

ELECTRONIC SUPPLEMENT INFORMATION

Insights into the performance and mechanism of Cr(VI) and U(VI) removal in water using innovative cross-linked chitosan adsorbent

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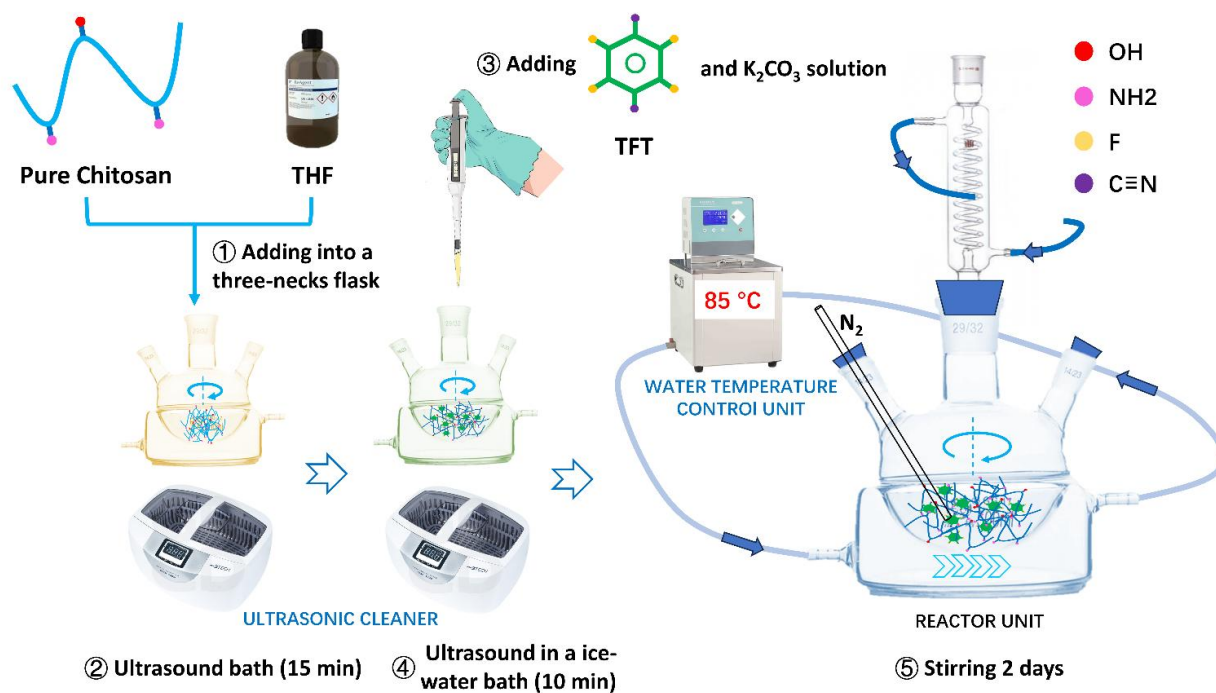


Figure S1. Scheme of the TFT cross-linked chitosan preparation.

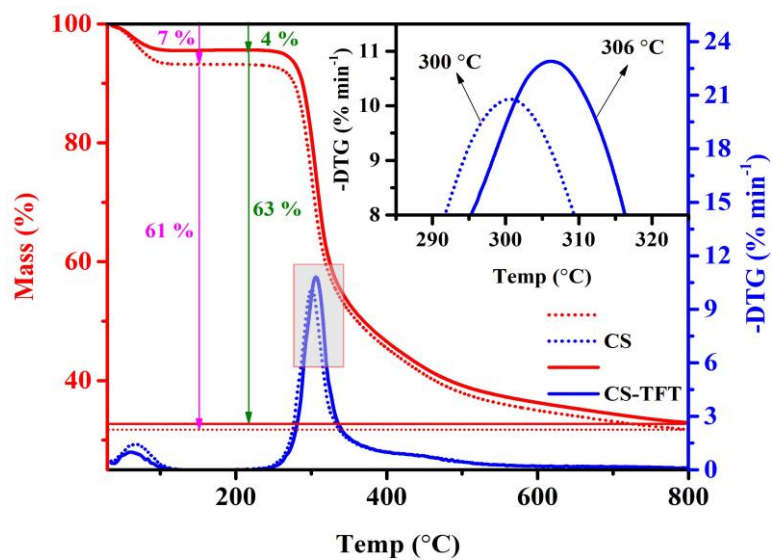


Figure S2. TG/DTG curves of CS-TFT and CS. The inset shows the peaks of DTG curves of CS-TFT and CS at the second mass loss.

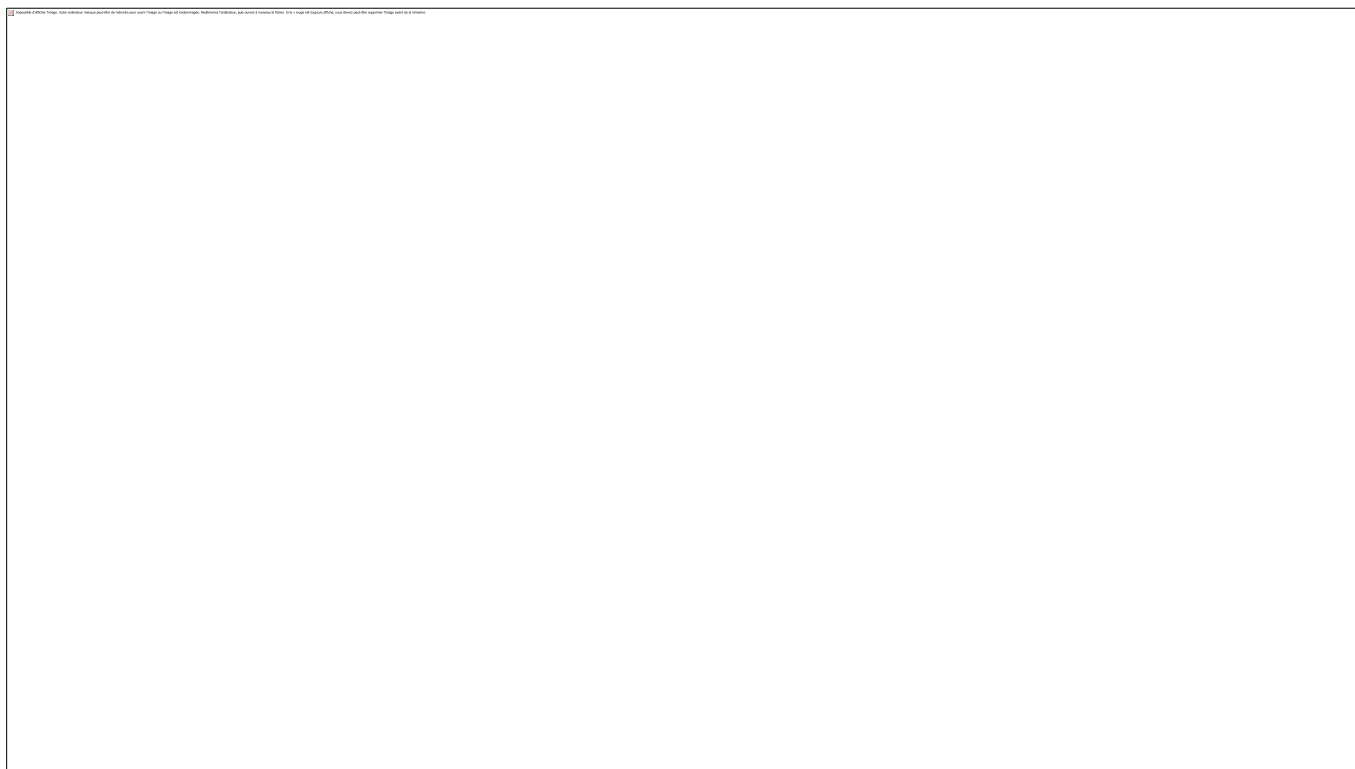


Figure S3. The cross-linking reaction of CS with TFT.

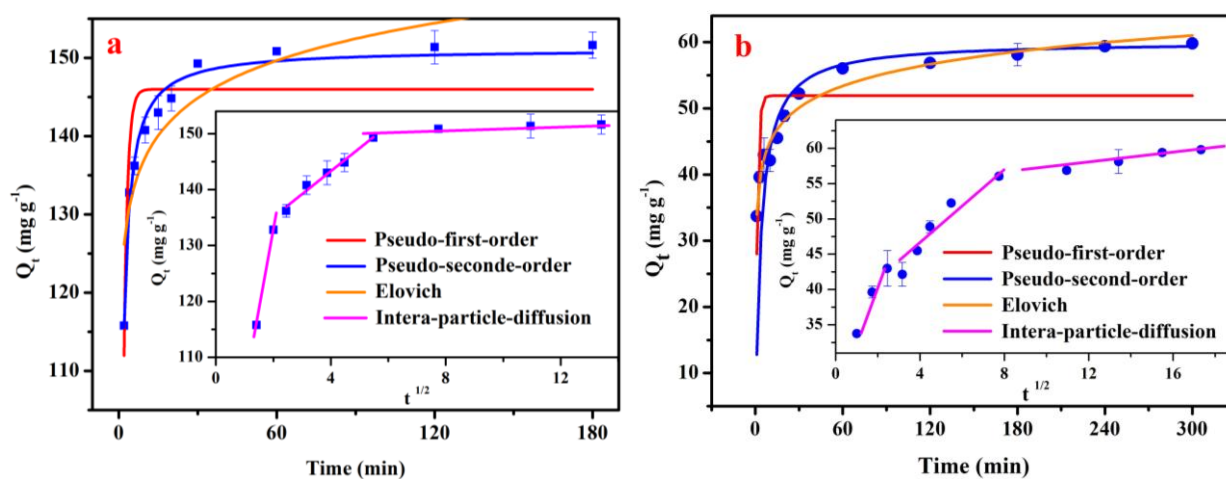


Figure S4. Adsorption kinetics of Cr(VI) U(VI) on CS-TFT. ((a) $[\text{Cr(VI)}] = 100 \text{ mg L}^{-1}$, $[\text{CS-TFT}] = 0.2 \text{ g L}^{-1}$, Ionic strength = 0.1 M , $\text{pH} = 3.0$, $\text{Temp} = 308\text{K}$); (b) $[\text{U(VI)}] = 20 \text{ mg L}^{-1}$, $[\text{CS-TFT}] = 0.2 \text{ g L}^{-1}$, Ionic strength = 1 M , $\text{pH} = 5.0$, $\text{Temp} = 308\text{K}$).

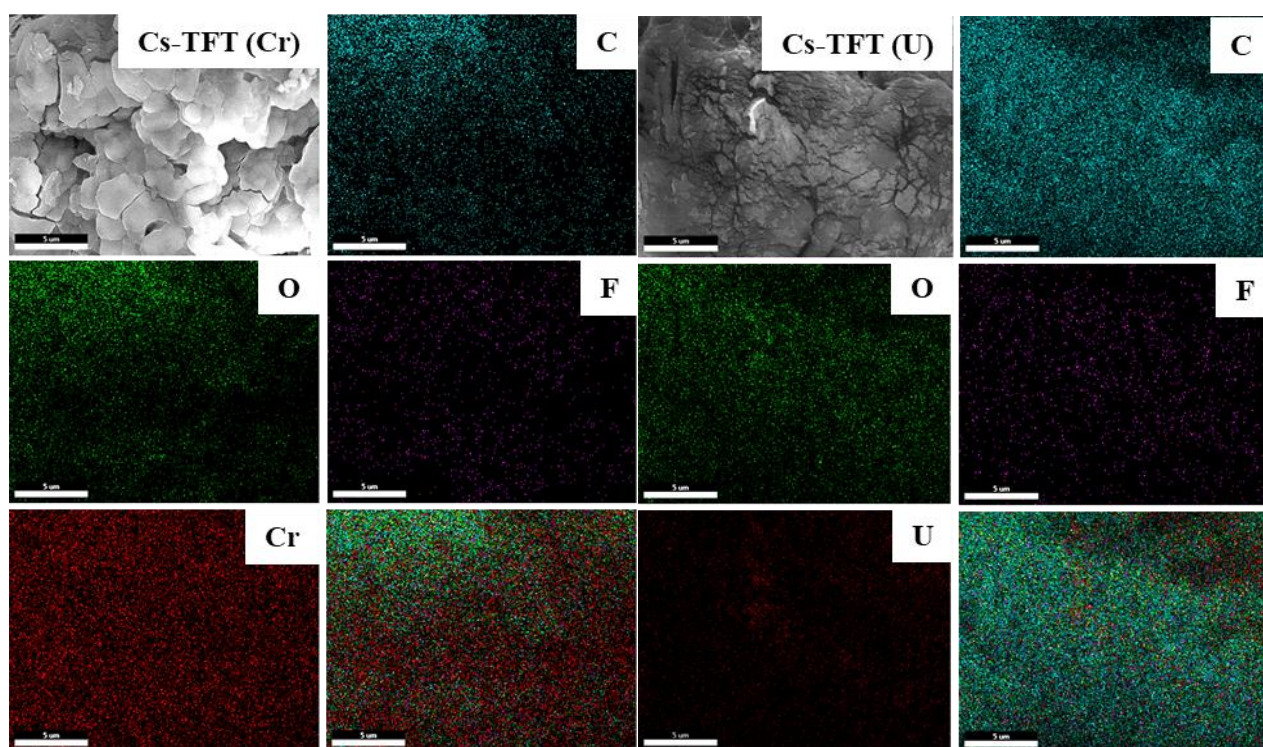


Figure S5. SEM-EDS images of adsorption of Cr(VI) and U(VI) on CS-TFT.

Table S1. The assignments of identified peaks from high-resolution XPS spectra of CS and CS-TFT. BE: binding energy; AC: atomic concentration; *n.d.*: not detected.

Peak	CS		CS-TFT		Assignment	Ref.
	BE (eV)	AC (%)	BE (eV)	AC (%)		
C1s	284.6	16.9	284.5	13.9	C-(C, H)	[1-3]
	286.0	33.2	286.2	29.6	C-(O, N)	[1,2]
	287.6	9.1	287.8	7.0	O-C-O/O=C-N	[1,2]
	<i>n.d.</i>	<i>n.d.</i>	292.6	3.9	Covalent C-F	[4,5]
	<i>n.d.</i>	<i>n.d.</i>	295.6	1.6	Semi-ionic C-F	[4,5]
O1s	<i>n.d.</i>	<i>n.d.</i>	531.1	3.9	O=C-NH ₂	[1,2,6]
	532.5	30.5	532.6	27.0	C-(O, OH)	[1,2,6]
N1s	399.0	8.4	399.1	8.8	C-NH ₂	[1,6]
F1s	<i>n.d.</i>	<i>n.d.</i>	687.2	0.7	Semi-ionic C-F	[4,5]
	<i>n.d.</i>	<i>n.d.</i>	689.1	3.6	Covalent C-F	[4,5]

Table S2. The results of BET analysis for CS and CS-TFT

Samples	CS	CS-TFT
Surface area (m ² mg ⁻¹)	2.61	2.93
Pore volume (cm ³ g ⁻¹)	0.004	0.032
Average pore diameter (nm)	13.15	4.96

Table S3. Kinetic parameter for adsorption of Cr (VI) and U(VI) on CS-TFT

Elements	pseudo-first-order			pseudo-second-order		
	Q _e (mg g ⁻¹)	K ₁ (h ⁻¹)	R ²	Q _e (mg g ⁻¹)	K ₂ (g (mg·min) ⁻¹)	R ²
Cr(VI)	17.05	0.040	0.76	152.21	8.83×10 ⁻³	0.99
U(VI)	51.91	0.775	0.35	60.10	4.50×10 ⁻³	0.99
Elements	Elovich			Intra-particle diffusion		
	α	β	R ²	C (mg g ⁻¹)	K _{int} (mg g ⁻¹ min ^{-0.5})	R ²
Cr(VI)	0.145	2.98×10 ⁸	0.79	126.85	4.11	0.97
U(VI)	0.211	6185.41	0.97	34.36	2.95	0.90

Table S4. Parameters for the Langmuir, Freundlich, Temkin, D-R models

Elements	T(K)	Langmuir model			Freundlich model		
		Q_{max} (mg g ⁻¹)	K_L (L mg ⁻¹)	R^2	K_F (mg ¹⁻ⁿ L ⁿ g ⁻¹)	1/n	R^2
Cr(VI)	298K	265.96	0.372	0.93	129.65	0.207	0.94
	308K	250.00	0.401	0.95	110.22	0.233	0.97
	318K	233.64	0.425	0.99	97.19	0.230	0.88
U(VI)	298K	346.02	0.045	0.94	26.90	0.538	0.97
	308K	170.94	0.055	0.94	24.35	0.432	0.89
	318K	127.55	0.067	0.94	20.06	0.409	0.85
Elements	T(K)	Temkin model			D-R model		
		A_T (L mg ⁻¹)	B_1 (mg g ⁻¹)	R^2	Q_s (mol ² kJ ⁻²)	B (mg g ⁻¹)	R^2
Cr(VI)	298K	39.55	40.53	0.98	237.07	9.85×10 ⁻⁸	0.85
	308K	17.80	38.21	0.99	218.88	1.67×10 ⁻⁷	0.74
	318K	8.42	34.95	0.95	209.33	5.05×10 ⁻⁷	0.94
U(VI)	298K	0.61	59.12	0.92	154.99	2.36×10 ⁻⁶	0.84
	308K	0.54	39.87	0.94	110.34	3.36×10 ⁻⁶	0.83
	318K	0.46	32.21	0.94	93.04	6.08×10 ⁻⁶	0.93

Table S5. Effect of pH, adsorption time, concentration of pollutants and temperature on the adsorption performance of CS-TFT.

Effect Factor	Cr(VI)			U(VI)			
	C_e (mg L^{-1})	Q_e (mg g^{-1})	Q_e/C_e ($\text{mg g}^{-1} \text{mM}^{-1}$)	C_e (mg L^{-1})	Q_e (mg g^{-1})	Q_e/C_e ($\text{mg g}^{-1} \text{mM}^{-1}$)	
pH	2	78.96	105.22	69.29	17.27	13.64	187.98
	3	60.08	199.59	172.75	16.43	17.84	258.44
	4	88.12	59.42	35.07	6.17	69.14	2666.37
	5	92.31	38.45	21.66	3.23	83.85	6181.00
	6	94.27	28.66	15.81	3.57	82.17	5485.72
	7	97.90	10.49	5.57	4.41	77.97	4211.95
	8	97.97	10.14	5.38	13.07	34.66	631.34
	9	98.39	8.04	4.25	13.57	32.14	563.68
	10	98.67	6.64	3.50	18.79	6.07	76.91
	Adsorption time (min)	1	79.66	101.72	66.40	13.25	33.74
10		62.04	189.81	159.09	11.57	42.15	867.01
20		56.24	218.82	202.34	10.23	48.87	1137.69
30		55.12	224.41	211.72	9.55	52.24	1301.62
60		50.43	247.83	255.53	8.80	56.02	1516.02
120		49.31	253.43	267.22	8.63	56.86	1568.77
180		48.62	256.92	274.81	8.38	58.12	1651.87
[Cr or U] (mg L^{-1})	20	0.41	97.96	12454.67	4.41	75.47	4076.81
	40	3.12	184.41	3075.46	16.09	119.53	1767.69
	60	12.64	236.78	973.85	29.13	154.36	1261.34
	80	29.33	253.36	449.23	40.90	195.49	1137.69
	100	43.09	284.54	343.35	53.51	232.43	1033.81
Temperature (K)	298	0.41	97.96	12297.37	4.41	75.47	4072.98
	308	0.69	96.56	7276.99	7.94	60.31	1807.78
	318	1.56	92.19	3073.00	9.45	52.74	1328.27

pH: [Cr(VI)] = 100 mg L^{-1} or [U(VI)] = 20 mg L^{-1} ; [CS-TFT] = 0.2 g L^{-1} ; Adsorption time = 4 h; Temperature = 308 K; [NaCl] = 0.01 M. **Adsorption time:** [Cr(VI)] = 100 mg L^{-1} or [U(VI)] = 20 mg L^{-1} ; [CS-TFT] = 0.2 g L^{-1} ; Temperature = 308 K; [NaCl] = 0 M and 1 M for Cr(VI) and U(VI), respectively; pH = 3.0 and 5.0 for Cr(VI) and U(VI), respectively. **Concentration of Cr(VI) or U(VI):** [CS-TFT] = 0.2 g L^{-1} ; Adsorption time = 6 h; Temperature = 298 K; [NaCl] = 0 M; pH = 3.0 and 5.0 for Cr(VI) and U(VI), respectively. **Temperature:** [Cr(VI)] = [U(VI)] = 20 mg L^{-1} ; [CS-TFT] = 0.2 g L^{-1} ; pH = 3.0 for Cr and pH = 5.0 for U; [NaCl] = 0.01 M; adsorption time = 2 h.

Elements	Material	Optimal pH	Adsorption Equilibrium Time (h)	Best Fitted Isotherm Model	PC (mg g ⁻¹ mM ⁻¹)	Ref
Cr(VI)	CS-TFT	3.0	1.0	Langmuir	12.45×10³	This study
	SDS-chitosan	4.0-5.0	96	Langmuir	9.5	[7]
	Mesopore-rich badam-shell biochar	1.0	5.0	Langmuir	18.82	[8]
	Cr(VI)-NIPs (non-imprinted polymers)	2.0	0.5	Freundlich	591	[9]
	Nitrogen-doped porous carbon material (PCM-N)	2.0	10.0	Freundlich	2.90×10 ³	[10]
	Tin metal-organic framework [Sn ^(II) -BDC MOF]	4.0	2.5	Langmuir	48.75×10 ³	[11]
U(VI)	CS-TFT	6.0	1.0	Langmuir	4.08×10³	This study
	EDTA-LDH	3.0	2.0	Freundlich	834	[12]
	Functionalized Maghemite (AMNP)	5.5	2.0	Langmuir	7585	[13]
	Graphene oxide–polyethyleneimine (GO-PEI)	5.3	-	-	531.40×10 ³	[14]

Table S6. Literature review of Cr(VI) and U(VI) adsorption using different adsorbents.

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