

Lignin-based nano-adsorbent for superfast and highly selective removal of phosphate

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The main equations used in this study are as follows:

$$\log(q_e - q_t) = \log q_e - \frac{k_1 t}{2.303} \quad (1)$$

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

Where q_t (mg g⁻¹) and q_e are the adsorbed capacities (mg g⁻¹) at time t (min) and equilibrium, respectively, respectively; k_1 (min⁻¹) and k_2 (g mg⁻¹ min⁻¹) are the related reaction rate constants.

$$q_t = k_{dr} \sqrt{t} + C \quad (3)$$

Where k_i (mg P g⁻¹ min^{-1/2}) is the diffusion rate constant whereas the C is the intercept for the intraparticle diffusion model. Values of k_i and C are calculated from the slope of the linear plot of q_t against $t^{1/2}$.

$$\frac{1}{q_e} = \frac{1}{q_m b C_e} + \frac{1}{q_m} \quad (4)$$

$$\ln q_e = \ln K_f + \frac{1}{n} \ln C_e \quad (5)$$

Where q_e and q_m represent the amount of adsorbing phosphate per unit weight of adsorbent at equilibrium and the maximum adsorption capacity (mg g⁻¹), respectively. C_e (mg L⁻¹), b (L mg⁻¹), K_f , and $1/n$ respectively refer to the equilibrium solution concentration, the Langmuir model constant, a rough indicator of adsorption capacity, and the heterogeneity factor.

$$R_L = \frac{1}{1 + bC_0} \quad (6)$$

Where C_0 is the highest initial phosphate concentration (mg L^{-1}), and the value of R_L can indicate whether the adsorption is irreversible ($R_L = 0$), favorable ($0 < R_L < 1$), linear ($R_L = 1$), or unfavorable ($R_L > 1$).

$$\Delta G^0 = -RT \ln K_d \quad (7)$$

$$\Delta G^0 = \Delta H^0 - T\Delta S^0 \quad (8)$$

$$\ln K_d = \frac{\Delta S^0}{R} - \frac{\Delta H^0}{RT} \quad (9)$$

Where K_d is the adsorption distribution coefficient at different temperatures, and the value is computed by the ratio of the equilibrium (q_e) to equilibrium (C_e)

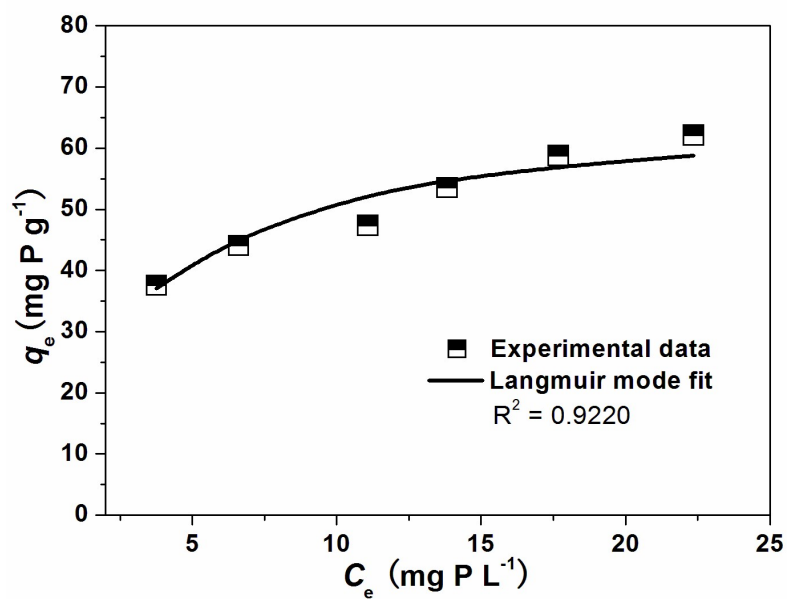


Fig. S1. Phosphate adsorption isotherm of AL-PEI-La in the ice-water bath at 273 K

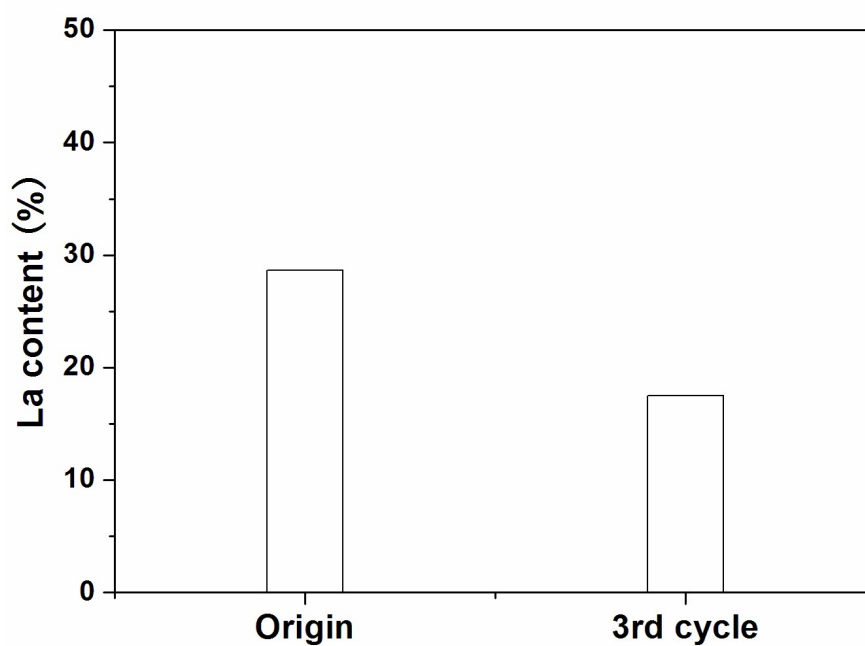


Fig. S2. The lanthanum content of AL-PEI-La origin AL-PEI-La and AL-PEI-LA after 3 cycles

Table S1. Adsorption kinetics fitting results for phosphate on AL-PEI-La by pseudo-first-order, pseudo-second-order, and intraparticle diffusion models.

C_0 (mg P L ⁻¹)	$(q_{e,exp})$	Pseudo-first-order kinetics			Pseudo-second-order kinetics		
		$(q_{e,cal})$ (mg P g ⁻¹)	k_1 (g mg ⁻¹ min ⁻¹)	R^2	$(q_{e,cal})$ (mg P g ⁻¹)	k_2 (g mg ⁻¹ min ⁻¹)	R^2
50	37.27	5.00	0.011	0.8830	37.59	0.07	1.0000
Intra-particle diffusion model							
C_1 (mg P g ⁻¹)	k_{d1} (mg P g ⁻¹ min ^{-1/2})	R_1^2	C_2 (mg P g ⁻¹)	k_{d2} (mg P g ⁻¹ min ^{-1/2})	R_2^2		
50	0	27.43	1.000	26.29	2.171	0.913	

Table S2. Equilibrium parameters of Langmuir and Freundlich models

Temperature (K)	Langmuir constans		isotherm	Freundlich constans		isotherm
	b (L mg ⁻¹)	q_m (mg g ⁻¹)	R^2	K_f	n	R^2
298	4.47	65.79	0.9700	52.25	12.74	0.8796
308	4.32	74.60	0.9249	51.46	8.12	0.7564
318	0.57	85.47	0.9213	56.39	9.46	0.8612

Table S3. Thermodynamic parameters of phosphate adsorption on AL-PEI-La at 298

K, 308 K, and 318 K, respectively.

Temperature (K)	Thermodynamic parameters		
	ΔG^0 (kJ mol ⁻¹)	ΔH^0 (kJ mol ⁻¹)	ΔS^0 (J mol ⁻¹ K ⁻¹)
298	-4.43	21.23	85.97
308	-5.21	21.23	85.97
318	-6.15	21.23	85.97