

## Supporting Information

### Water-stable Zeolite-like Metal-Organic Framework for Selective Separation of Organic Dyes

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## Materials and Instrumentation

All reagents were purchased commercially and used without further purification. All Powder X-ray diffraction (PXRD) analyses were recorded on a Rigaku Dmax2500 diffractometer with Cu K $\alpha$  radiation ( $\lambda = 1.54056 \text{ \AA}$ ) with a step size of  $0.05^\circ$ . Thermal stability studies were carried out on a NETSCHZ STA-449C thermoanalyzer with a heating rate of  $10 \text{ }^\circ\text{C}/\text{min}$  under an air atmosphere. Gas adsorption measurement was performed in the ASAP (Accelerated Surface Area and Porosimetry) 2020 System. High-performance liquid chromatography (HPLC) separation experiment was performed in LC-20AD System.

**Synthesis of [AgIn(ina)<sub>4</sub>] $\cdot$ 2DMF (1):** Hina (246 mg, 2 mmol), AgNO<sub>3</sub> (85 mg, 0.5 mmol) and In(NO<sub>3</sub>)<sub>3</sub> (150 mg, 0.5 mmol) were dissolved in 5 mL DMF, which were placed in a small vial. The mixture was heated at  $100 \text{ }^\circ\text{C}$  for 8 hours, and then cooled to room temperature. Colorless block crystals of the product were formed and collected by filtration and washed with DMF several times (Yield: 75% based on H<sub>2</sub>ina).

**Synthesis of [CuIn(ina)<sub>4</sub>] $\cdot$ 2DMF (2):** Hina (246 mg, 2 mmol), CuI (95 mg, 0.5 mmol) and In(NO<sub>3</sub>)<sub>3</sub> (150 mg, 0.5 mmol) were dissolved in 5 mL DMF, which were placed in a small vial. The mixture was heated at  $100 \text{ }^\circ\text{C}$  for 3 days, and then cooled to room temperature. Red block crystals of the product were formed and collected by filtration and washed with DMF several times (Yield: 43% based on H<sub>2</sub>ina).

**X-ray diffraction analysis:** The diffraction data for compounds were collected on an Oxford Xcalibur diffractometer equipped with a graphite-monochromatized Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 293(2) K. The structures were solved by direct methods and refined on  $F^2$  by full-matrix, least-squares methods using the SHELXL-97 program package. CCDC-902245 & 902246 (1 and 2) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via [www.ccdc.cam.ac.uk/conts/retrieving.html](http://www.ccdc.cam.ac.uk/conts/retrieving.html).

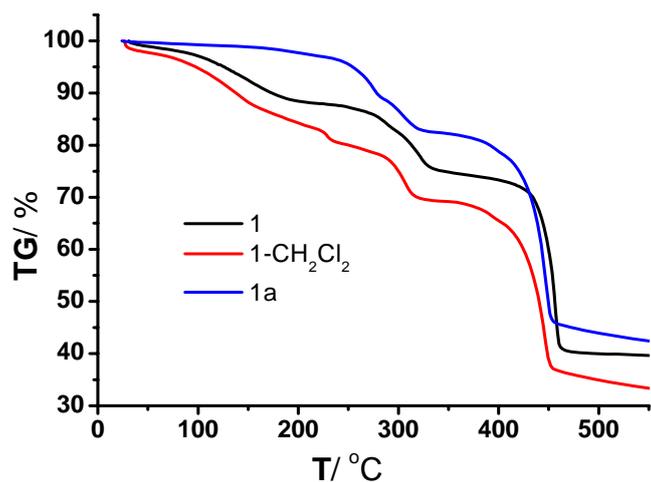


Figure S1. The TG plots of **1**, CH<sub>2</sub>Cl<sub>2</sub>-exchanged **1** and hollow phase of **1a**.

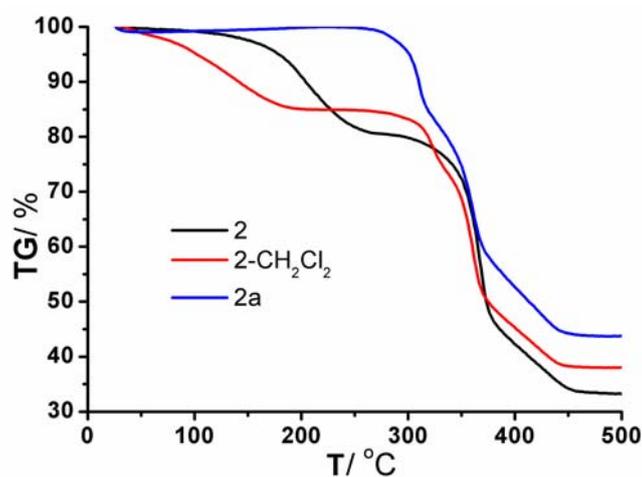


Figure S2. The TG plots of **2**, CH<sub>2</sub>Cl<sub>2</sub>-exchanged **2** and hollow phase of **2a**.

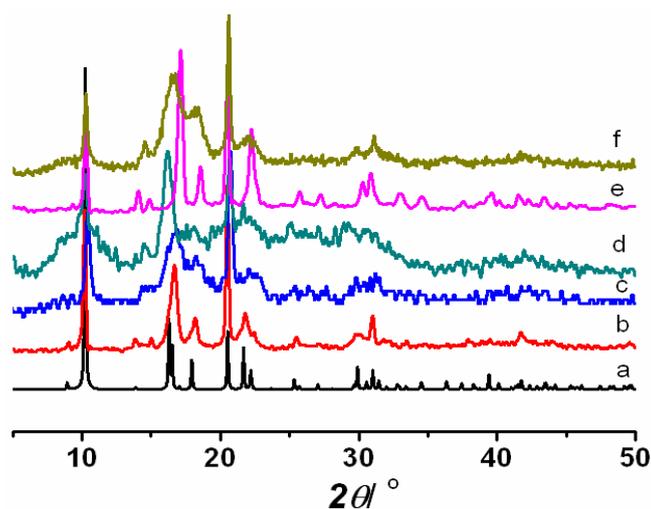


Figure S3. PXRD patterns: a) simulated from the single-crystal data of **1**, b) as-synthesized **1**, c) hollow phase of **1a**, d) MO-loading phase of **1a'**, e) the sample of **1a'** soaked in DMSO and f) the sample of **1a** soaked in water.

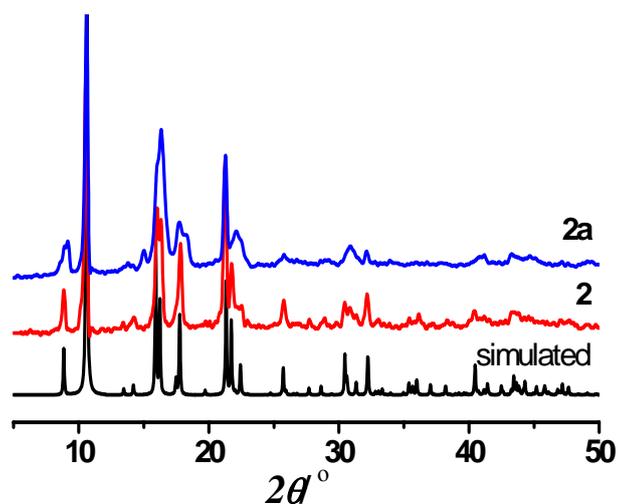


Figure S4. PXRD patterns: simulated from the single-crystal data of **2**, as-synthesized **2**, hollow phase of **2a**.

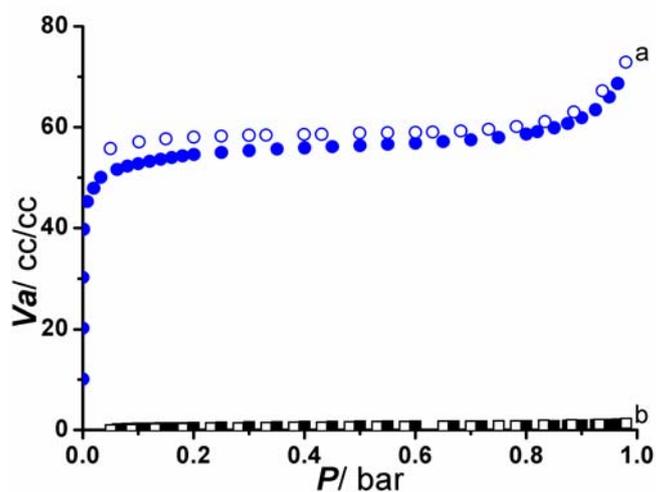


Figure S5.  $N_2$  sorption isotherms at 77 K for **1a** (b) and **2a** (a).

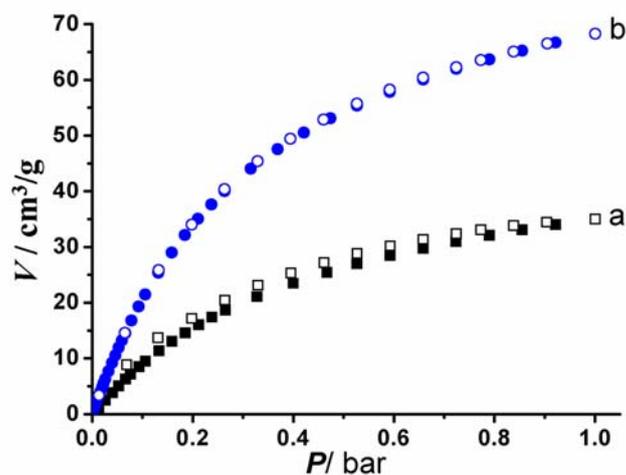


Figure S6.  $CO_2$  sorption isotherms: a)  $CO_2$  at 273 K for **1a**; b)  $CO_2$  at 273 K for **2a**.



Figure S7. Photos of MO enrichment progress over **2a** in 6 mins.

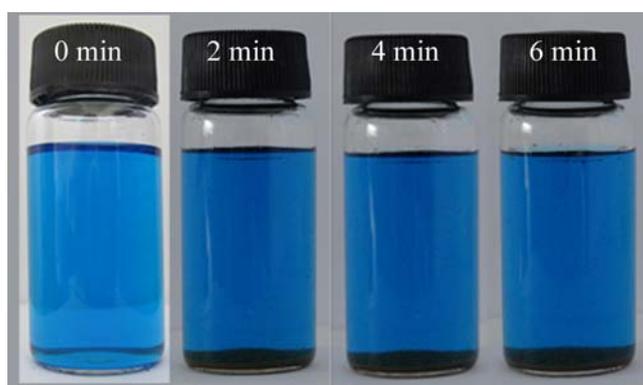


Figure S8. Photos of MB enrichment progress over **2a** in 6 mins.

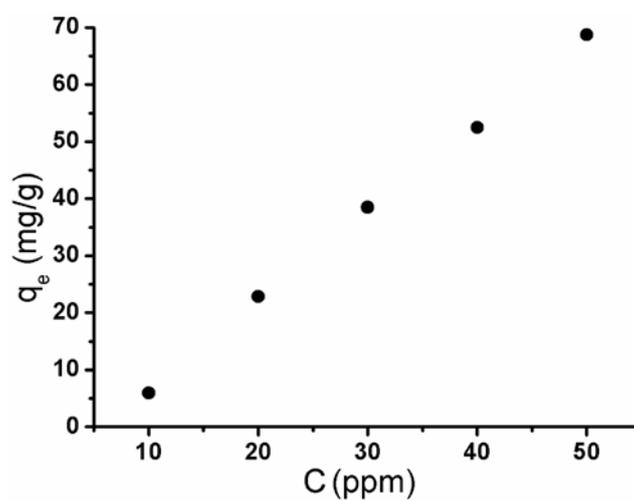


Figure S9. Adsorption isotherm for MO adsorption over **1a**.

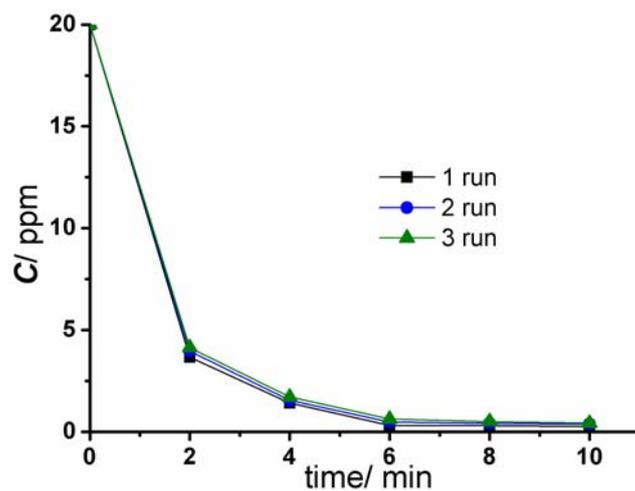


Figure S10. Measured concentration curves of MO enrichment progress over **1a**. A recycling test with three consecutive runs.

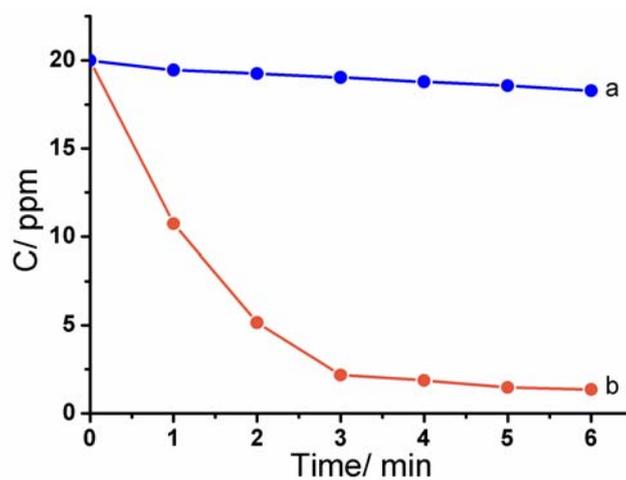


Figure S11. The concentrations of mixed MB (a) and MO (b) in water solution.

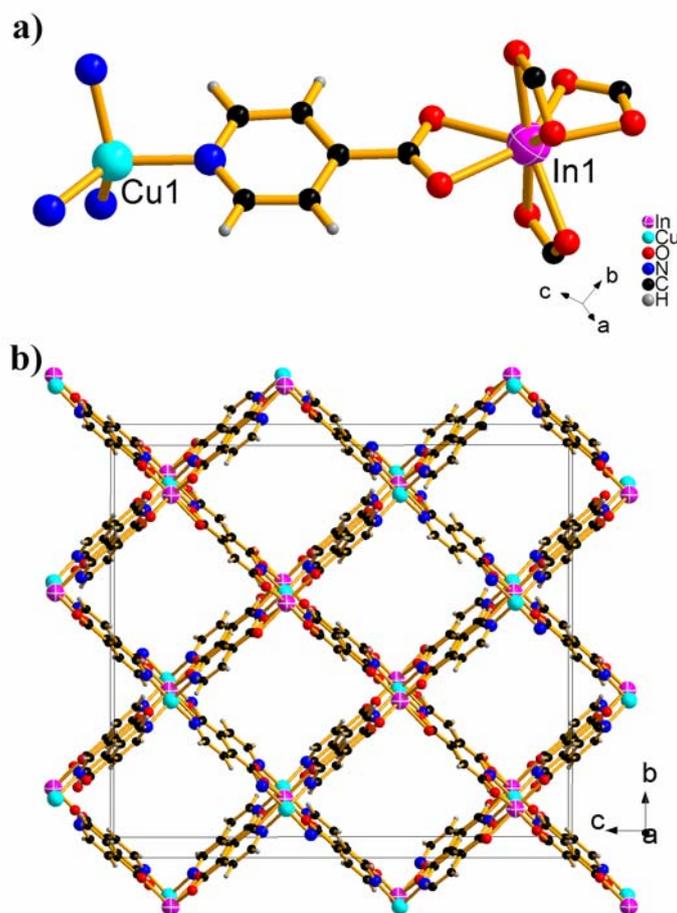


Figure S12. (a) Two tetrahedral building units ( $[\text{CuN}_4]^+$  and  $[\text{In}(\text{COO})_4]^-$ ) linked by the ina ligand in **2**; (b) The 3D framework of **2**.