

Preparation and Characterization of an Electrospun Whey Protein/Polycaprolactone Nanofiber Membrane for Chromium Removal from Water

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Table S1. Classical kinetic models.

Model	Equation
Pseudo first order	$q_t = q_{te}(1 - e^{-K_1 t})$
Pseudo Second order	$q_t = \frac{q_{te}^2 K_2 t}{1 + q_{te} K_2 t}$
Intraparticle diffusion	$q_t = k_{te} t^{0.5} + C$

Where q_t (mg/g) and q_{te} (mg/g) are the quantity of chromium adsorbed per mass unit of membrane at a given time t , and at equilibrium, respectively; K_1 and K_2 (mg min⁻¹) are the first-order rate constant and second-order rate constant, respectively; k_{te} (mg/(g min^{1/2})) is the Intraparticle diffusion rate constant; C is a model constant (mg/g).

Table S2. Classical isotherm models.

Model	Equation
Langmuir	$q_e = \frac{q_m K_L C_e}{1 + K_L C_e}$
Freundlich	$q_e = K_F C_e^{1/n}$
Sips	$q_e = \frac{q_s K_s C_e^{n_s}}{1 + K_s C_e^{n_s}}$

Where q_e and C_e are the adsorption capacity (mg/g) and concentration (mg/L) at equilibrium, q_m and q_s are the theoretical maximum adsorption capacity (mg/g), K_L (L/mg), K_F (mg^{1-1/n} L^{1/n} g⁻¹), K_s (L^{ns}/mg^{ns}) represents the Langmuir, Freundlich and Sips equilibrium constants, n is the parameters characteristic of the adsorbent-adsorbate system and n_s is the heterogeneity Sips parameter.

Table S3. Results of data correlation of adsorption isotherms to classical models for chromium removal from aqueous solutions using and WPI-PCL adsorptive membrane.

Temperature (°C)	pH	Model					
		Langmuir			Freundlich		
		q_m	K_L	R^2	K_F	n	R^2
20	2	26.4	0.039	0.96	3.1	2.4	0.87
	2	31.4	0.072	0.98	5.7	2.8	0.94
30	3	13.5	0.069	0.98	2.0	2.4	0.92
	5	10.5	0.110	0.98	2.3	2.8	0.96
	9	7.5	0.327	0.96	3.2	5.3	0.92

11	3.1	0.561	0.99	1.4	5.1	0.86
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Table S4. Contributions of individual chemical moieties in the high-resolution spectra of the WPI-PCL adsorptive membrane before and after chromium adsorption.

Element	Chemical moiety	Before		After	
		Binding Energy	% Relative Content	Binding Energy	% Relative Content
Cr 2p 3/2	Cr (VI)	-	-	577.6	23.73
	Cr (III)	-	-	579.3	41.25
Cr 2p 1/2	Cr (VI)	-	-	586.89	14.98
	Cr (III)	-	-	589.56	20.04
C1 s	C-(C,H)	284.8	31.92	284.81	41.07
	C-O	286.1	49.71	285.9	43.49
	C=O	288.73	18.37	288.43	15.45
O1 s	C-O	533.66	71.88	533.32	48.1
	C=O	532.13	28.12	531.91	51.9
N1 s	NHC=O	401.26	38.17	400.36	36.83
	NH2	399.87	48.07	399.93	44.43
	NH3	401.91	13.76	400.75	18.75

Table S5. Results of the atomic concentration of the general XPS before and after chromium adsorption by the membrane.

Atomic concentration [%]		
Element	Before	After
C	74.95	75.07
O	18.18	19.8
N	6.86	4.37
Cr	-	0.76