Supplementary material for

Investigating the potential of N-methylglucamine modified cellulose microspheres for Sb(III) and Sb(V) removal from actual mine inflow

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Text S1:

Specifically, 5.0 g Celp sealed in polyethylene bag was purged with nitrogen gas for 3 min. The samples were irradiated at dose of 30 kGy by EB accelerator (1MeV, 10 kGy/pass) under the cooling of dry-ice, followed by injecting 50 mL GMA emulsion solution (30 % GMA, 3 % surfactant Tween 20) into the sample bag. Subsequently, the mixture was placed in a water bath at 50 ℃ for 2 h. The resulting product was labelled as Celp-g-GMA and purified from copolymer and unreacted monomer using acetone and ultrapure water. And the grafted polymers Celp-g-GMA were desiccated in vacuum at 60 ℃.

The equations for PFO and PSO models (Eq.S1- Eq.S2) are presented as follows:

$$q_t = q_e(1-e^{-k_1 t}) \quad \text{(S1)}$$

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \quad \text{(S2)}$$

where k_1 (h^{-1}) and k_2 (h^{-1} g mg^{-1}) were rate constant for PFO and the PSO model, respectively. q_e (mg/g) and q_t (mg/g) represented the amounts of Sb adsorbed per gram adsorbent at equilibrium and at time t (h), respectively.

The isotherm data for the capture of Sb(III) and Sb(V) by Celp-g-GMA-NMG were fitted using the Langmuir (Eq. S3) and Freundlich models (Eq. S4).

$$C_e / Q_e = C_e / Q_m + 1/(K_L \times Q_m) \quad \text{(S3)}$$

$$\ln Q_e = \ln K_F + \frac{1}{n}\ln C_e \quad \text{(S4)}$$

where the equilibrium concentration and adsorption capacity of Sb are denoted by C_e (mg/L) and Q_e (mg/g). Q_m (mg/g) is the theoretical maximum adsorption capacity of Sb on Celp-g-GMA-NMG. The Langmuir and Freundlich constants are expressed by K_L (L/mol) and K_F ((mg/g)/(L/mg)$^{1/n}$), respectively. The Freundlich exponent (n) represents the adsorption intensity.

The thermodynamic data for the adsorption of Sb(III) and Sb(V) onto Celp-g-GMA-NMG were fitted using Eq. (S5) and Eq. (S6).

$$\lg K_d = \frac{-\Delta H}{2.303RT} + \frac{\Delta S}{2.303R} \quad \text{(S5)}$$

$$\Delta G = \Delta H - T\Delta S \quad \text{(S6)}$$

where ΔG (kJ/mol), ΔS (J/mol), and ΔH (kJ/mol) were Gibbs free energy, entropy and enthalpy, respectively. R was the molar gas constant (8.314 J/mol K) and T (K) represented the adsorption absolute temperature.

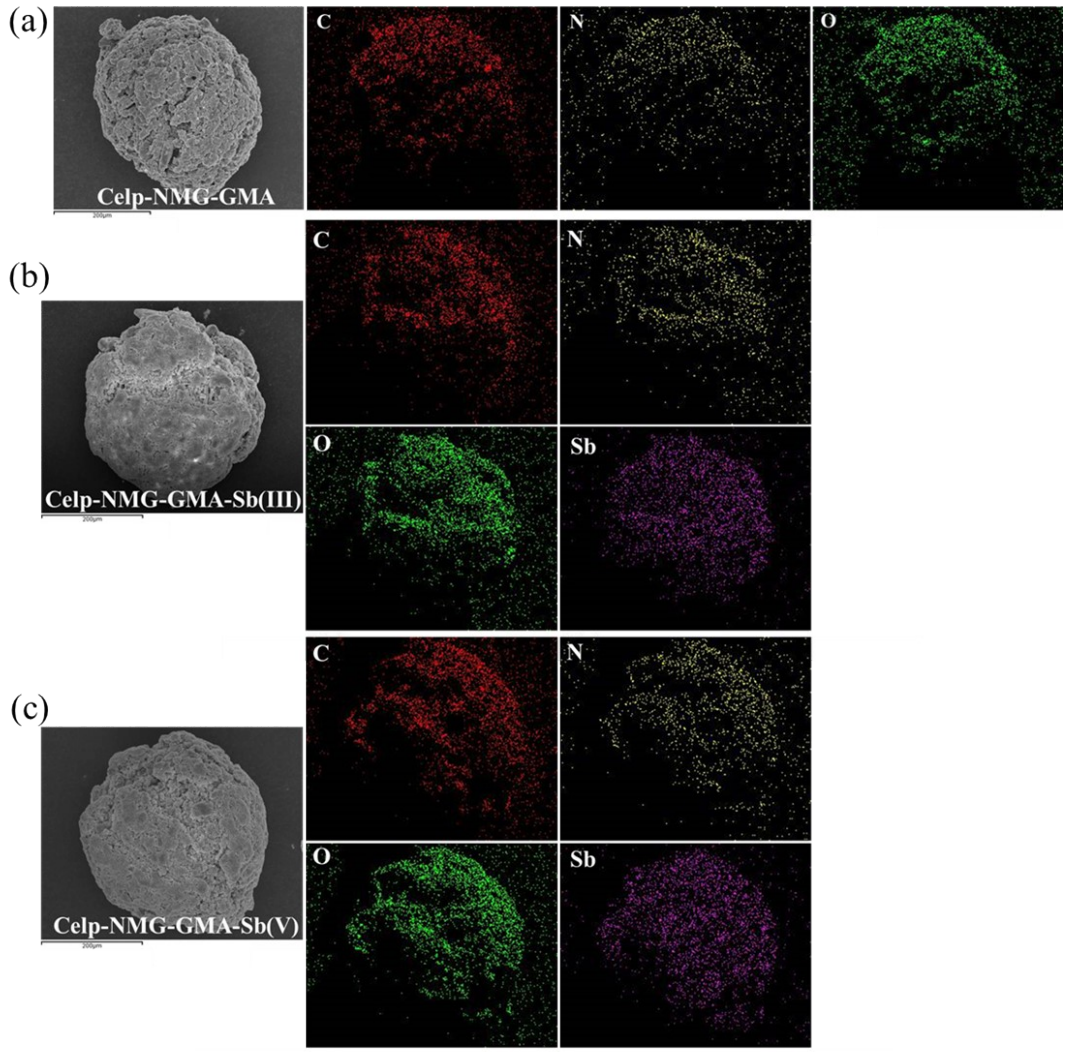

Fig. S1 SEM and elemental mapping images of Celp-g-GMA-NMG before and after adsorption.

Table S1 Kinetic parameter of Sb(III/V) individual adsorption onto Celp-g-GMA-NMG.

Parameter	Sb(III)	Sb(V)
$q_{e,exp}$ / (mg·g^{-1})	10.26	11.74
t_e / (h)	6	1.5
Pseudo-first order model		
$q_{e,est}$ / (mg·g^{-1})	9.4048	9.4048
k_1 / (h^{-1})	0.1031	0.0832
R^2	0.9214	0.9606
R^2_{adj}	0.9127	0.9550
χ^2_{red}	0.6128	0.1197
RSS	5.5150	0.8382
Pseudo-second order model		
$q_{e,est}$ / (mg·g^{-1})	10.1926	11.5340
k_2 / (g·mg^{-1}·h^{-1})	0.0103	0.0152
R^2	0.9999	0.9998
R^2_{adj}	0.9998	0.9998
RSS	1.8384	0.8048

k_1 and k_2: Adsorption kinetic rate constants of Pseudo-first order and Pseudo-second order models, respectively;
R^2: correlation coefficient;
R^2_{adj}: adjusted R^2;
χ^2_{red}: Reduced chi-square;
RRS: Residual Sum of Squares.

Table S2 Isotherm parameter of Sb(III/V) individual adsorption onto Celp-g-GMA-NMG.

Parameter	Sb(III)	Sb(V)
	Langmuir model	
$q_{e,est}$ / (mg·g^{-1})	217.61	49.11
k_L / (L·mg^{-1})	0.1505	3.7466
R^2	0.9827	0.9639
R^2_{adj}	0.9802	0.9567
χ^2_{red}	135.5199	18.5917
RSS	948.6390	92.9585
	Freundlich model	
n	4.2676	6.3154
k_F / (mg/g)/(L/mg)$^{1/n}$)	62.7840	23.2958
R^2	0.9592	0.90502
R^2_{adj}	0.9533	0.88602
χ^2_{red}	319.6012	48.9039
RSS	2237.2086	244.5196

K_L: the Langmuir constant:

K_F and n: the Freundlich adsorption coefficient and constant, respectively:

R^2: correlation coefficient;

R^2_{adj}: adjusted R^2;

χ^2_{red}: Reduced chi-square;

RRS: Residual Sum of Squares.

Table S3 Calculated thermodynamic parameters of Celp-g-GMA-NMG.

	Δ H (kJ/mol)	ΔS (J/mol)	T (K)	ΔG (kJ/mol)	R^2
Sb(III)	24.21	103.94	298	-6.7382	0.9949
			303	-7.3169	
			308	-7.8228	
			313	-8.2998	
Sb(V)	44.32	185.91	298	-11.1119	0.9982
			303	-11.9704	
			308	-12.9302	
			313	-13.8929	

Table S4 The main composition of actual mine inflow.

Composition	Concentration(mg/L)	Composition	Concentration(mg/L)
Ca	147.40	As	18.20
Sb	10.16	Si	9.07
Sr	0.21	Mg	46.80