Mesoporous Magnetic Cysteine Functionalized Chitosan Nanocomposite for Selective Uranyl Ions Sorption: Experimental, Structural Characterization, and Mechanistic Studies

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Supporting Information section

Table S1. Adsorption modeling Equations: kinetics and isotherms [1, 2]

Process	Model	Equation	Parameters	
Kinetics	PFORE	$q(t) = q_{eq,1}(1 - e^{k_1 t})$	$q_{eq,1}$ (mmol^U/g)	k_1 (min^{-1})
	PSORE	$q(t) = \dfrac{q_{eq,2}^2 \times k_2 \times t}{1 + q_{eq,2} \times k_2 \times t}$	$q_{eq,2}$ (mmol^U/g^{-1})	k_2 (L mmol^{-1} min^{-1})
	sRIDE (Weber & Morris)	$q_{(t)} = k_{int.,i} \cdot t^{0.5} + C$ Several linear sections corresponding to different regimes of resistance (i) to intraparticle diffusion may co-exist ($K_{int, i}$) (linear regression calculation)	$K_{int.,i}$ (mmol g^{-1} min$^{-0.5}$)	
Isotherms	Langmuir	$\dfrac{C_{eq}}{q_{eq}} = \dfrac{C_{eq}}{q_{max}} + \dfrac{1}{b q_{max}}$	q_{max} (mmol^U/g)	b_L (L/mmol)
	Freundlich	$q = k_F\, C_{eq}^{1/n}$	k_F	N (dimensionless)
	Temkin	$q_{eq} = B_T\, lnC_{eq} + B_T\, lnA_T$ Where, $B_T = \dfrac{RT}{b_T}$	A_T (L/mmol)	b_T (J/mol)

Figure S1. XPS core level spectra for C 1s, O 1s, N 1s, P 2p, Fe 2p, and U 4f for Cys-sorbent before and after UO_2^{2+} sorption.
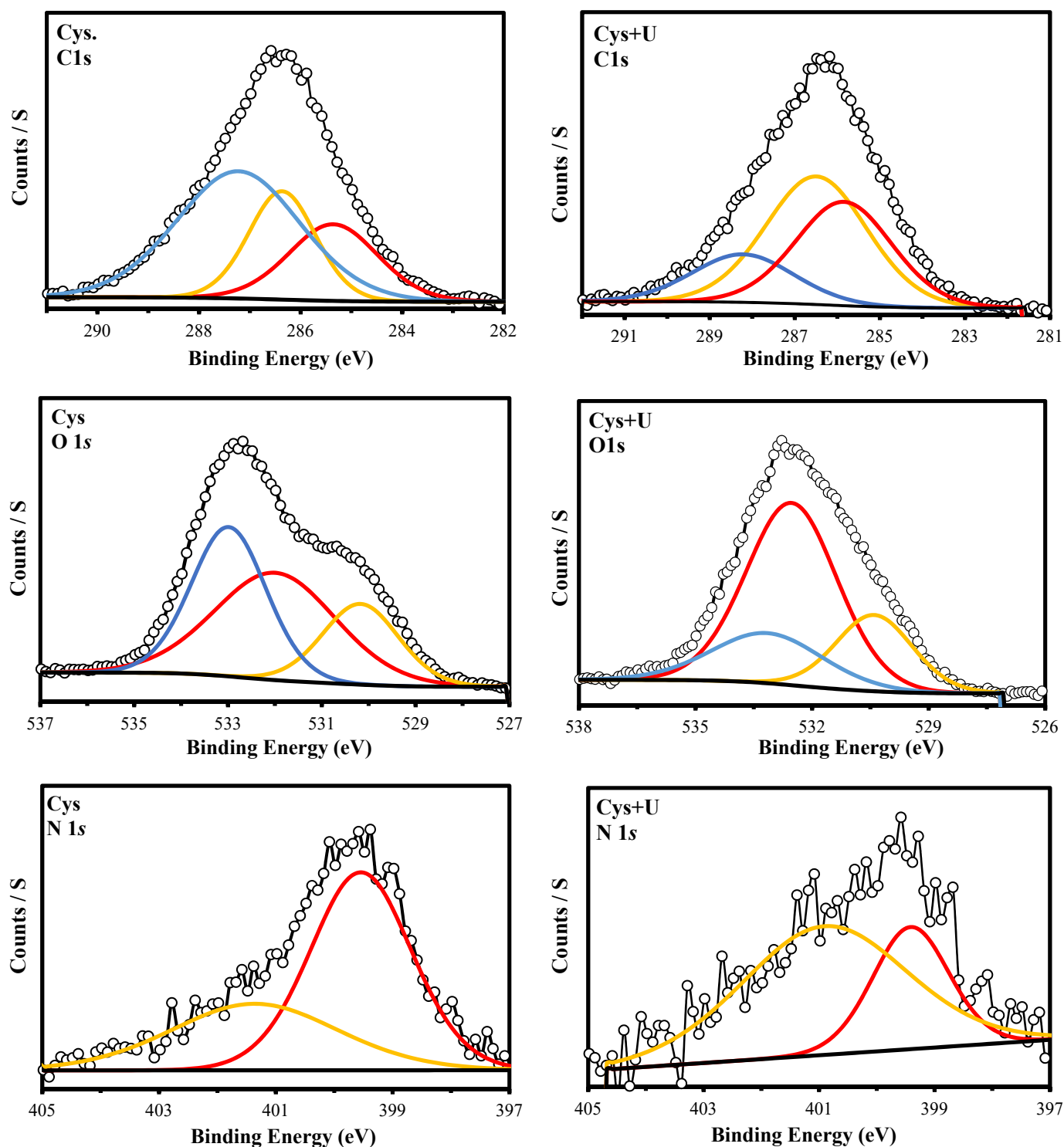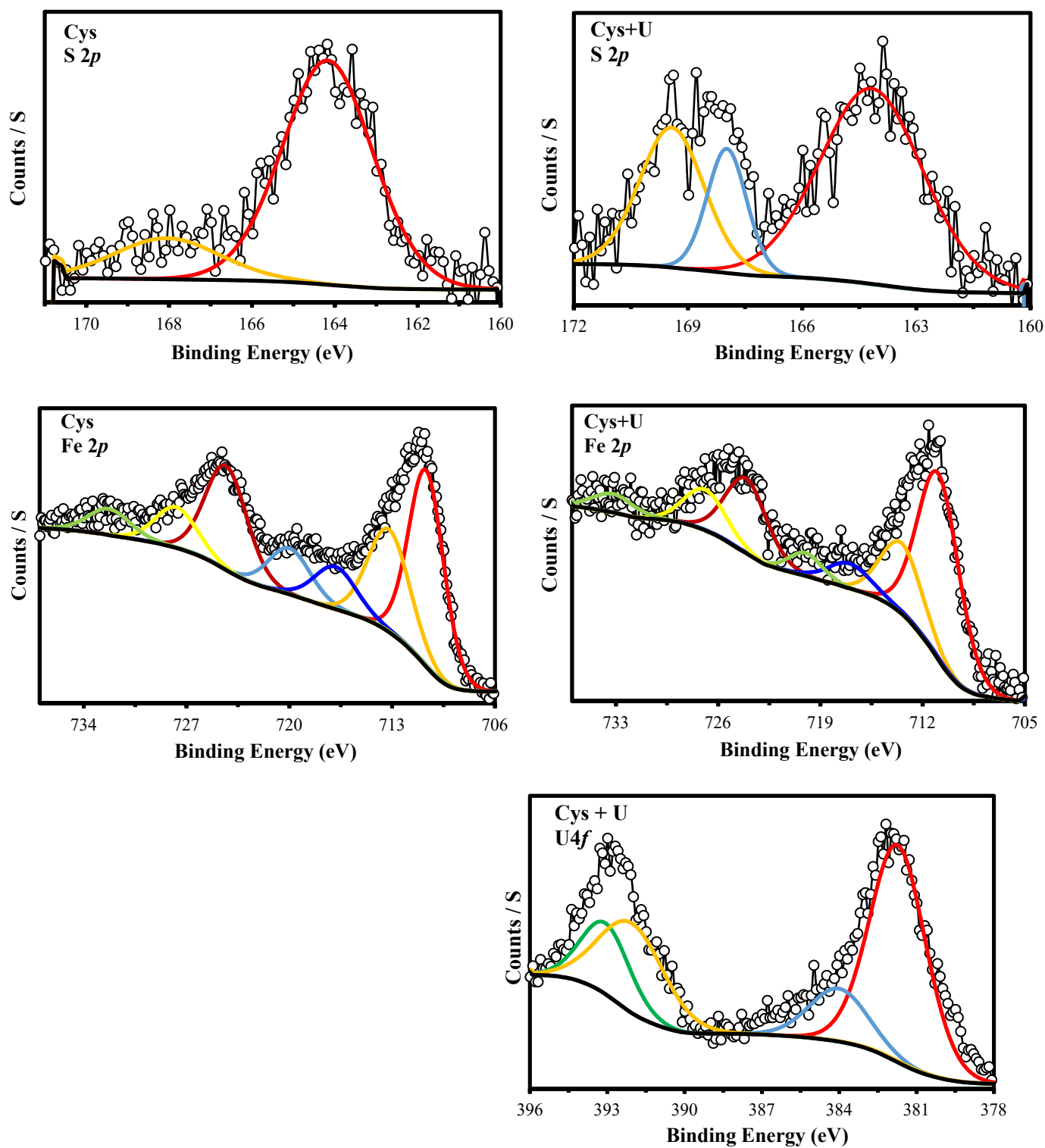
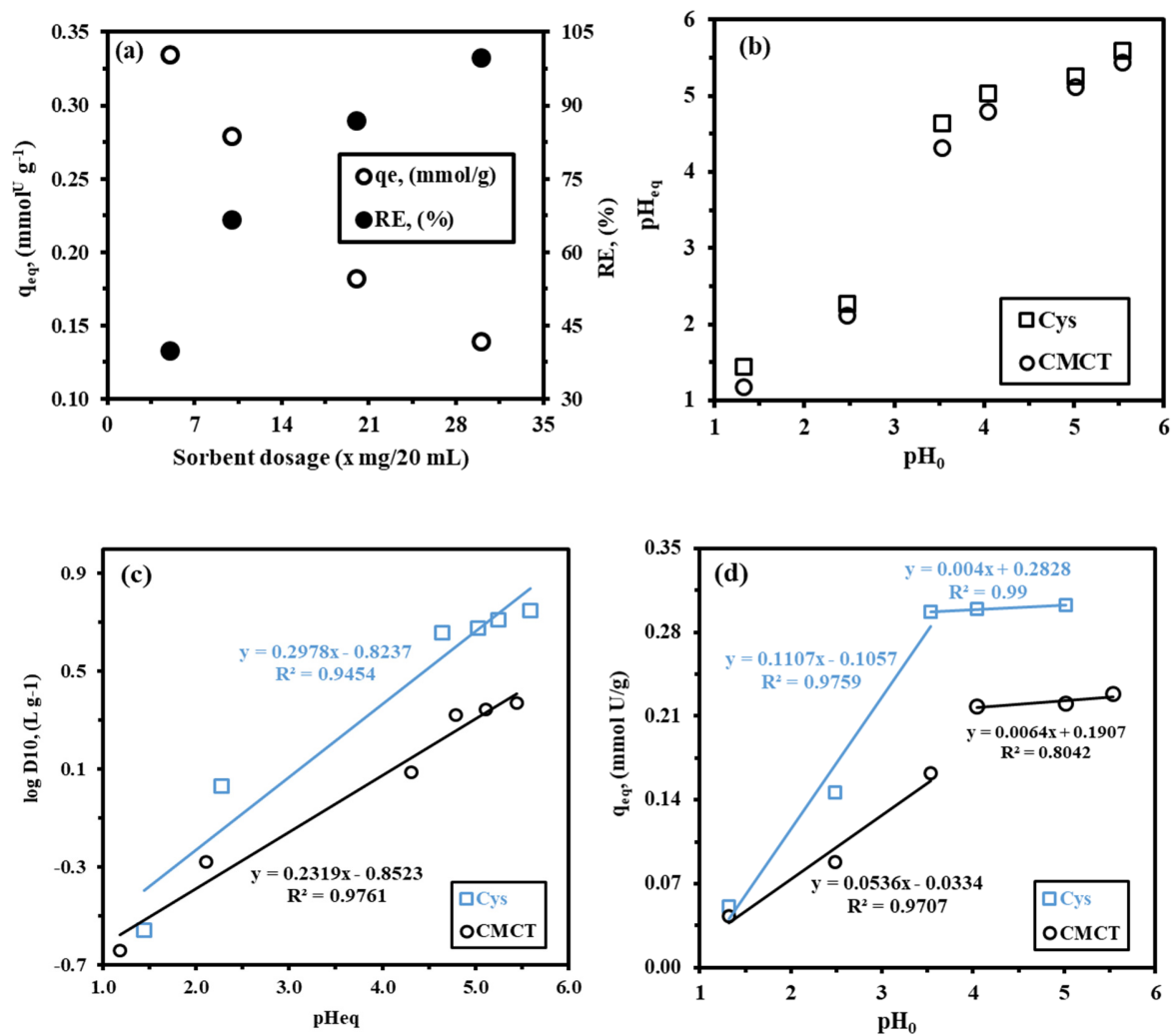**Figure S1. (*cont.*)**

Figure S2. Effect of sorbent dosage (a), Plot of pH_0 vs. pH_{eq} (b), $\log_{10}D$ plot vs. pH_{eq} (b), and plot of pH_0 vs. q_{eq} (c) for
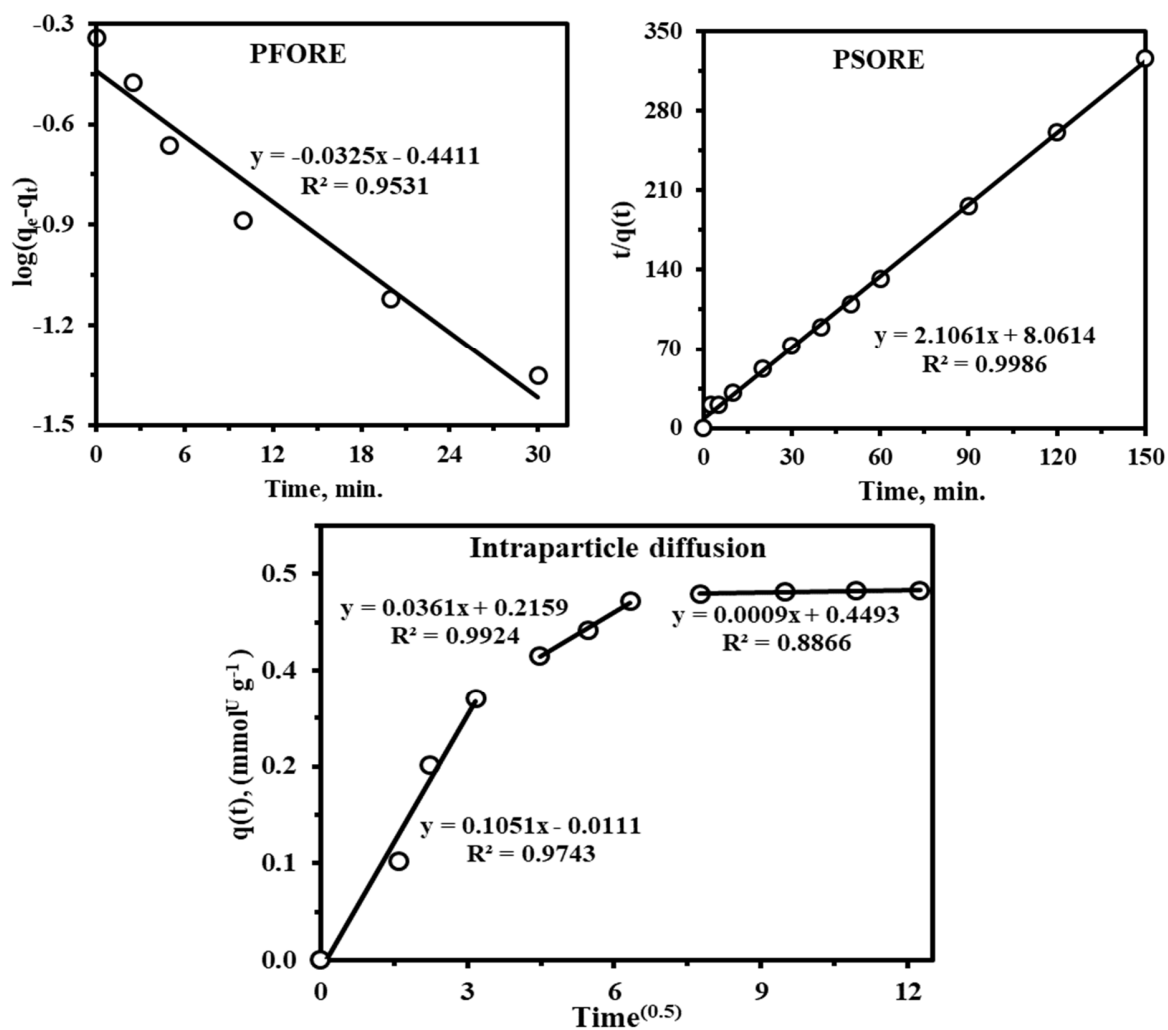
UO_2^{2+} sorption.

Figure S3. Sorption kinetics for PFORE, PSORE, and Intraparticle diffusion. (C_0: 0.425 mmol U/L, SD: 0.5g/L, time 60 min., room temp. 298 K)
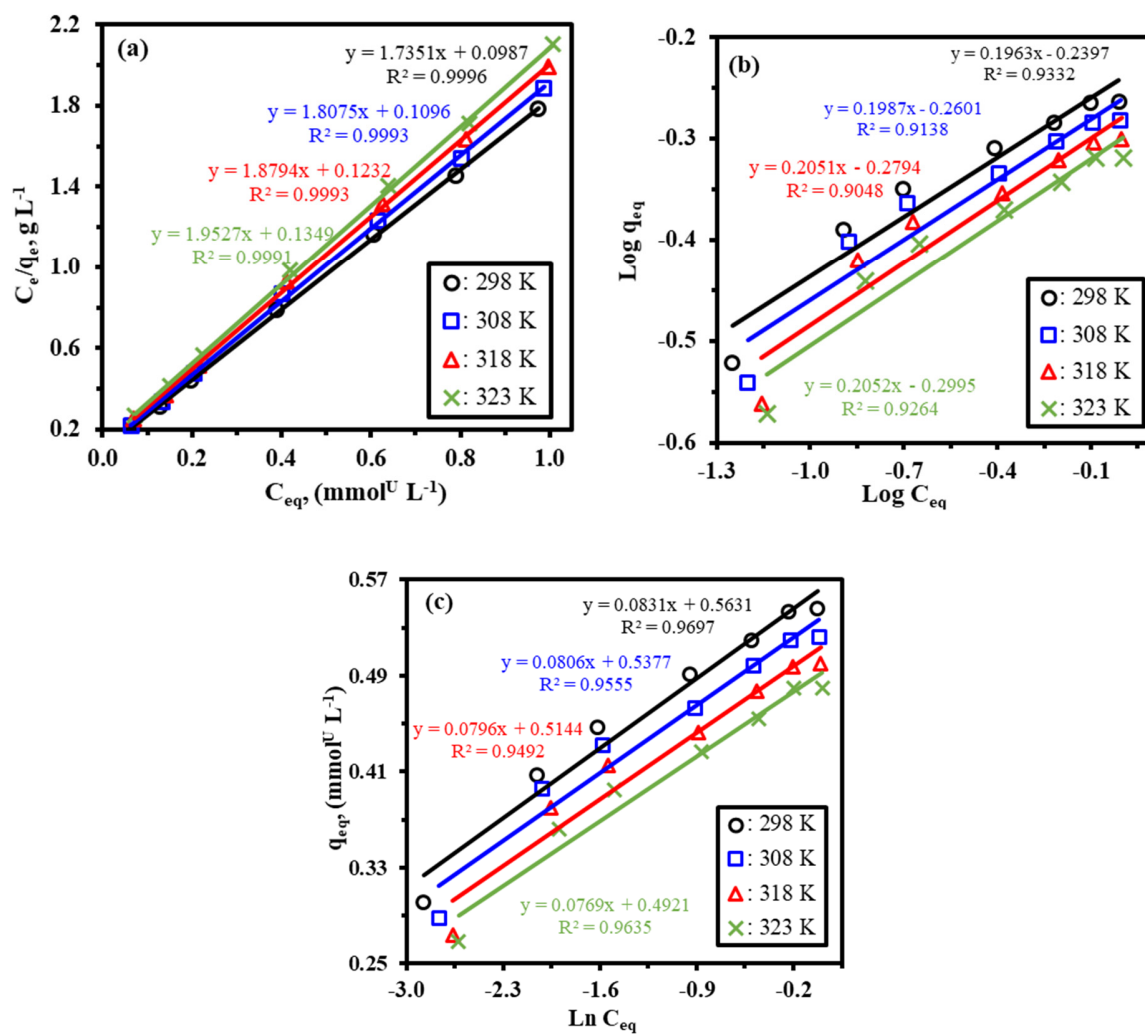
Figure S4. Linearization plots of Langmuir (a), Freundlich (b), and Timken isotherm (c): for UO_2^{2+} sorption. (pH$_0$: 4.0,

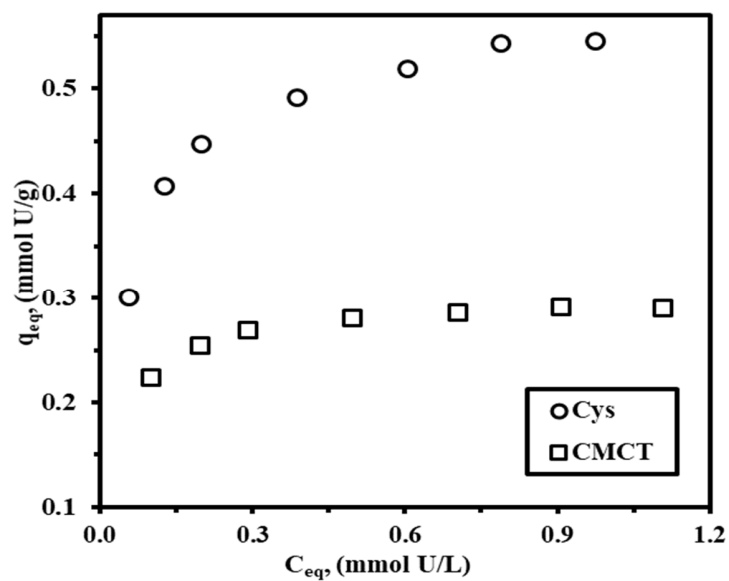SD: 0.5 g L^{-1}, C$_0$: 0.21–1.26 mmol U/L; T: 298–328 K, Time: 60 min.).

Figure S5. Sorption isotherm using both CMCT and Cys nanocomposites for UO_2^{2+} sorption. (pH$_0$: 4.0, SD: 0.5 g/L,

C$_0$: 0.21–1.26 mmol U/L, T: 298–328 K, Time: 60 min for Cys and 180 min for CMCT).

References

[1] X. Hu, C. Chen, D. Zhang, Y. Xue, Kinetics, isotherm and chemical speciation analysis of Hg(II) adsorption over oxygen-containing MXene adsorbent, Chemosphere 278 (2021) 130206.
[2] C. Tien, Adsorption calculations and modeling, Butterworth-Heinemann, Boston, 1994.