Polyethylenimine functionalized mesoporous silica-chitosan composites and their performance on Pb(II) adsorption

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Equations

The adsorption percentage (A%) and adsorption capacity (q_e, mg g^{-1}) of Pb(II) on the adsorbents were calculated on the basis of equation (S1) and (S2):

$$A\% = \frac{(C_i - C_e)}{C_i} \times 100\% \qquad \text{(S1)}$$

$$q_e = \frac{(C_i - C_e) \times V}{W} \qquad \text{(S2)}$$

Where C_i and C_e represent the initial and equilibrium adsorption concentration of metal ions in the solution, respectively. V (L) is the volume of Pb(II) solution, and W (mg) is the mass of adsorbent in the solution.

The pseudo-first-order (equation S1), pseudo-second-order (equation S2), Elovich equations (S3) and intraparticle diffusion kinetic model (equation S4) are as follows:

$$\ln(q_e - q_t) = \ln q_e - k_1 t \qquad \text{(S3)}$$

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \qquad \text{(S4)}$$

$$q_t = \frac{1}{b}\ln(ab) + \frac{1}{b}\ln t \qquad \text{(S5)}$$

$$q_t = k_p t^{0.5} + C \qquad \text{(S6)}$$

where q_e (mg g^{-1}) and q_t (mg g^{-1}) are the adsorption amount at equilibrium time and a certain time t (h), respectively. k_1 (h^{-1}), k_2 (g mg^{-1} h^{-1}) and k_p (mg g^{-1} h$^{0.5}$) are the rate constant of the homologous kinetics equations, respectively. And a (mg g^{-1} h^{-1}) represents Elovich constant and b (g mg^{-1}) represents a coefficient associated with the activation energy of the adsorption. C is a constant related to the boundary layer thickness.

The Gibbs free energy change (ΔG^0), enthalpy change (ΔH^0), and entropy change (ΔS^0) of the adsorption process were calculated by the following equations (S7-S10):

$$K_{\mathrm{d}} = \frac{C_{\mathrm{a}}}{C_{\mathrm{e}}} \quad \text{(S7)}$$

$$\Delta G^0 = -RT \ln K_d \quad \text{(S8)}$$

$$\ln K_d = \frac{\Delta S^0}{R} - \frac{\Delta H^0}{RT} \quad \text{(S9)}$$

$$\Delta G^0 = \Delta H^0 - T\Delta S^0 \quad \text{(S10)}$$

Where C_{a} (mg·L^{-1}) is the adsorbed concentration at equilibrium, C_{e} (mg·L^{-1}) is the equilibrium concentration of the solution, K_{d} is the equilibrium constant, R (8.314 J·mol^{-1}·K^{-1}) is the universal gas constant and T (K) is the absolute temperature.

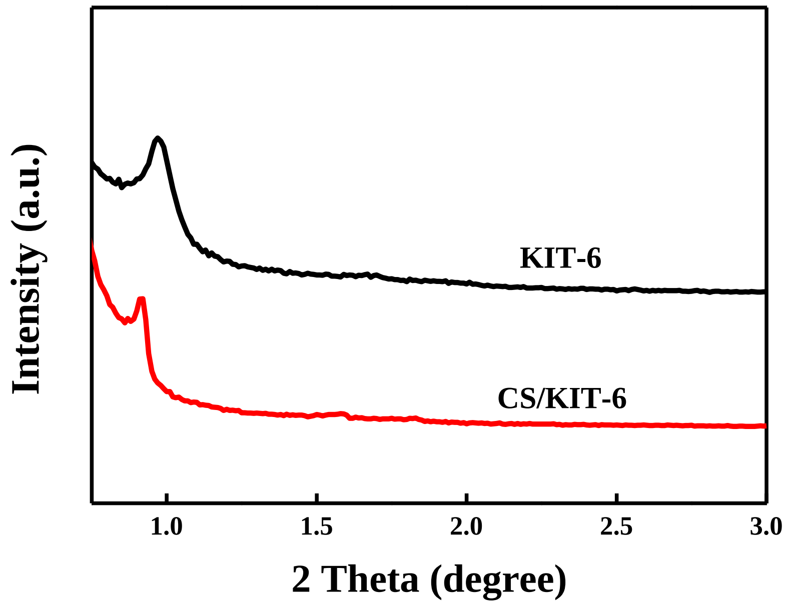

Fig. S1 Small angle XRD patterns of the synthesized KIT-6 type composites.

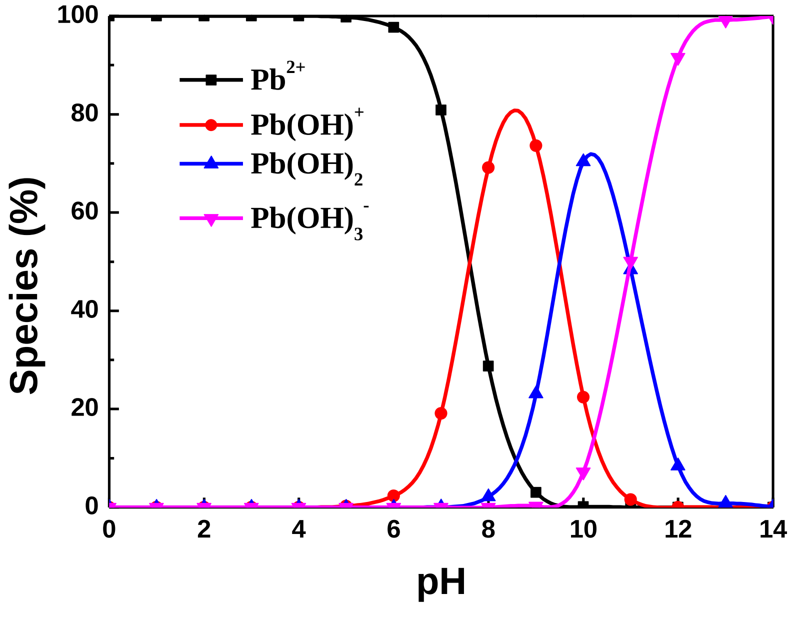

Fig. S2 The speciation diagram of Pb at varies pH values.

Table S1 Adsorption kinetic parameters of different temperatures for Pb(II) adsorption on CK-T_{50}/t_{20}-$m_{0.2}$.

Temperature	q_e	pseudo first-order equation			pseudo second-order equation			Elovich equation			Intraparticle diffusion	
(K)	(mg·g^{-1})	q_e (mg·g^{-1})	k (g·mg^{-1}·h^{-1})	R^2	q_e (mg·g^{-1})	k (g·mg^{-1}·h^{-1})	R^2	α (mg·g^{-1}·h^{-1})	β (g·mg^{-1})	R^2	k_p (mg·g^{-1}·h$^{1/2}$)	R^2
303	18.43	14.78	-0.19	0.97	19.36	0.59	0.99	43.5124	0.33	0.94	3.74	0.91
313	18.87	14.29	-0.18	0.97	20.00	0.68	0.99	55.4857	0.33	0.94	3.67	0.90
323	21.21	15.14	-0.25	0.97	20.41	0.89	1.00	13.8459	0.32	0.88	3.65	0.88

Table S2 Adsorption isotherm parameters for Pb(II) adsorption onto the prepared adsorbents at 303 K, pH 6.

Adsorbent	Langmuir			Freundlich			Temkin		
	q_{max} (mg g^{-1})	K_L (mg L^{-1})	R^2	K_F (L mg^{-1})	n	R^2	A (L·g^{-1})	b	R^2
CK-T_{50}/t_5-$m_{0.2}$	211.89	0.0144	0.9689	16.7171	2.6666	0.9380	0.3943	83.6101	0.9380
CK-T_{50}/t_{10}-$m_{0.2}$	159.57	0.0076	0.9813	17.1101	2.6949	0.8958	0.2363	74.2388	0.9621
CK-T_{50}/t_{20}-$m_{0.2}$	279.08	0.0251	0.9938	22.6417	2.6621	0.9671	0.3352	59.6432	0.9646
CK-T_{70}/t_{20}-$m_{0.2}$	219.60	0.0145	0.9718	12.8447	2.4281	0.9536	0.4462	92.6737	0.8725
CK-T_{50}/t_{20}-$m_{0.1}$	146.72	0.0115	0.9856	6.6441	2.2094	0.9626	0.1161	99.3063	0.9708
CK-T_{50}/t_{20}-$m_{0.3}$	149.70	0.0091	0.9888	19.6447	3.0155	0.9195	0.7251	104.5448	0.9190
CK-T_{50}/t_{20}-$m_{0.4}$	160.10	0.0102	0.9959	30.4245	3.6095	0.8596	0.8188	92.3555	0.9385