polymers

MDPI

Supplementary Information

1. Experimental

1.1. Swelling experiments

To evaluate the durability of XMPC, deionized water (pH = 7), acidic (pH = 3, aqueous hydrochloric acid), and basic media (pH = 11, aqueous sodium hydroxide) were used for the swelling test. 1 g of sample immersed in 200 mL deionized water, acidic, and basic media for 10 days, respectively. Then the swollen samples were weighted immediately after removing excess water. The swelling ratio (Sw) is calculated as:

$$Sw = (Ws–Wd)/W\ d \quad (S1)$$

where *Wd* and *Ws* are the masses before and after immersed for 10 days, respectively.

2. Results and discussion

2.1. Adsorption studies

The adsorption capacity Q_e (mg/g) of XMPC toward metal ions at equilibrium was calculated as following Equation S1:

$$Q_e = (Co - Ce)V/m \quad (S2)$$

where C_0 and C_e are the initial and equilibrium concentrations (mg/L) of metal ions in solution, respectively. V (L) is the volume of solution and m (g) is the mass of XMPC.

2.2. Adsorption kinetics

Pseudo-first-order model:

$$\lg(Q_e - Q_t) = \log Q_e - k_1 t \quad (S3)$$

Pseudo-second-order model:

$$\frac{t}{Q_t} = \frac{1}{k_2 Q_e^2} + \frac{1}{Q_e} t \quad (S4)$$

Intraparticle diffusion model:

$$Q_t = k_3 t^{1/2} + C \quad (S5)$$

Where k_1 (1/min) and k_2 g/(mg·min) are the rate constants for first-order and second-order models, respectively; k_3 [mg/(g·min$^{1/2}$)] is a constant related to the diffusion coefficient in intraparticle diffusion model; C is the intercept for the intraparticle diffusion model; Q_e is the fitted adsorption value (mg/g) at equilibrium, and Q_t is the experimental value (mg/g) at set time t (min), respectively.

2.3. Adsorption isotherms

Langmuir model:

$$\frac{C_e}{Q_e} = \frac{C_e}{Q_m} + \frac{1}{K_l Q_m} \quad (S6)$$

Freundlich model:

$$\log Q_e = b_F \log C_e + \log K_F \quad (S7)$$

Where Q_m is the maximum adsorption capacity (mg/g), C_e is the final equilibrium mercury concentration (mg/L), K_L is the Langmuir constant (L/mg) related to the adsorption strength. K_F is the Freundlich constant related to the adsorption strength (mg/g) (L/mg),

Langmuir isotherm describes a monolayer adsorption which takes place at homogeneous sites within the adsorbent where all the adsorption sites are energetically identical. Freundlich isotherm expresses adsorption at multilayer and on the energetically heterogeneous surface and active sites.

2.4. Absorption thermodynamics

$$\Delta G^{\circ} = -RT\ln K_0 \quad \text{(S8)}$$

$$\ln K_0 = \frac{\Delta S^{\circ}}{R} - \frac{\Delta H^{\circ}}{RT} \quad \text{(S9)}$$

Where K_0 is distribution coefficient, R is the gas constant (8.314 J / (mol·K)), T is the temperature (K).ΔG_0 is the standard Gibbs free energy change, $\Delta H0$ is the standard enthalpy change (J/mol), and ΔS_0 is the standard entropy change (J/(mol·K)). K_0 was obtained from the intercept of plotting ln(qe/Ce) versus Ce at three different temperatures by extrapolating Ce to zero. ΔH_0 and ΔS_0 were obtained from the slope and intercept in the curve of $\ln K_0$ versus T^{-1}.

2.5. Selective adsorption behaviors of heavy metals

The selectivity of XMPC for metal ions over other metal ions can be evaluated using the selectivity coefficient (Ks). It is an important parameter to express the removal selectivity of the adsorbent toward objective metal ions in a complex components solution, which can be derived by the following Equation S10:

$$K_s = \frac{K_d(T)}{K_d(I)} \quad \text{(S10)}$$

where Kd is the distribution coefficient of metal ions and was calculated by Equation S11:

$$K_d = \frac{Q_e}{C_e} \quad \text{(S11)}$$

Table S1. Swelling ratio of XMPC.

pH	W_d (g)	W_S (g)	S_w
3	0.20	1.52	6.6
7	0.20	1.37	5.8
11	0.20	1.29	5.5

Table S2. Adsorption and desorption data of heavy metal ion adsorption by XMPC.

Time	Qe(mg/g)			Adsorption rate (%)			Desorption rate (%)		
	Pb(II)	Cu(II)	Cd(II)	Pb(II)	Cu(II)	Cd(II)	Pb(II)	Cu(II)	Cd(II)
1	62.19	89.96	116.28	33.05	54.18	86.95	89.35	81.82	84.86
2	54.78	84.26	100.15	27.32	49.06	66.83	79.52	79.43	70.13
3	48.60	78.97	97.15	24.68	44.76	41.65	62.66	72.80	63.20
4	42.93	81.51	81.60	22.00	43.03	48.46	60.33	53.85	61.63
5	40.09	60.17	77.56	18.79	35.91	44.71	59.01	57.37	49.27
6	40.35	55.39.	64.99	18.42	34.98	34,23	55.27	47.54	45.67
7	36.10	55.09	54.00	17.18	31.13	26.74	41.19	41.99	42.57
8	26.62	84.81	34.37	12.13	25.50	19.46	38.05	34.56	41.93
9	26.81	49.94	26.48	12.72	26.53	14.38	40.65	35.30	41.21
10	24.60	41.81	37.41	10.99	20.15	16.38	39.68	42.96	30.26

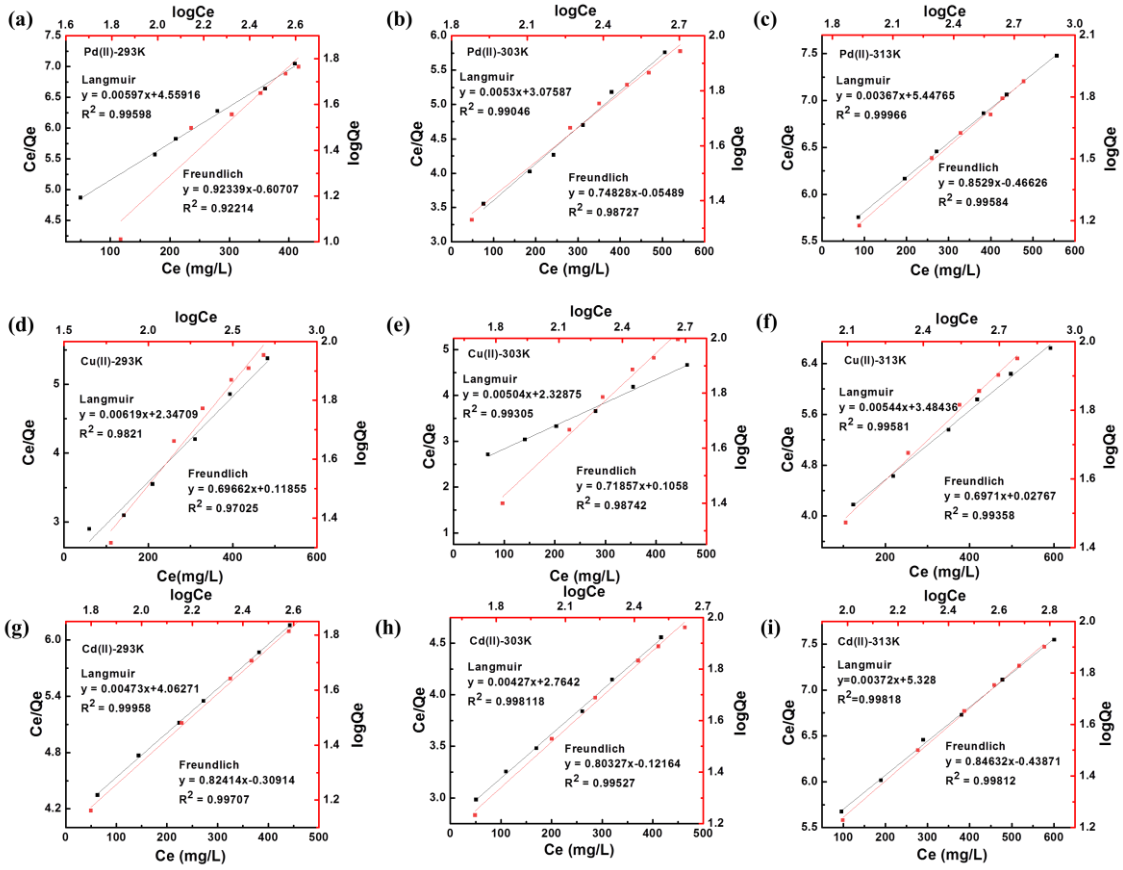

Figure S1. Adsorption isotherms for metal ions on XMPC. (**a**) Pd(II) at 293K, (**b**) Pd(II) at 303K, (**c**) Pd(II) at 313K, (**d**) Cu(II) at 293K, (**e**) Cu(II) at 303K, (**f**) Cu(II) at 313K, (**g**) Cd(II) at 293K, (**h**) Cd(II) at 303K, and (**i**) Cd(II) at 313K.