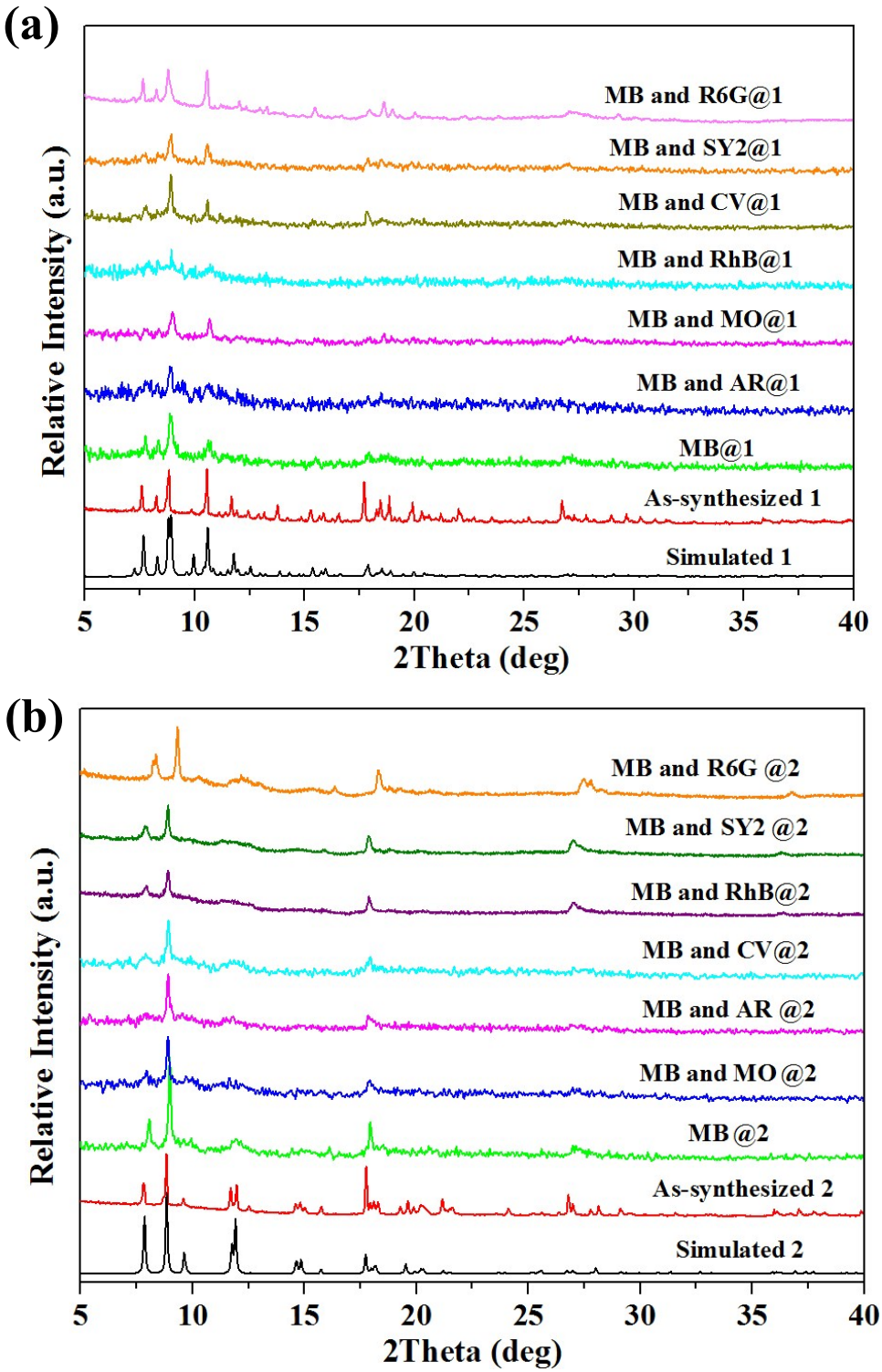


Fig. S7 PXRD patterns for **1** and **2**: a simulated PXRD pattern from the single-crystal structure, as-synthesized and after dye adsorption, respectively.

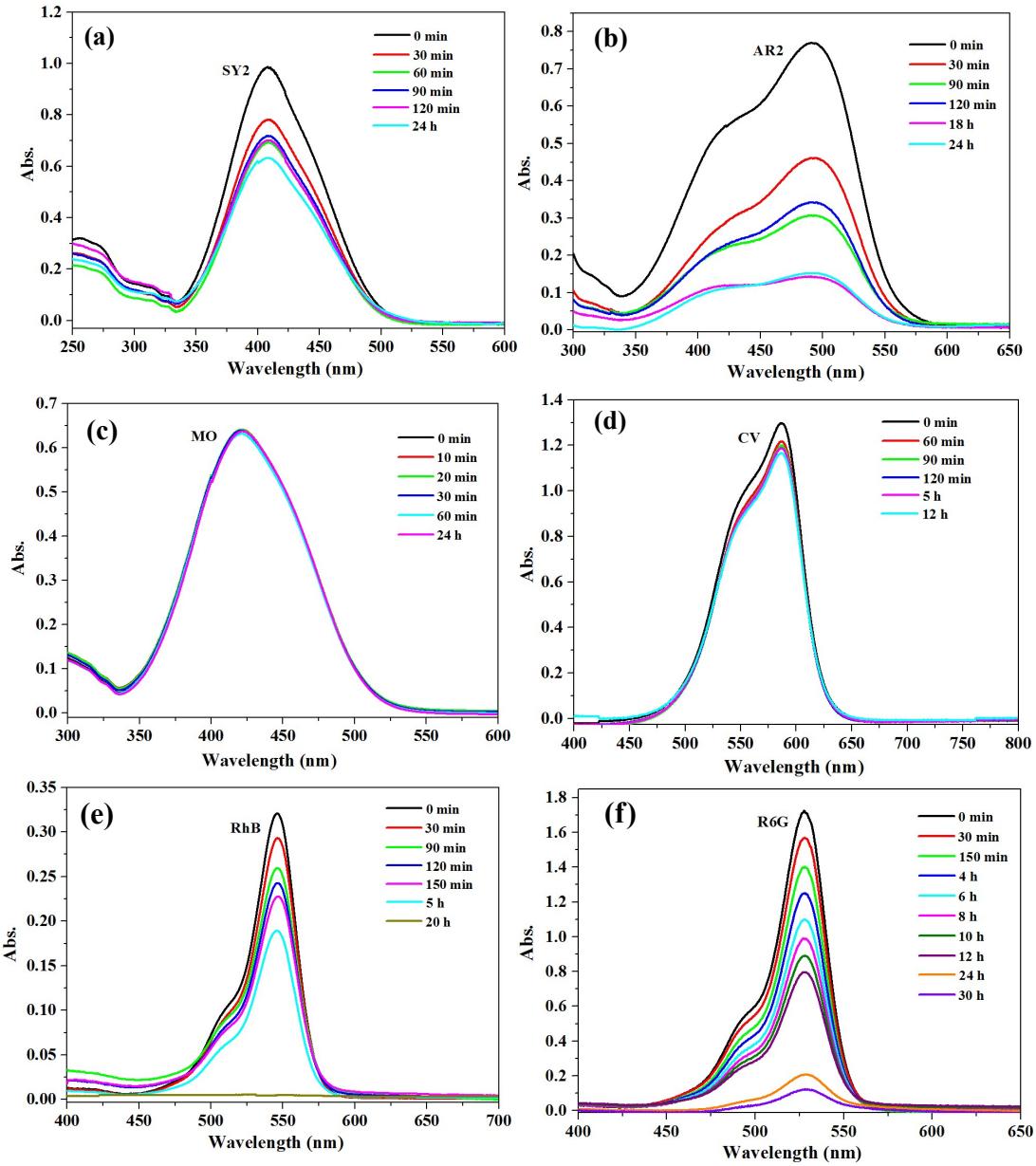


Fig. S8 UV-vis spectra of SY2 (a), AR2 (b), MO (c), CV (d), RhB (e) and R6G (f) in MeOH solution at different time during the adsorption with **1** as the host.

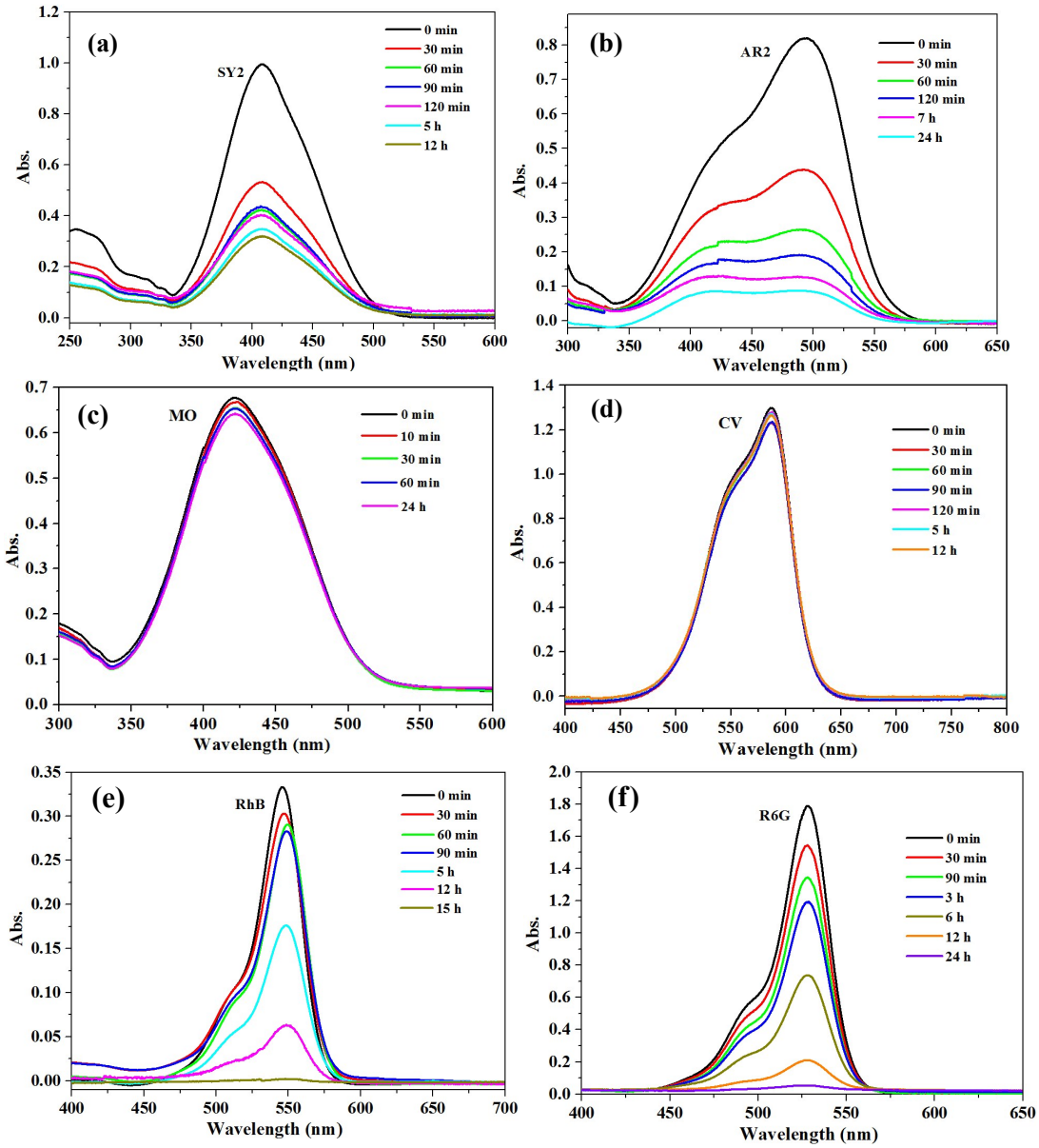


Fig. S9 UV-vis spectra of SY2 (a), AR2 (b), MO (c), CV (d), RhB (e) and R6G (f) in MeOH solution at different time during the adsorption with **2** as the host.

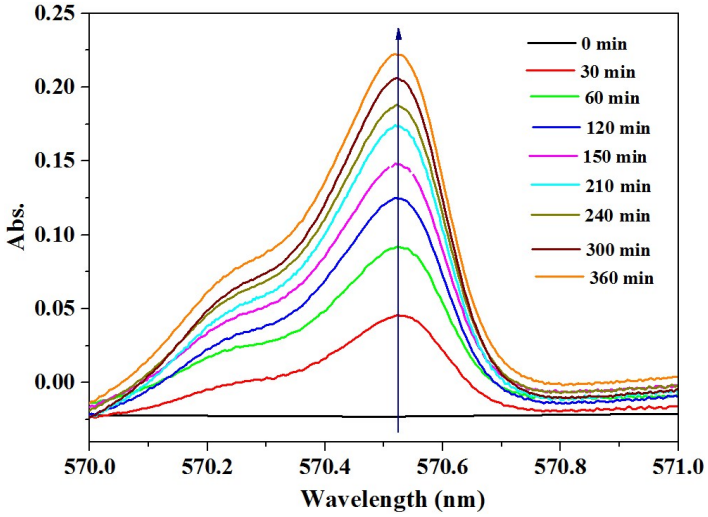


Fig. S10 The MB released from the **MB@2** in a saturated solution of NaCl in DMF monitored by UV-vis spectra.

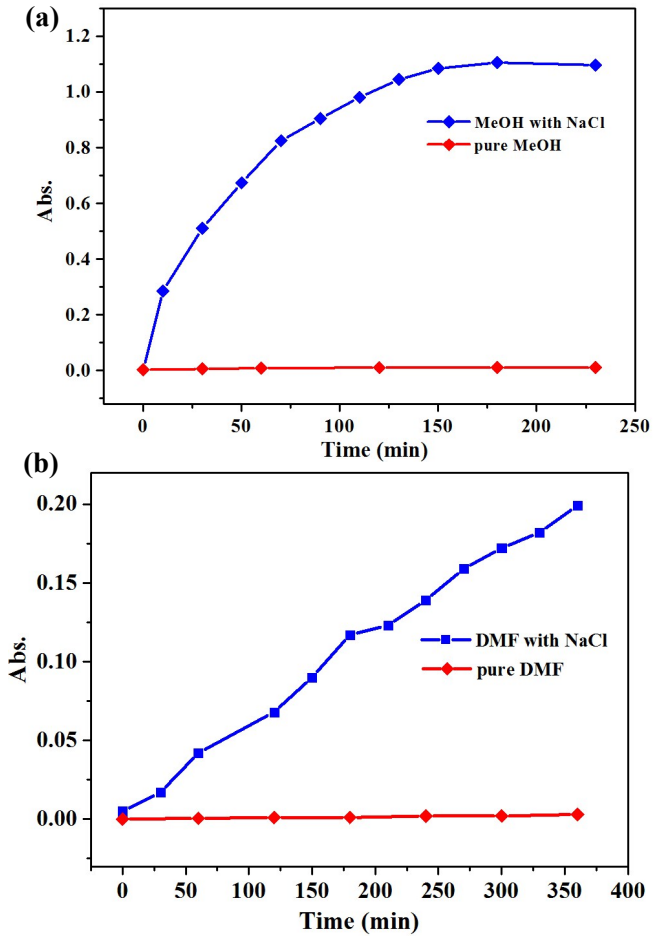


Fig. S11 The release-rate comparison of MB from **MB@1** (a) **and MB@2** (b) in pure MeOH and DMF, and a saturated solution of NaCl in MeOH and DMF, respectively.

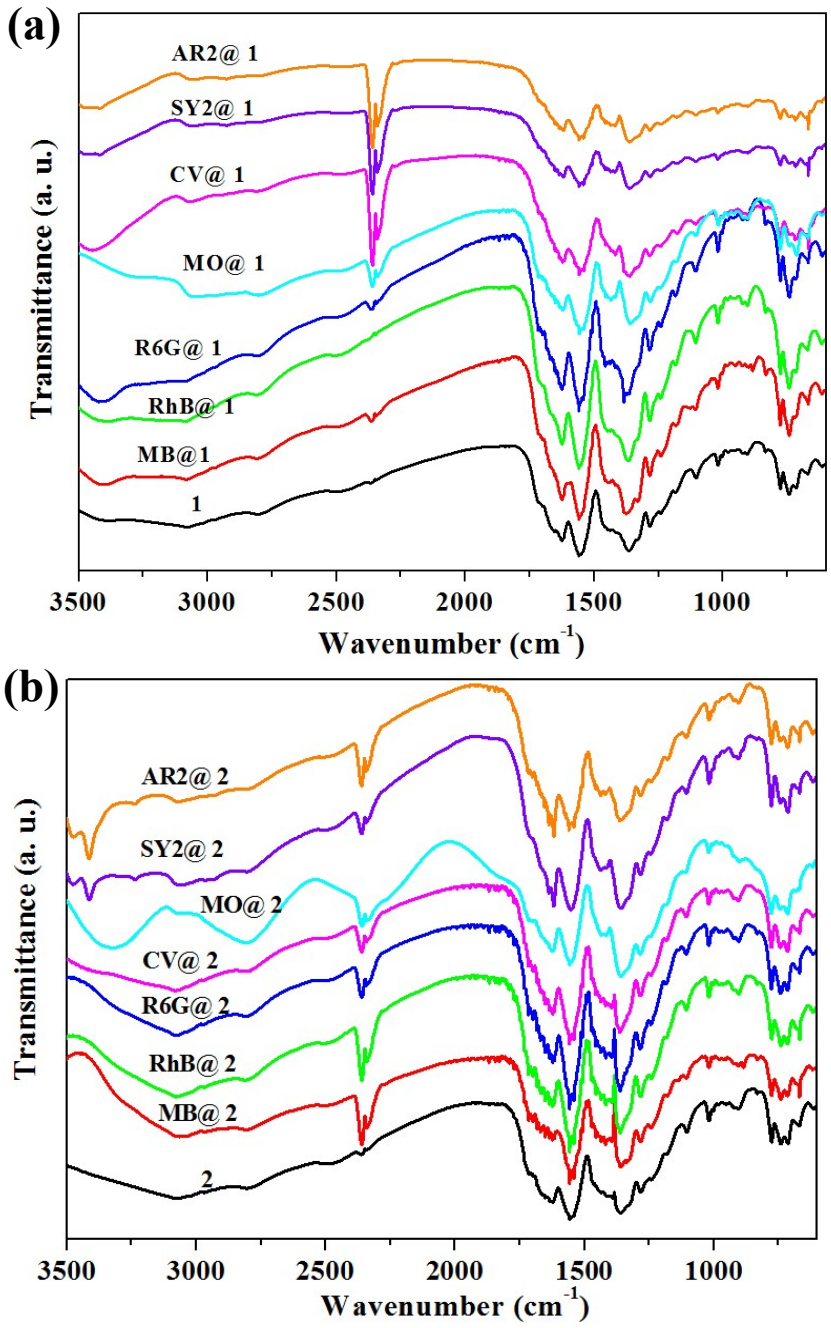


Fig. S12 The infrared spectra for **1** and **2** and after dyes adsorption, respectively.

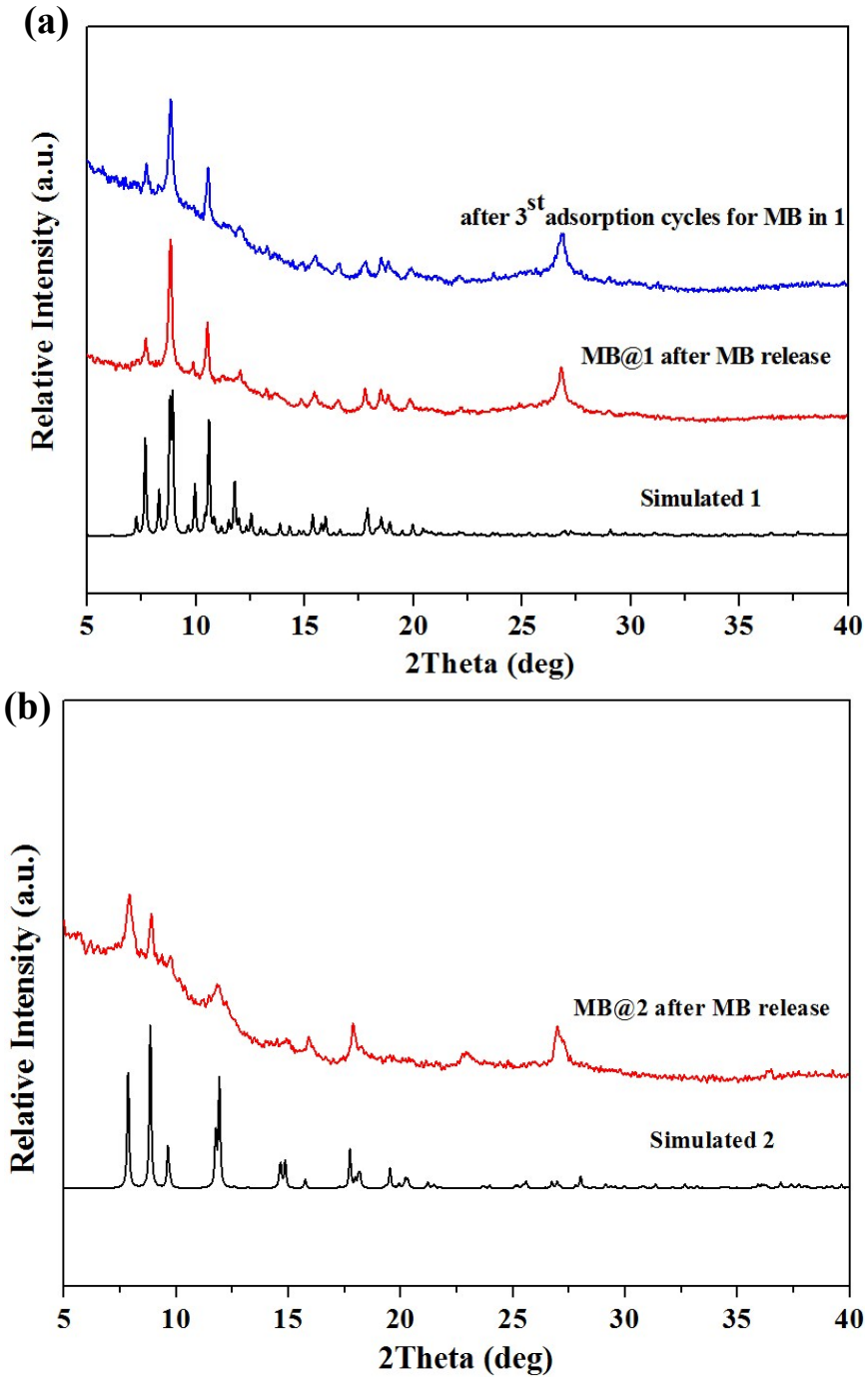


Fig. S13 (a) PXRD patterns for simulated **1, MB@1** after MB release in a saturated solution of NaCl in MeOH, and after 3st adsorption cycles for MB in **1**. (b) PXRD patterns for simulated **2**, and **MB@2** after MB release in a saturated solution of NaCl in DMF.

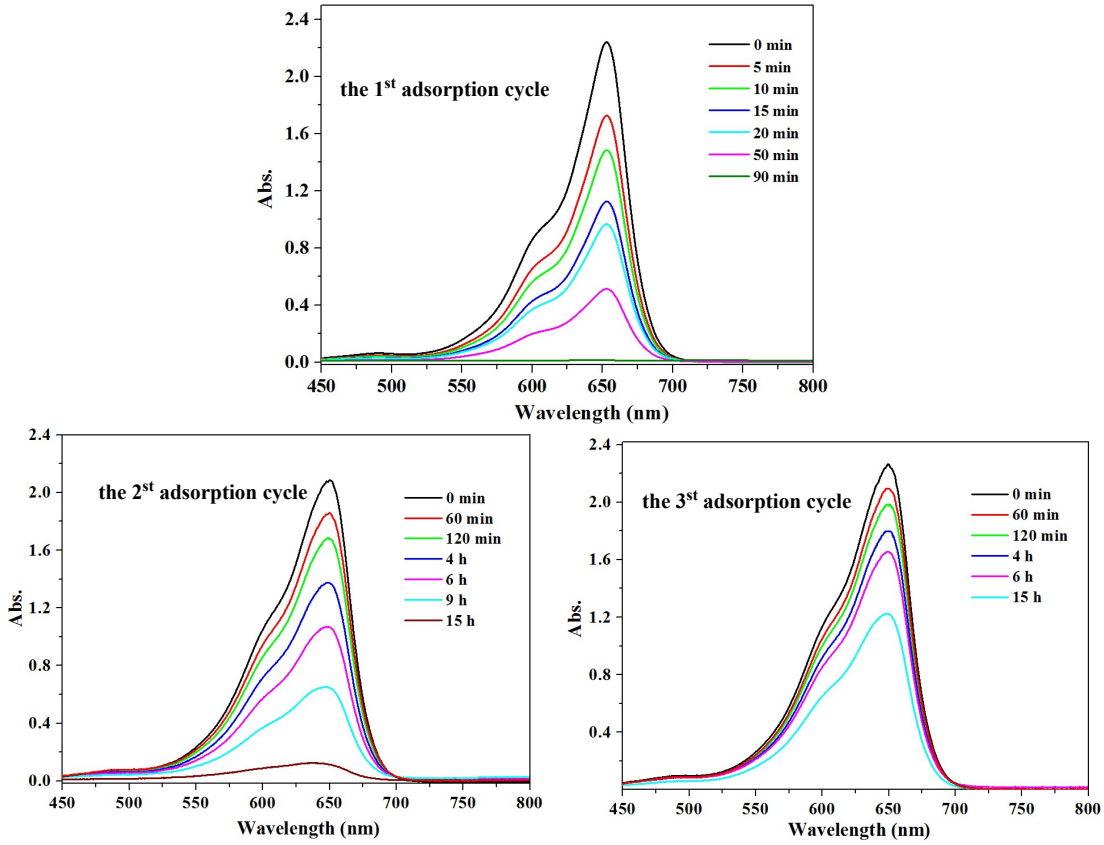


Fig. S14 UV-vis spectra of three adsorption cycles of **1** for MB.

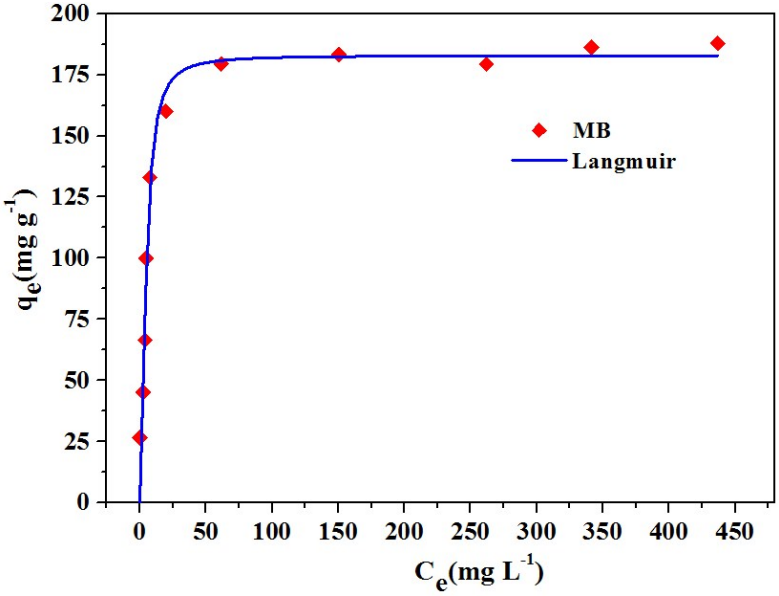


Fig. S15 Langmuir fitting plots for the adsorptions of MB on **2**.

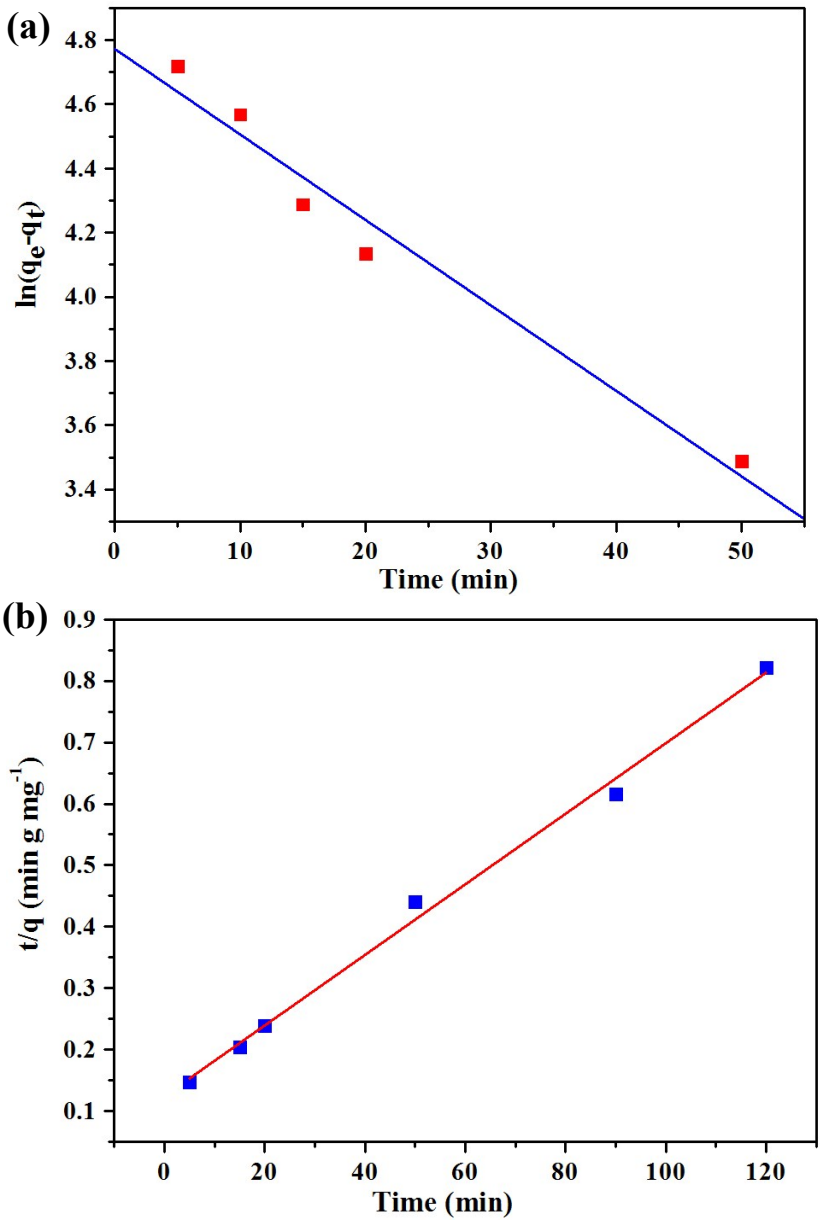


Fig. S16 Plots of pseudo-first-order (a) and pseudo-second-order (b) kinetics for the adsorption of MB on **1**.

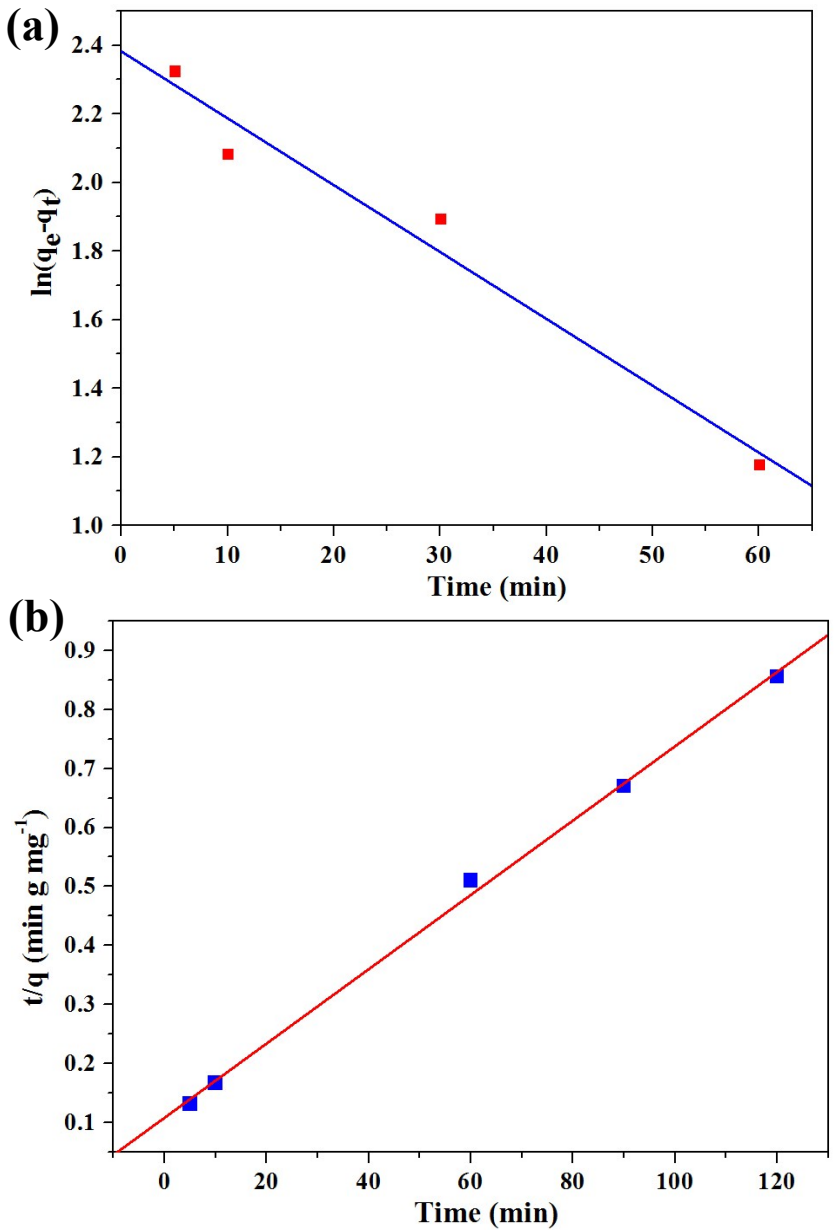
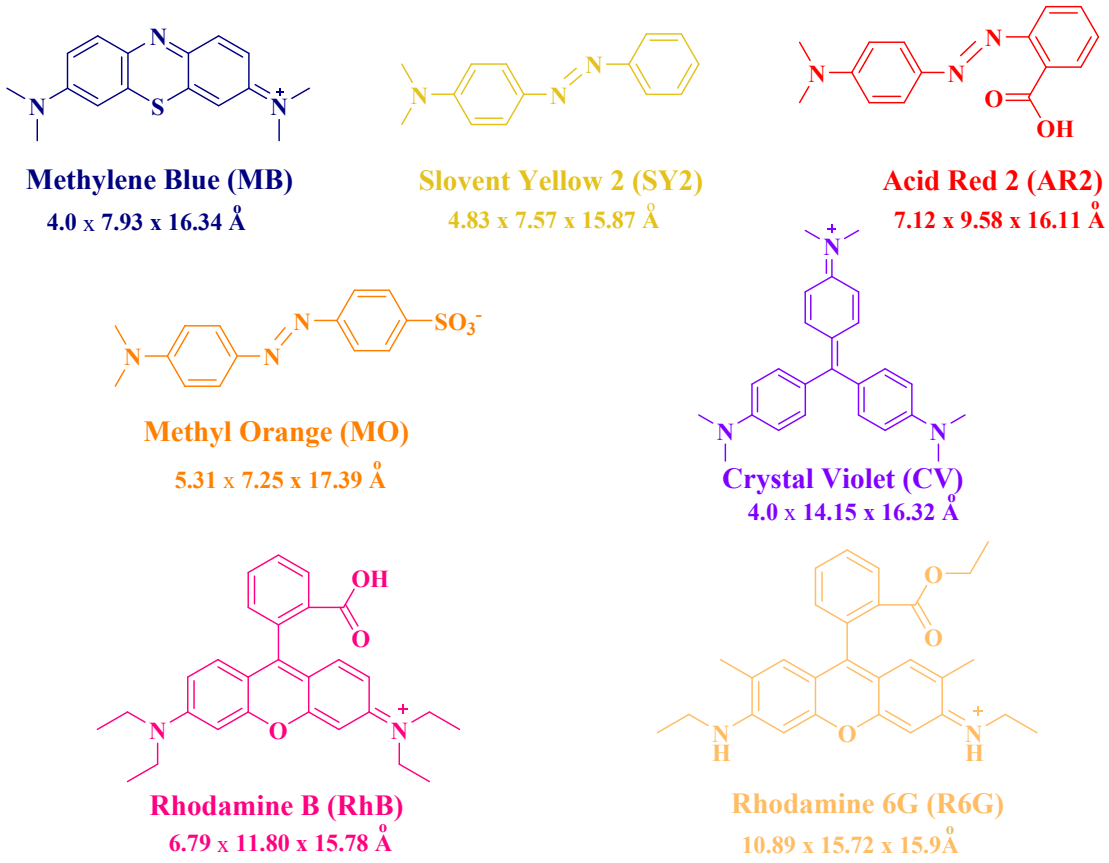


Fig. S17 Plots of pseudo-first-order (a) and pseudo-second-order (b) kinetics for the adsorption of MB on **2**.



Scheme S1 Schematic structural illustration of seven dyes used with different charged and dimension.

Table S1 Summary of adsorption efficiencies of **1** and **2** towards different dyes and proposed interaction mechanism between dyes and frameworks

dyes		adsorption efficiencies (adsorption time)		proposed interactions
		1	**2**	
cationic dyes	MB	99.6 (1.5 h)	99.0 (2 h）	electrostatic attractions
	CV	10.8 (8 h)	5.4 (8 h)	size-exclusion effect
	RhB	93.7 (20 h)	99.4 (14 h)	hydrogen-bonding interactions
	R6G	92.7 (30 h)	97.2 (24 h)	hydrogen-bonding interactions
neutral dyes	SY2	35.7 (24 h)	67.7 (7 h)	repulsive electrostatic effect
	AR2	80.4 (24 h)	83.6 (24 h)	repulsive electrostatic effect

anionic dyes	MO	1.5 (24 h)	6.0 (24 h)	repulsive electrostatic effect

Table S2 Comparison of adsorption capacities of MB obtained in this study with various materials reported in literature.

adsorbents	dye	adsorption capacity (mg g^{-1})	reference
activated carbon	MB	263.2	1
GO	MB	243.9	1
muli-walled CT	MB	196.1	1
OND-4.5	MB	47.6	2
activated carbon	MB	26.0	3
MOF-235	MB	187	3
UiO-66	MB	90.9	4
NH_2-UiO-66	MB	96.5	4
NH_2-MIL-101-SO_3H	MB	141	5
JLU-liu39	MB	308	6
$\{[Cd_2(BPTC)(DMA)_2(DMPU)_{0.5}(H_2O)_{0.5}](DMPU)_{0.5}\}_n$	MB	73.0	7
$\{[Cd_4(BPTC)_2(DMA)_4(H_2O)_2](DMA)\}_n$	MB	79.4	7
$[(CH_3)_2NH_2]_{1.5}[Tb_{1.5}(TATAT)(H_2O)_{4.5}]\cdot x(solvent)$	MB	147	8
1	MB	281	This work
2	MB	181	This work

Table S3 Kinetic parameters for the adsorption of MB on **1** and **2**.

MOFs	pseudo-first-order model			pseudo-second-order model		
	k_1 (min^{-1})	R^2	q_e (cal.) (mg g^{-1})	k_2 (g mg^{-1} min^{-1})	R^2	q_e (cal.) (mg g^{-1})
1	2.66×10^{-2}	0.95485	11.8	2.54×10^{-3}	0.99422	17.4
2	1.95×10^{-2}	0.95311	10.8	3.67×10^{-4}	0.99741	15.9

Reference

(1) Y. Li, Q. Du, T. Liu, X. Peng, J. Wang, J. Sun, Y. Wang, S. Wu, Z. Wang, Y. Xia and L. Xia, *Chem. Eng. Res. Des.*, 2013, **91**, 361.

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