

Supporting information

Phosphorylated cellulose nanofibers exhibit exceptional capacity for uranium capture

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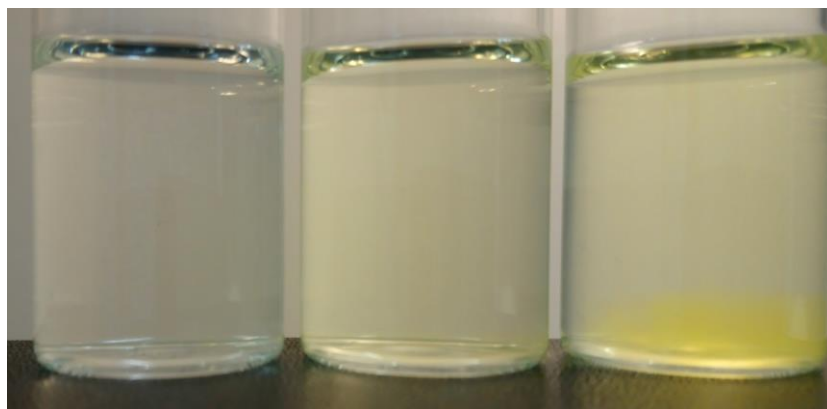


Fig. S1. Gelling of PHO-CNF_{1.00} as initial uranium concentration increases. The photos were taken after 1 h contact of PHO-CNF_{1.00} with uranium solutions of initial concentrations of 100, 300 and 500 mg/L (vials from left to right, respectively)

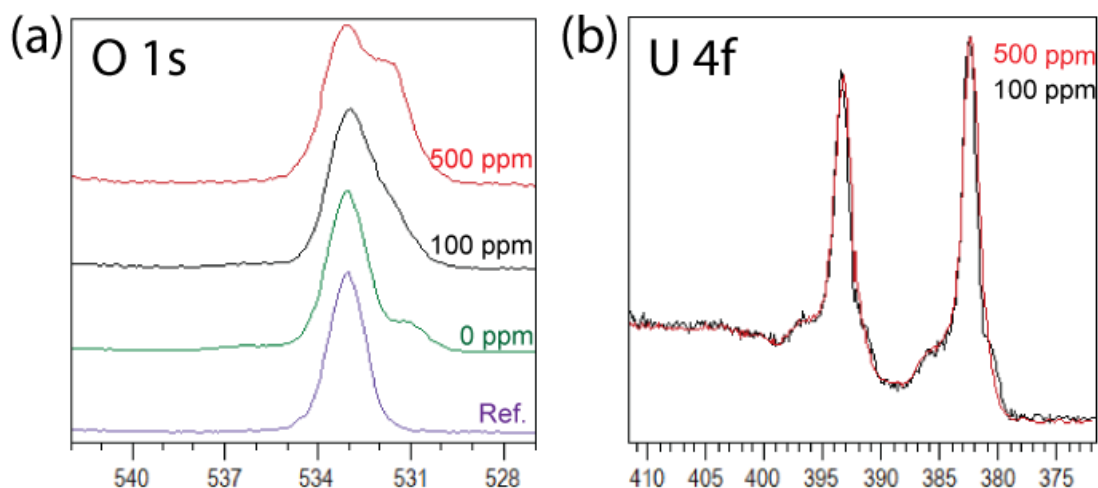


Fig. S2. High-resolution XPS spectra of (a) oxygen for PHO-CNF_{1.00} samples with initial U(VI) concentrations of 0, 100 and 500 mg/L and for the in situ cellulose reference and (b) uranium for PHO-CNF_{1.00} samples with initial U(VI) concentrations of 100 and 500 mg/L

Table S1. The ionic composition of water used for selectivity studies

Ion	mg/L
Cl ⁻	89
SO ₄ ²⁻	33
NO ₃ ⁻	1.8
Carbonates	54
Na ⁺	46
Mg ²⁺	8.3
K ⁺	1.2
Ca ²⁺	28

Table S2. Uranyl speciation with initial uranium concentration of 100 mg/L at pH 3-7

	pH 3		pH 4		pH 5		pH 6		pH 7	
	<i>m</i> (mol/kg)	%*	<i>m</i> (mol/kg)	%*	<i>m</i> (mol/kg)	%*	<i>m</i> (mol/kg)	%*	<i>m</i> (mol/kg)	%*
(UO ₂) ₃ (OH) ₅ ⁺	1.21E-11	0.00	8.03E-07	0.57	1.04E-04	73.96	1.38E-04	98.60	1.40E-04	99.88
(UO ₂) ₂ (OH) ₂ ⁺²	4.00E-07	0.19	2.95E-05	14.04	3.39E-05	16.12	1.97E-06	0.94	8.93E-08	0.04
UO ₂ OH ⁺	4.70E-07	0.11	4.07E-06	0.97	4.40E-06	1.05	1.05E-06	0.25	2.26E-07	0.05
UO ₂ ⁺²	4.19E-04	99.69	3.55E-04	84.41	3.74E-05	8.90	9.19E-07	0.22	1.92E-08	0.00

* Percent of total uranium in the indicated form

Table S3. Uranyl speciation in simulated drinking water at pH 6

	<i>m</i> (mol/kg)	%*
$(\text{UO}_2)_3(\text{OH})_5^+$	8.40E-06	53.10
UO_2CO_3	1.56E-05	32.88
$\text{UO}_2(\text{CO}_3)_2^{-2}$	4.89E-06	10.31
$(\text{UO}_2)_2(\text{OH})_2^{+2}$	3.89E-07	1.64
UO_2^{+2}	4.64E-07	0.98
UO_2OH^+	4.14E-07	0.87
UO_2SO_4	1.09E-07	0.23
$\text{UO}_2(\text{CO}_3)_3^{-4}$	9.07E-09	0.02

* Percent of total uranium in the indicated form

Table S4. XPS surface elemental concentrations, in at-%

Sample	C 1s	O 1s	U 4f _{7/2}	Na 1s	P 2p	Si 2s
Whatman	59.2	40.8	b.d.l.	b.d.l.	b.d.l.	b.d.l.
0 ppm	52.8	41.0	b.d.l.	2.5	3.2	0.6
100 ppm	53.8	36.8	1.2	1.1	2.5	4.6
500 ppm	55.1	37.9	3.8	0.3	1.9	0.9

Table S5. Langmuir, Freundlich and Sips isotherm parameters

Langmuir	q_m (mg/g)	1413
	K_L (L/g)	0.048
	R^2	0.972
Freundlich	K_F (mg/g)	72.86
	n	1.47
	R^2	0.962
Sips	q_m (mg/g)	1550
	n	1.09
	K_s (L/mg)	0.0485
	R^2	0.986