Supporting information

pH-Induced different crystalline behaviors in extended metal–organic frameworks based on the same reactants

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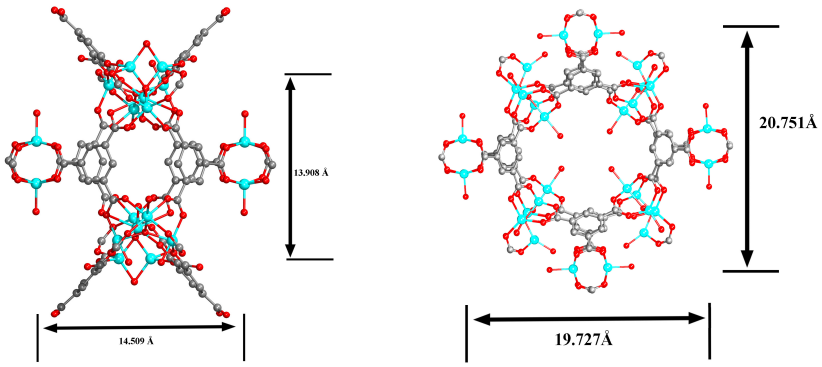

Fig. S1 The size of two kinds of cages (**A** and **B**) of compound **2**. Some of the coordination molecules are omitted for clearly.

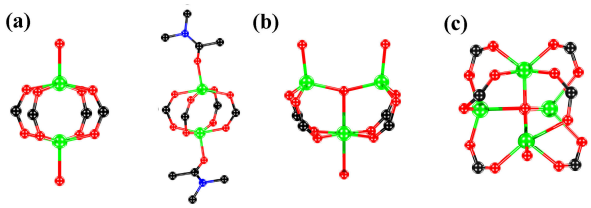

Fig. S2 Three kinds of Zn-SBUs in compound **2**.

Preparation of desolvated 2

The bulky crystals of **2** were immersed in the dichloromethane. After 24 h, the CH_2Cl_2 was decanted from the vial and fresh CH_2Cl_2 was added. The solution was replaced with fresh CH_2Cl_2 every 24 h for a total of 3 days and the crystals were stored in CH_2Cl_2 until further used. Finally, the sample was heated at 120 °C for 24

hours in vacuum.

Drug Loading Dissolving 5-FU (40 mg) and desolvated **2** (20 mg) in methanol (10 mL) three days yielded heterogeneous solution. The precipitation was isolated by centrifuging and washed with methanol. After that, the precipitation dried at room temperature. The 5-FU content was calculated using UV method (λ = 264 nm).

Drug Release The same accounts of drug-loaded **2** (10 mg) was dissolved into 1.5 mL of PBS buffer solution (pH 7.4) and acetate buffer (pH 5.0) respectively, and loaded into a dialysis bag, which was dialyzed against 8 mL of deionized water at 37°C. During each time interval, about 1 mL of the solution was pulled out to test, and decanted back when the test was over. The content of 5-FU in the samples taken out was monitored by fluorometry, in which the detection wavelength was 453 nm.

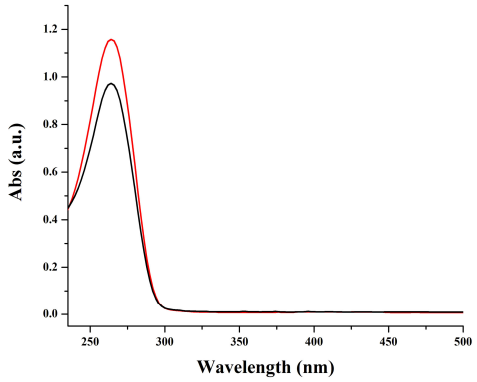

Fig. S3 The UV–Vis absorption spectra of 5-FU methanol solution before and after the interaction with **2**.

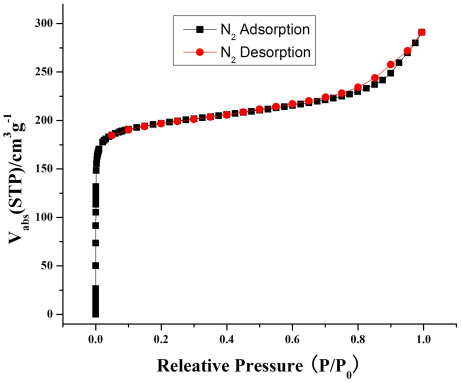

Fig. S4 N_2 sorption isotherms of **2**.

Table S1. Estimated 5-Fu content under several impregnation parameters

Impregnation parameters		g 5-FU/g dehydrated **2**
5-FU/**2** weight ratio	1:1	0.156
	3:2	0.227
	2:1	0.288
Immersion time (days)	1	0.154
	2	0.214
	3	0.288

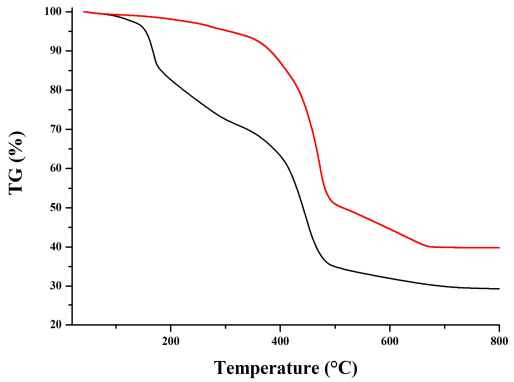

Fig. S4 TG profile of **2** (black: synthesized; red: desolvated).

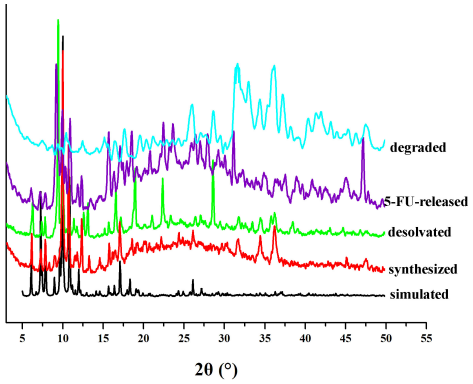

Fig. S5 Experimental and simulated powder X-Ray diffraction patterns for **2**. The purple and cyan lines represent the PXRD patterns of **2** after the drug release experiments in PBS (pH 7.4) and acetate buffer (pH 5.0).