

Supporting Information

An Anionic Potassium-Organic Framework for Selective Removal of Uranyl Ions

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Table S1. Crystallographic data of UPC-K1.

empirical formula	C ₅₆ H ₄₂ NO ₈ K
formula weight	896.03
temperature (K)	293(2)
crystal system	Orthorhombic
space group	<i>C</i> 222(1)
<i>a</i> (Å)	10.2471 (2)
<i>b</i> (Å)	43.0335 (8)
<i>c</i> (Å)	10.3618 (2)
<i>α</i> (deg)	90
<i>β</i> (deg)	90
<i>γ</i> (deg)	90
volume (Å ³)	4569.23(15)
<i>Z</i>	4
ρ _{calc} (g/cm ³)	1.302
μ (mm ⁻¹)	1.494
<i>F</i> (000)	1872
Data/ restraints/parameters	4351/31/318
GOF on <i>F</i> ²	1.035
Independent reflections	4351 [<i>R</i> _{int} = 0.0236, <i>R</i> _{sigma} = 0.0195]
Final <i>R</i> indexes [<i>I</i> ≥ 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0424, <i>wR</i> ₂ = 0.1232
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0449, <i>wR</i> ₂ = 0.1274
Flack parameter	0.013(5)
<i>N</i> _{ref}	4351

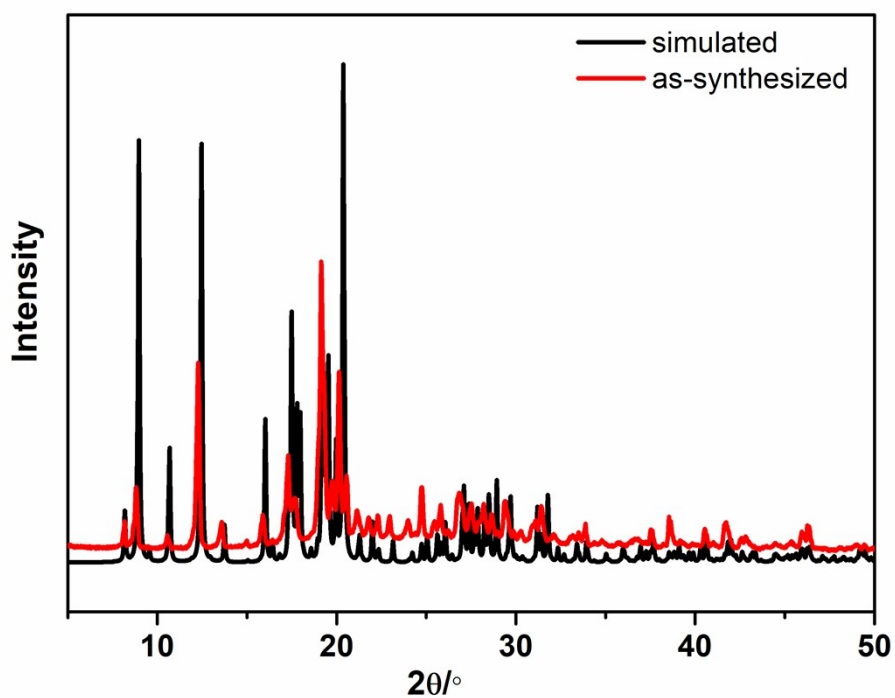


Fig. S1 The simulated (black) and as-synthesized (red) PXR D patterns of UPC-K1.

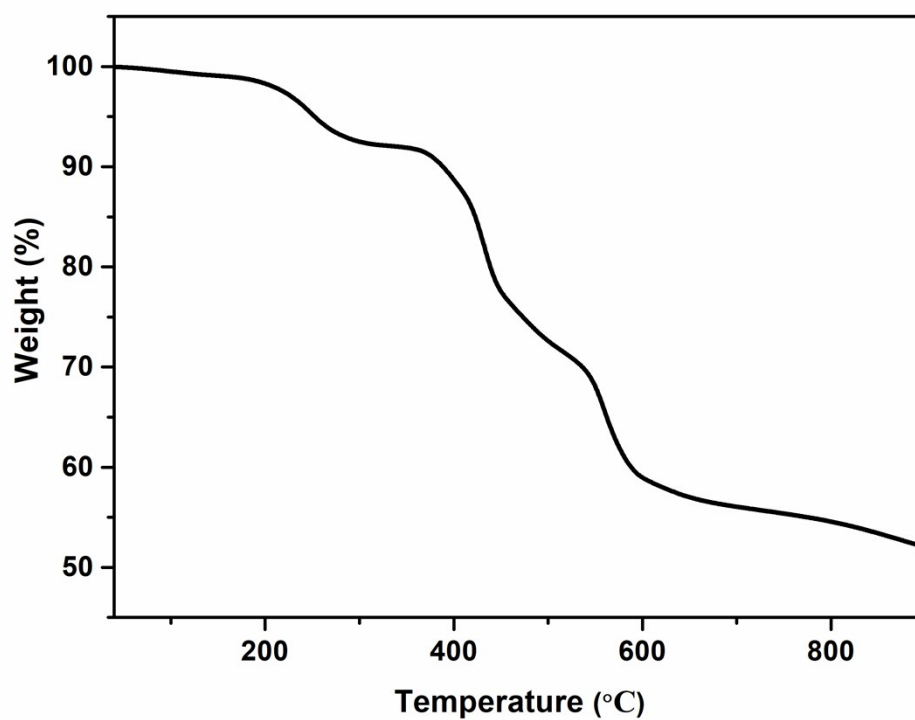


Fig. S2 TGA curve of UPC-K1.

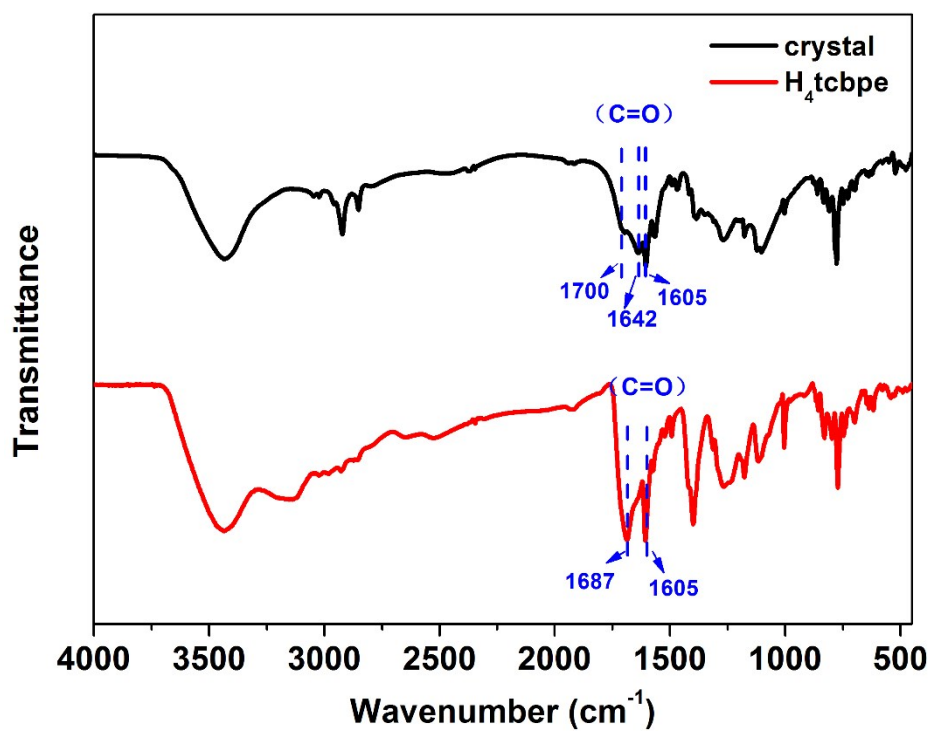


Fig. S3 IR spectra of H₄tcbpe and UPC-K1.

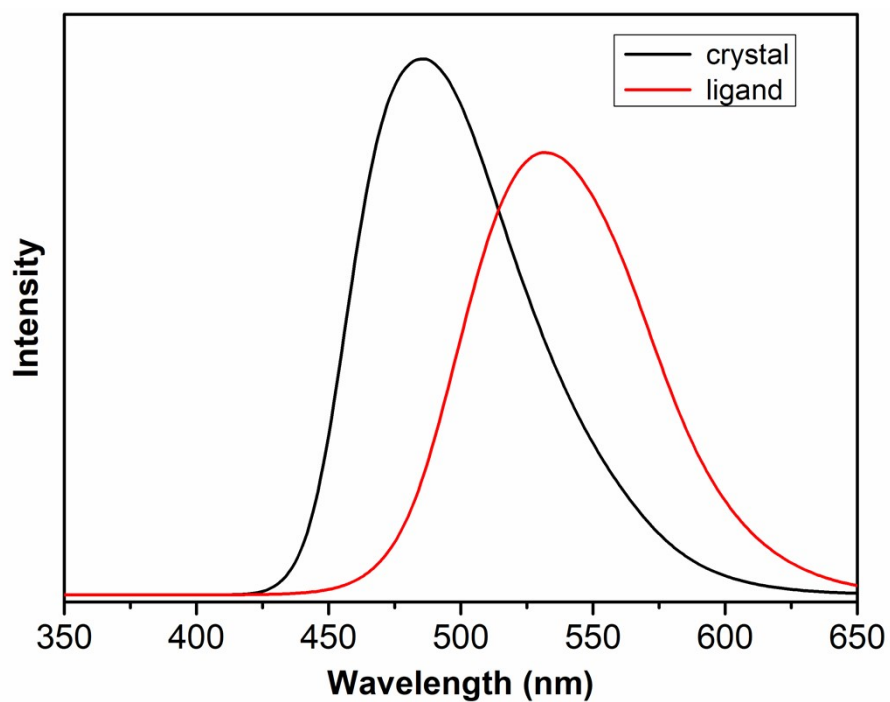


Fig. S4 The fluorescent spectra of H₄tcbpe and UPC-K1 in the solid state at room temperature.

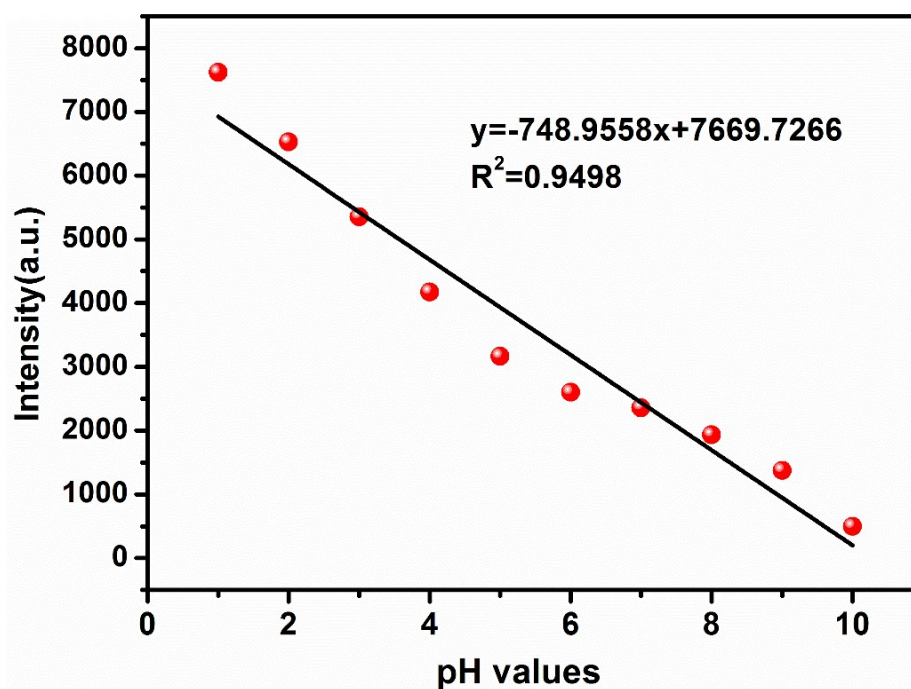
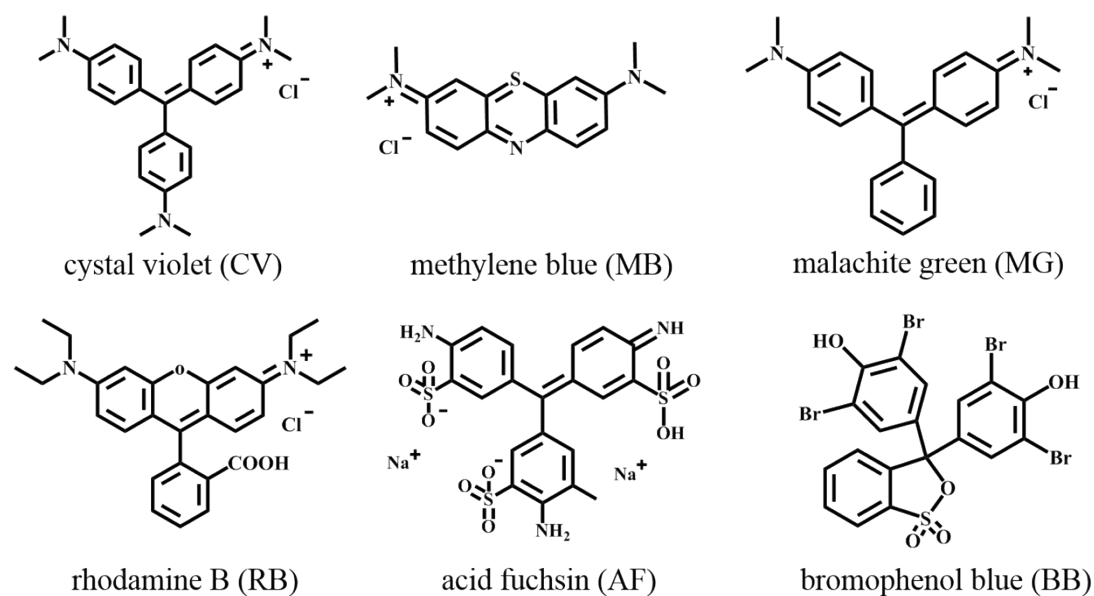


Fig. S5 The linear relation between the peak intensities of fluorescent spectra and the related pH values of solutions after immersing 2 mg of UPC-K1 in 2 mL of different pH value aqueous solutions.



Scheme S1. Schematic molecular structures of crystal violet (CV), methylene blue (MB), malachite green (MG), rhodamine B (RB), acid fuchsin (AF) and bromophenol blue (BB).

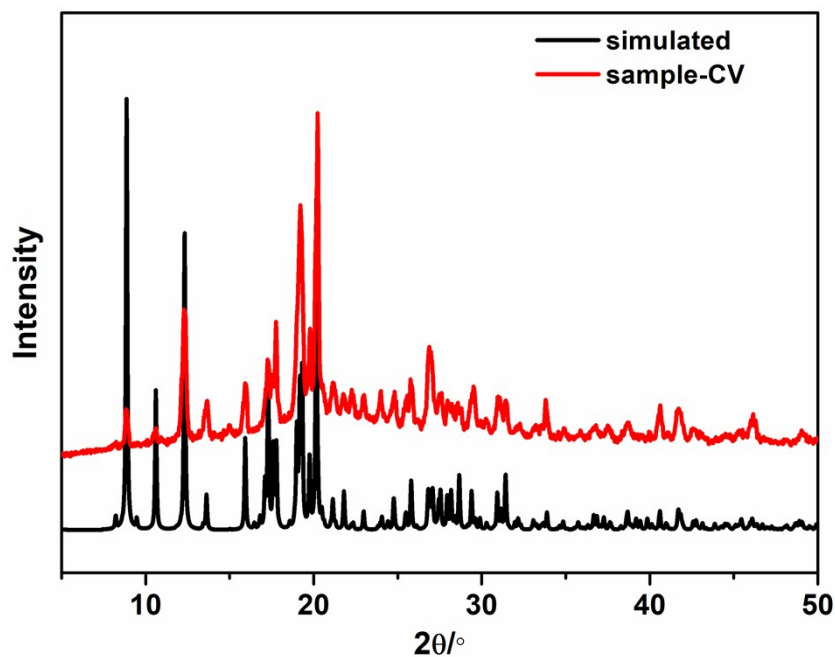


Fig. S6 The PXR D patterns of UPC-K1 before (black) and after (red) adsorbing crystal violet (CV).

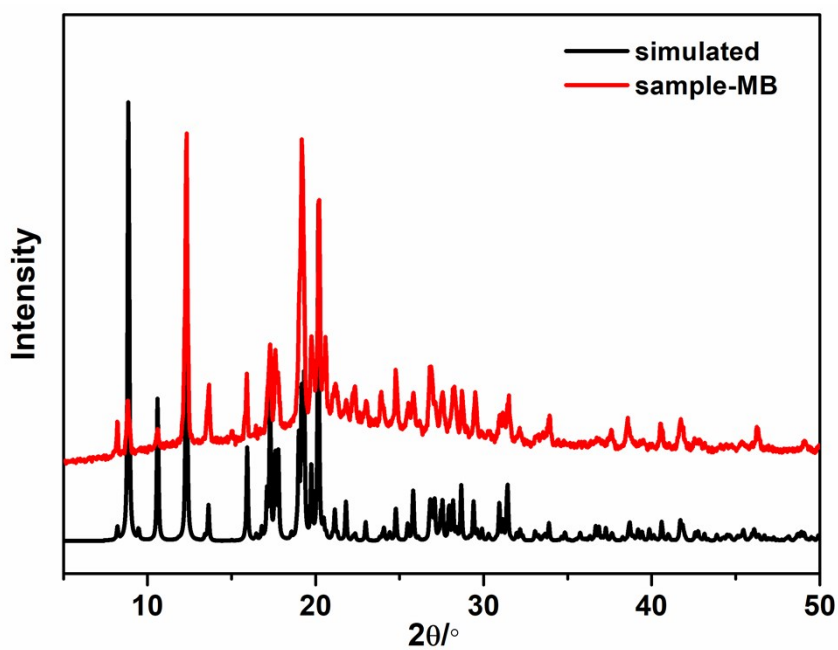


Fig. S7 The PXR D patterns of UPC-K1 before (black) and after (red) adsorbing methylene blue (MB).

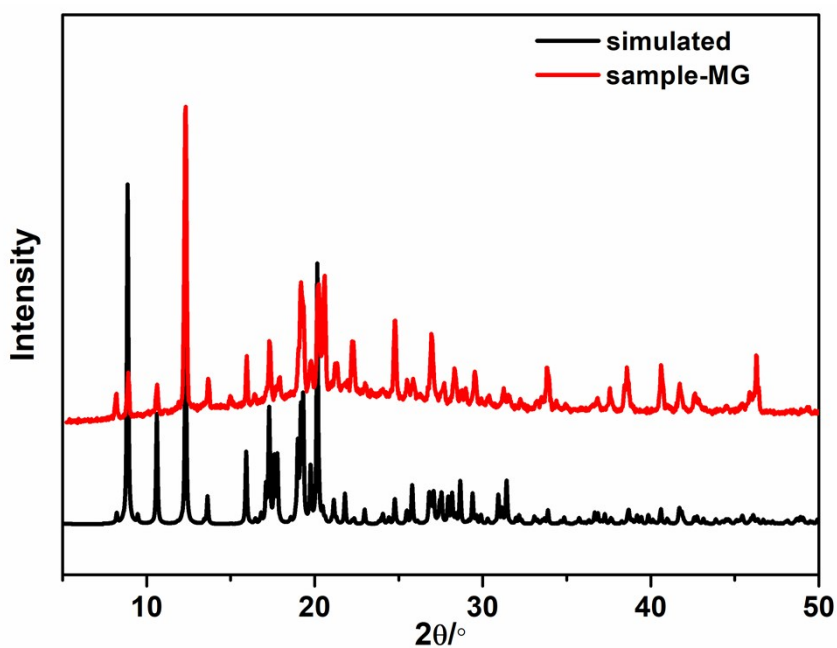


Fig. S8 The PXRD patterns of UPC-K1 before (black) and after (red) adsorbing malachite green (MG).

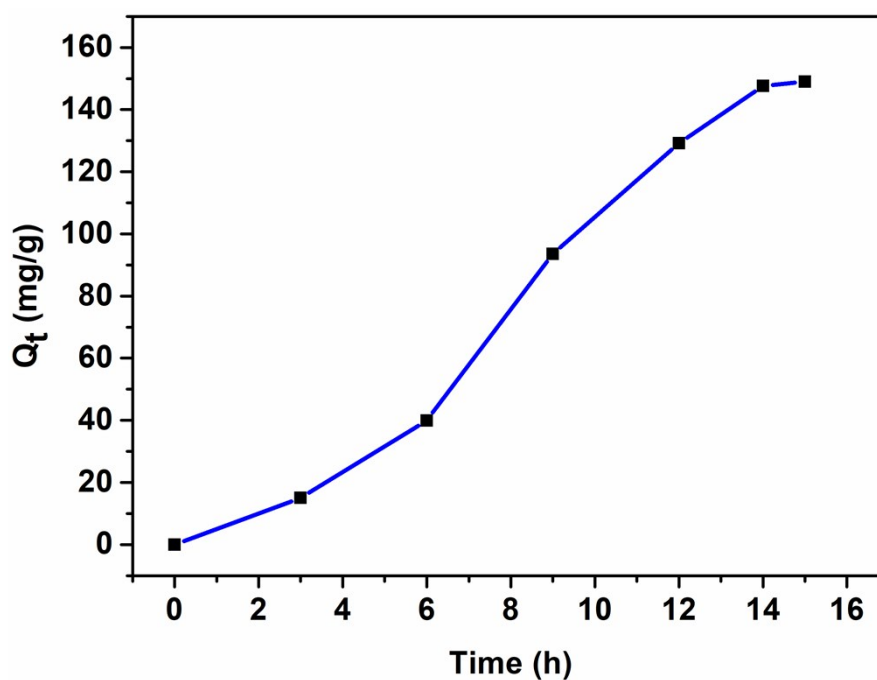


Fig. S9 The UO_2^{2+} adsorption quantity (Q_t) in different times after immersing 30 mg of UPK-1 into 4 mL of 2.2 mmol/L $\text{Zn}(\text{UO}_2)_2(\text{CH}_3\text{OO})_6$ aqueous solutions.

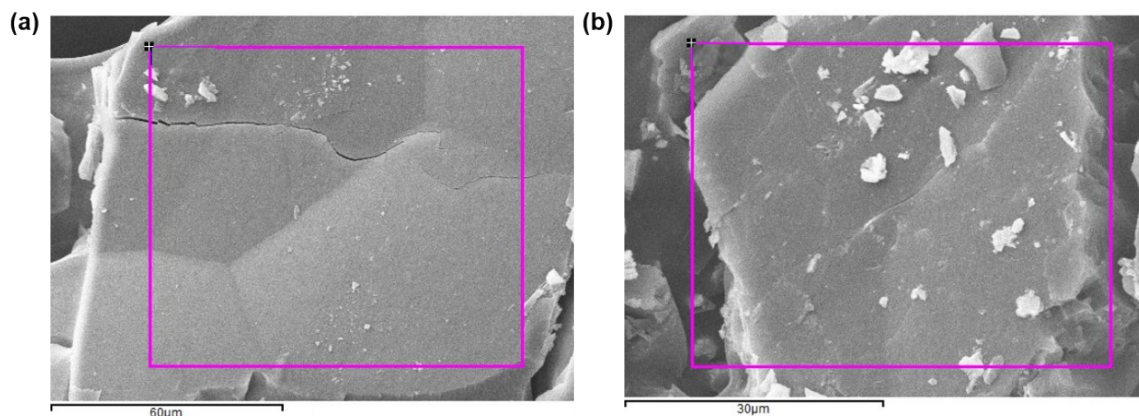


Fig. S10 The SEM images of UPC-K1 (30 mg) before (a) and after (b) adsorbing UO_2^{2+} in 4 mL of 2.2 mmol/L uranyl zinc acetate solution for 15 hours.

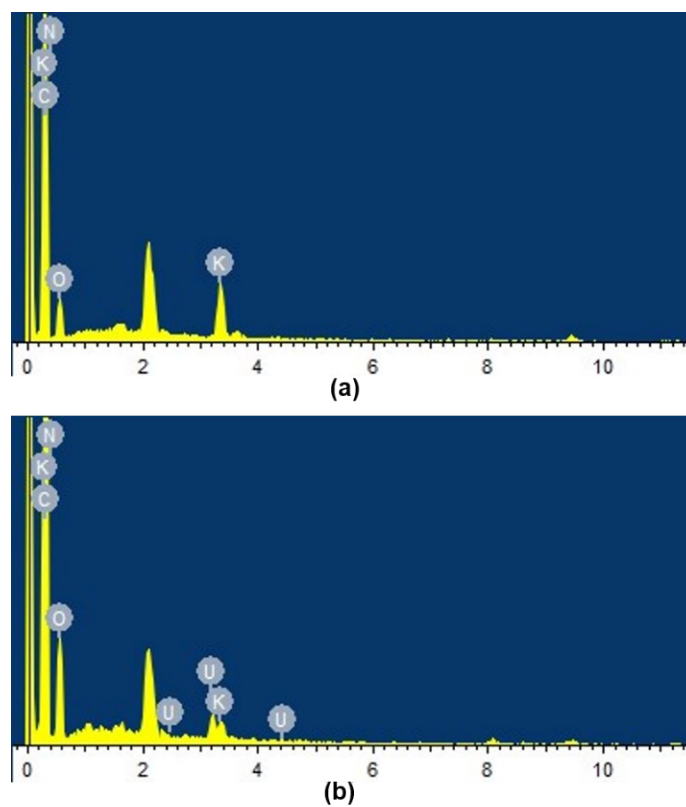


Fig. S11 The EDS spectra of UPC-K1 (30 mg) before (a) and after (b) adsorbing UO_2^{2+} in 4 mL of 2.2 mmol/L uranyl zinc acetate solution for 15 hours.

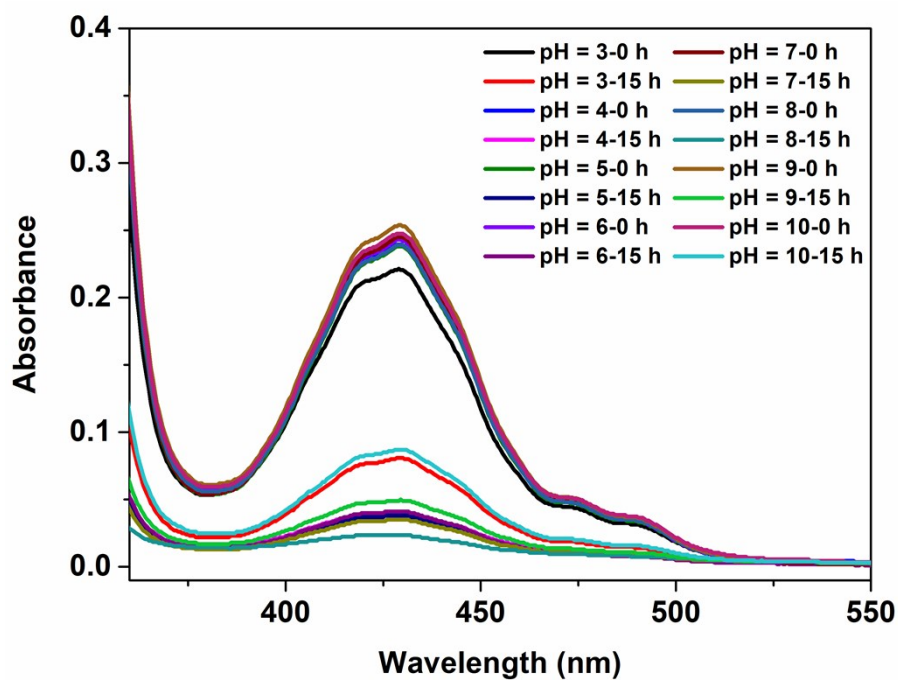


Fig. S12 The pH-dependent UO_2^{2+} adsorption of UPC-K1 detected by the UV-vis spectra. Note: 30 mg of crystals immersed in 4 mL of 2.2 mmol/L $\text{Zn}(\text{UO}_2)_2(\text{CH}_3\text{OO})_6$ solution.

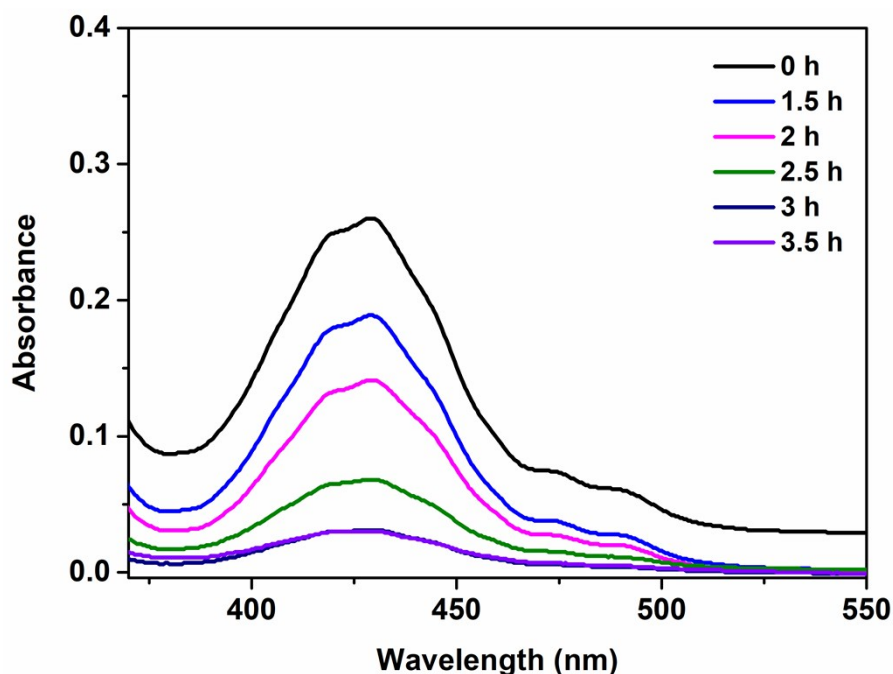


Fig. S13 UV-vis spectra of the filtered solutions after immersing 15 mg of slightly ground UPC-K1 in 4 mL of 2.2 mol/L $\text{Zn}(\text{UO}_2)_2(\text{CH}_3\text{OO})_6$ solutions under stirring for 24 hours.

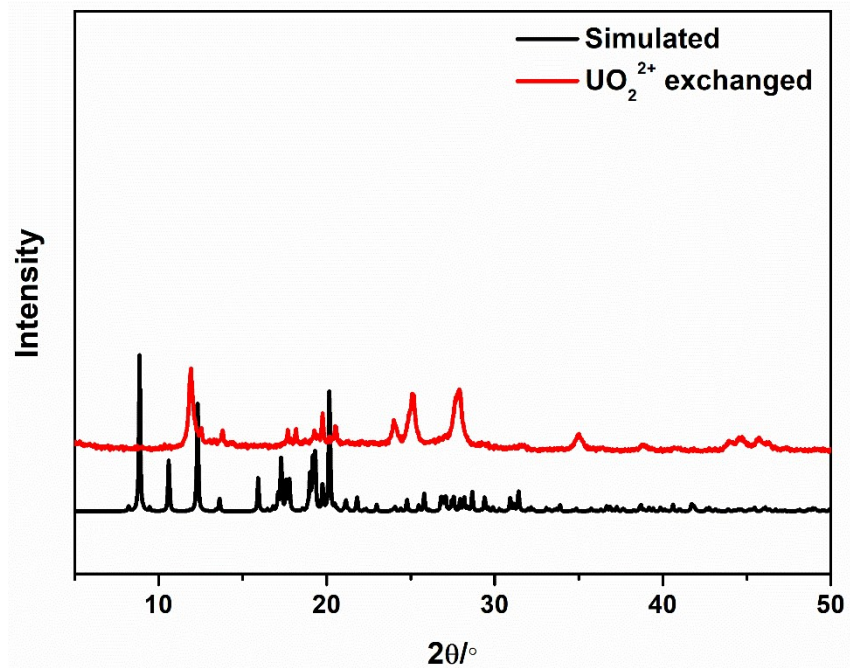


Fig. S14 PXR D patterns of UPC-K1 before and after immersing 15 mg of slightly ground UPC-K1 in 4 mL of 4.4 mmol/L Zn(UO₂)₂(CH₃OO)₆·7H₂O solutions under stirring for 5.5 hours.

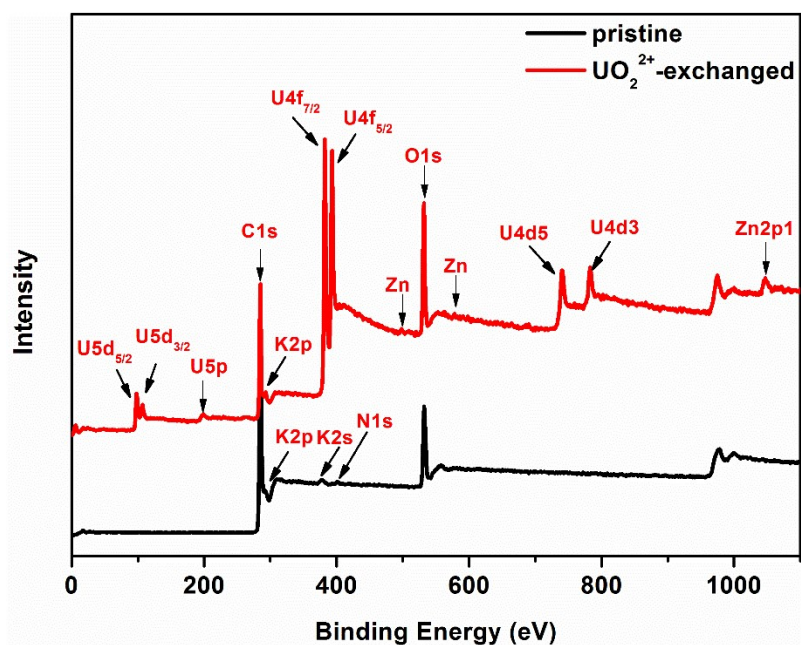


Fig. S15 XPS spectra of UPC-K1 before and after immersing 15 mg of slightly ground UPC-K1 in 4 mL of 4.4 mmol/L Zn(UO₂)₂(CH₃OO)₆·7H₂O solutions under stirring for 5.5 hours.

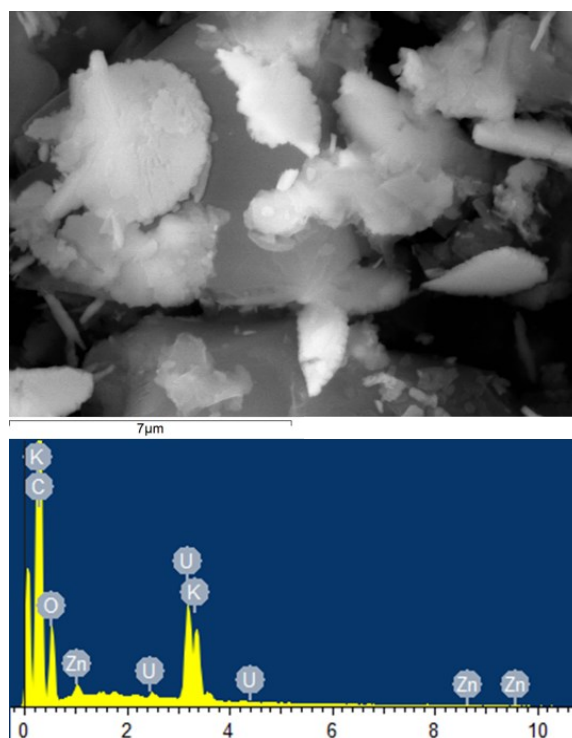


Fig. S16 The SEM image and EDS spectrum of UPC-K1 after immersing 15 mg of slightly ground UPC-K1 in 4 mL of 4.4 mmol/L $\text{Zn}(\text{UO}_2)_2(\text{CH}_3\text{OO})_6 \cdot 7\text{H}_2\text{O}$ solutions under stirring for 5.5

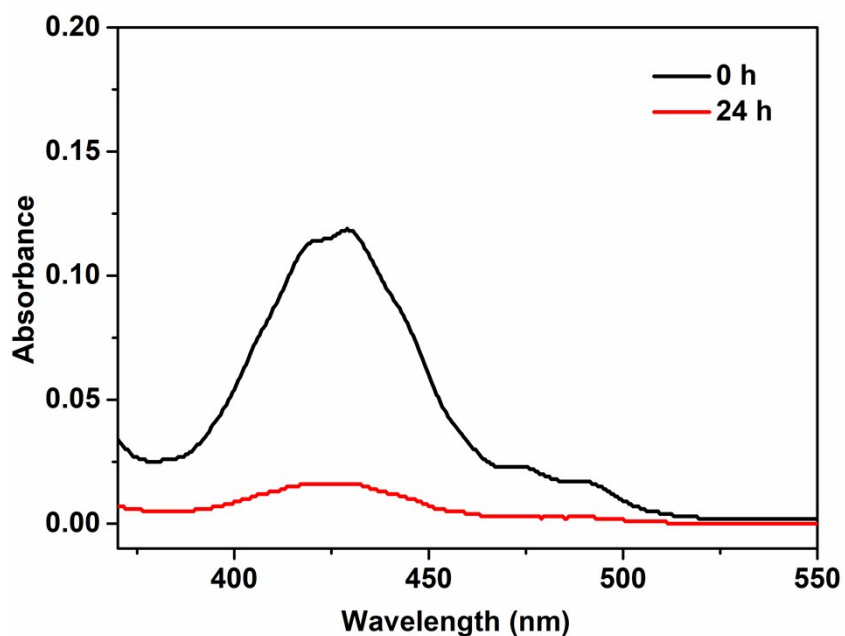


Fig. S17 UV-vis spectra of the filtered solutions after immersing 15 mg of slightly ground UPC-K1 in 16 mL of 1.1 mmol/L $\text{Zn}(\text{UO}_2)_2(\text{CH}_3\text{OO})_6$ solutions under stirring for different times.

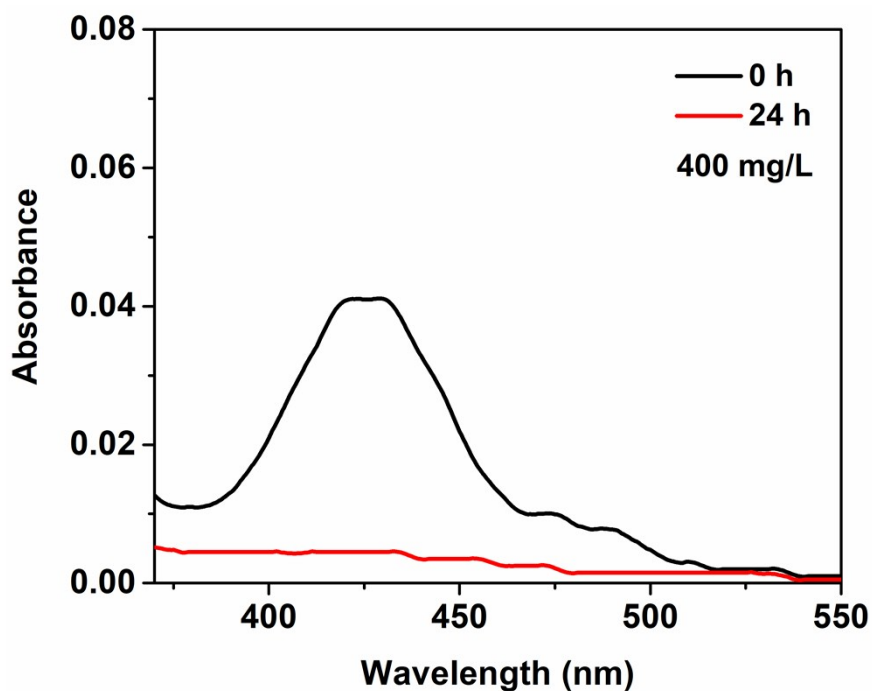


Fig. S18 UV-vis spectra of the filtered solutions after immersing 5 mg of as-synthesized UPC-K1 in 4 mL of 400 mg/L uranyl zinc acetate solutions at static state for 24 hours.

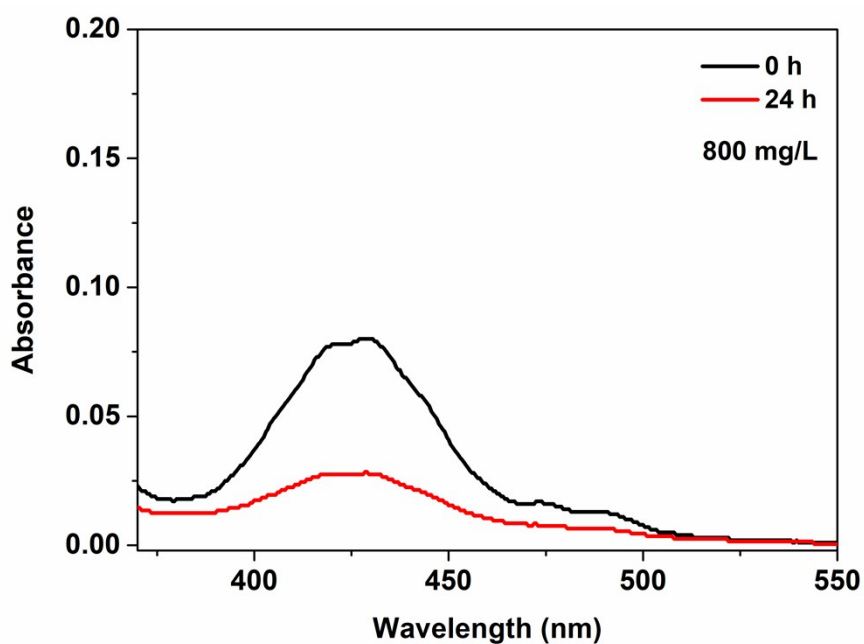


Fig. S19 UV-vis spectra of the filtered solutions after immersing 5 mg of as-synthesized UPC-K1 in 4 mL of 800 mg/L uranyl zinc acetate solutions at static state for 24 hours.

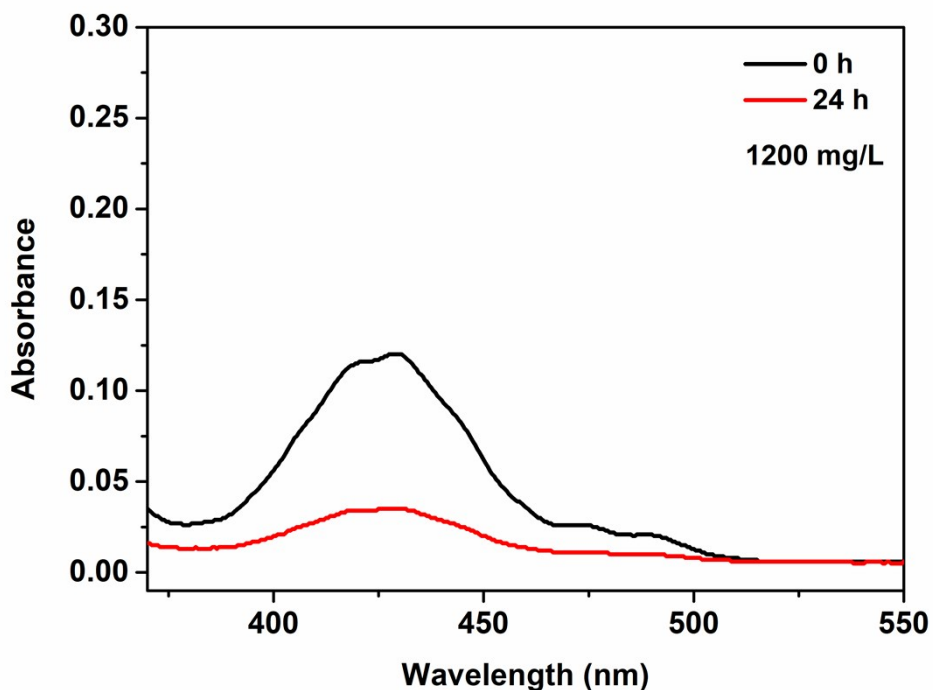


Fig. S20 UV-vis spectra of the filtered solutions after immersing 5 mg of as-synthesized UPC-K1 in 4 mL of 1200 mg/L uranyl zinc acetate solutions at static state for 24 hours.

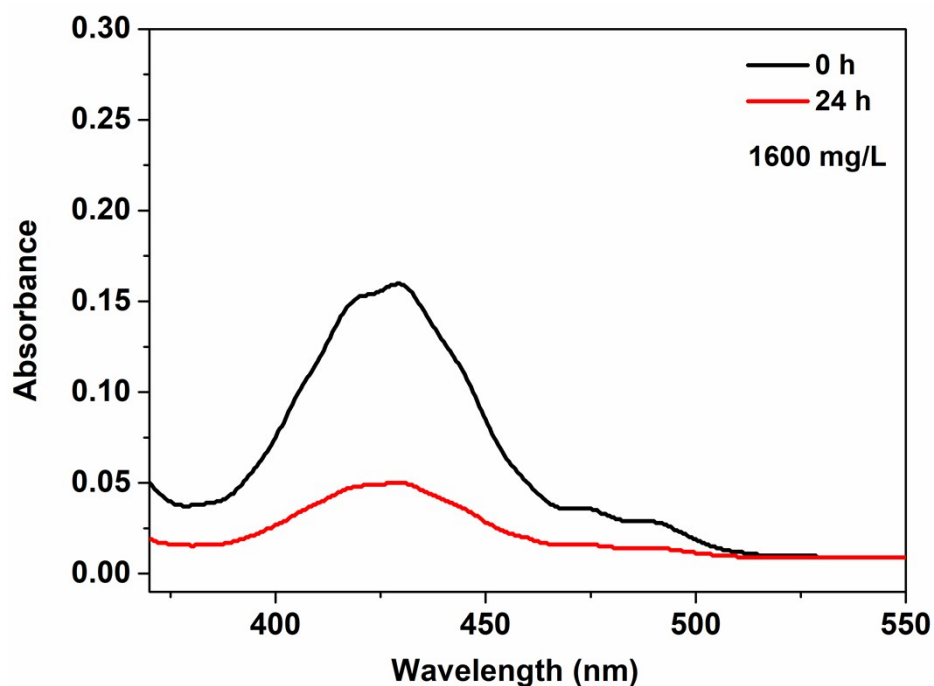


Fig. S21 UV-vis spectra of the filtered solutions after immersing 5 mg of as-synthesized UPC-K1 in 4 mL of 1600 mg/L uranyl zinc acetate solutions at static state for 24 hours.

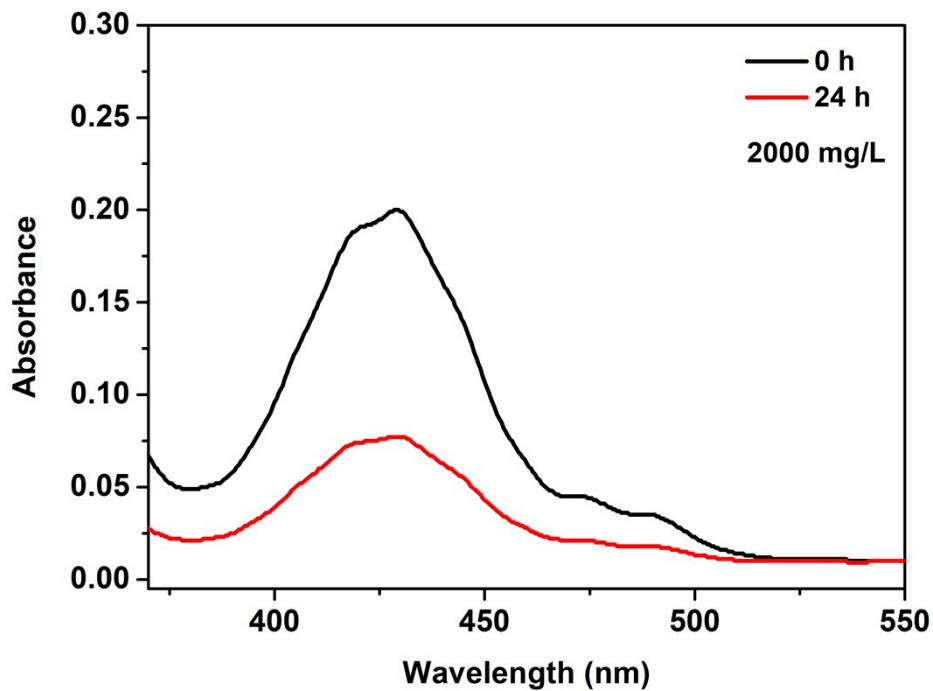


Fig. S22 UV-vis spectra of the filtered solutions after immersing 5 mg of as-synthesized UPC-K1 in 4 mL of 2000 mg/L uranyl zinc acetate solutions at static state for 24 hours.

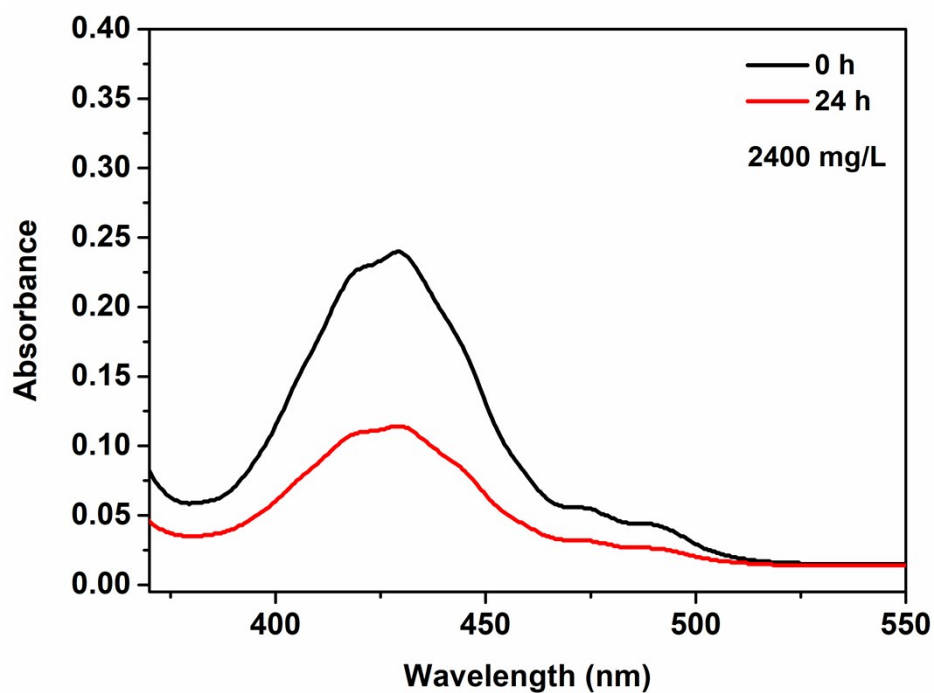


Fig. S23 UV-vis spectra of the filtered solutions after immersing 5 mg of as-synthesized UPC-K1 in 4 mL of 2400 mg/L uranyl zinc acetate solutions at static state for 24 hours.

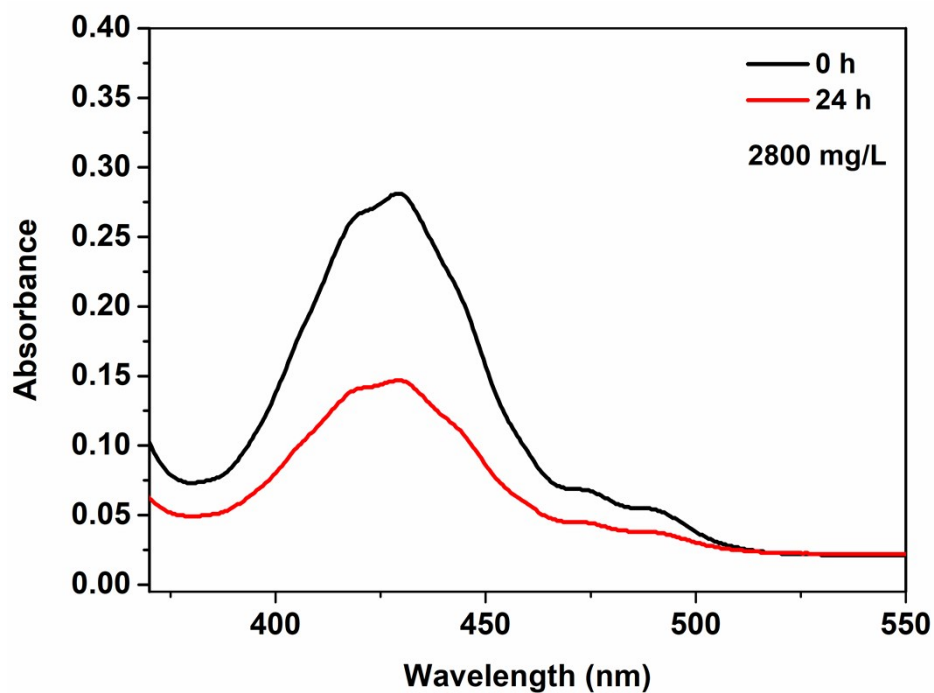


Fig. S24 UV-vis spectra of the filtered solutions after immersing 5 mg of as-synthesized UPC-K1 in 4 mL of 2800 mg/L uranyl zinc acetate solutions at static state for 24 hours.

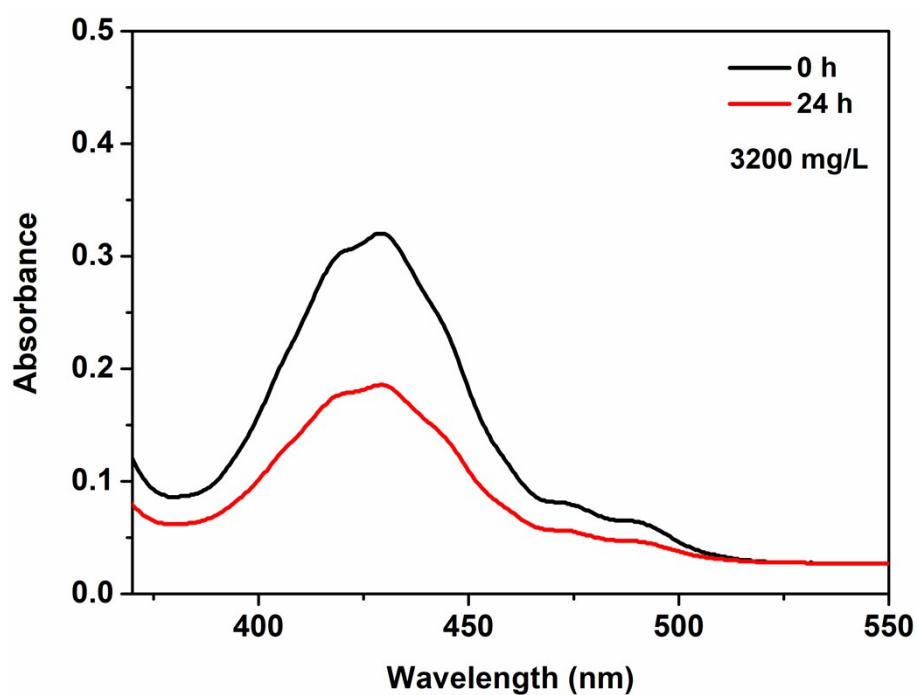


Fig. S25 UV-vis spectra of the filtered solutions after immersing 5 mg of as-synthesized UPC-K1 in 4 mL of 3200 mg/L uranyl zinc acetate solutions at static state for 24 hours.

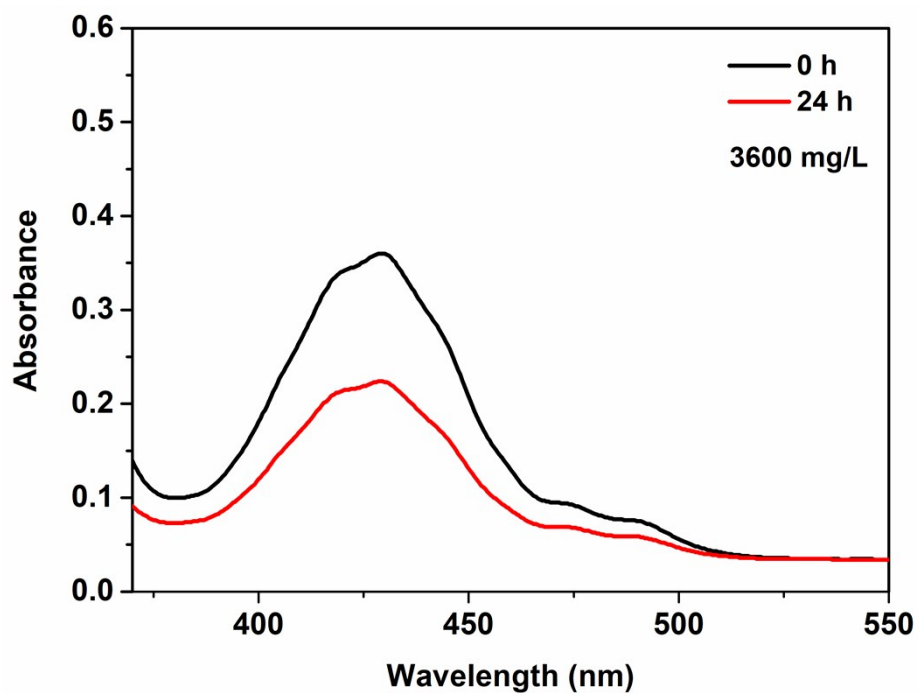


Fig. S26 UV-vis spectra of the filtered solutions after immersing 5 mg of as-synthesized UPC-K1 in 4 mL of 3600 mg/L uranyl zinc acetate solutions at static state for 24 hours.

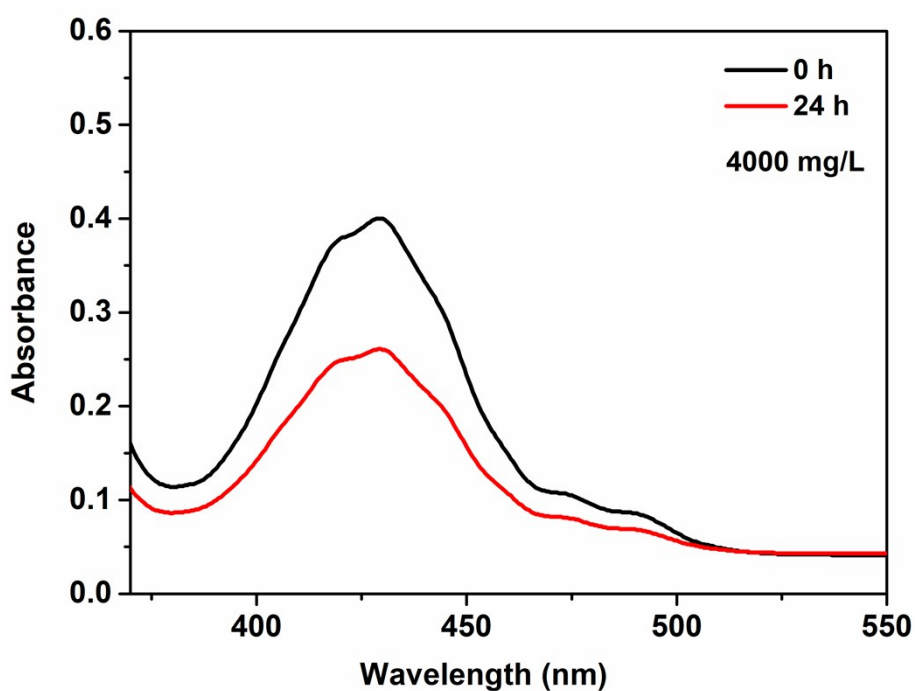


Fig. S27 UV-vis spectra of the filtered solutions after immersing 5 mg of as-synthesized UPC-K1 in 4 mL of 4000 mg/L uranyl zinc acetate solutions at static state for 24 hours.

Table S2 Comparison of uranium adsorption data with the reported materials except for the data listed or described in Ref. 1.

Materials	Adsorption capacity (mg/g)	pH range	Selectivity	Ref.
δ -MnO ₂ @TpPa-1	1147.773	6.5	-	8
δ -MnO ₂	499.41	6.5	-	8
BSA–BT-NSs	487.805	5	vs. Mn ²⁺ , Cs ⁺ , Co ²⁺ , Sr ²⁺	9
UPC-K1	486	3-10	vs. various metal ions	This work
GOANS	311.5	4	-	6
Fe@ZIF-8	277.77	4.5	vs. Ce ³⁺ , Na ⁺ , Fe ³⁺ , Cu ²⁺ , Ca ²⁺	11
FJSM-GAS-1	196	2.9-10.5	vs. Na ⁺ , Ca ²⁺	3
NU6CN	195.55	5	-	12
MoS ₂ -IP6 NRA/CC	183.3	5.5	vs. K ⁺ , Li ⁺ , Cr ³⁺ , Cu ²⁺ , Ca ²⁺	7
FJSM-GAS-2	144	2.9-10.5	vs. Na ⁺ , Ca ²⁺	3
CNFs	125	1-11	-	4
HCTC	96.99	5.5	-	5
MoS ₂ nanosheets	45.7	6	-	10

Crystal hydrogel	40.4	2.5-5.5	vs. various metal ions	2
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Reference

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