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# 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:

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

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

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.

$$q_t = k_{di}\sqrt{t} + C \qquad (3)$$

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 $t^{1/2}$.

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

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

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.

$$R_L = \frac{1}{1 + bC_0} \tag{6}$$

Where $C_o$ 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 ($R_L > 1$).

$$\Delta G^0 = -RT\, lnK_d \tag{7}$$

$$\Delta G^0 = \Delta H^0 - T\Delta S^0 \tag{8}$$

$$lnK_d = \frac{\Delta S^0}{R} - \frac{\Delta H^0}{RT} \tag{9}$$

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 ($C_e$)

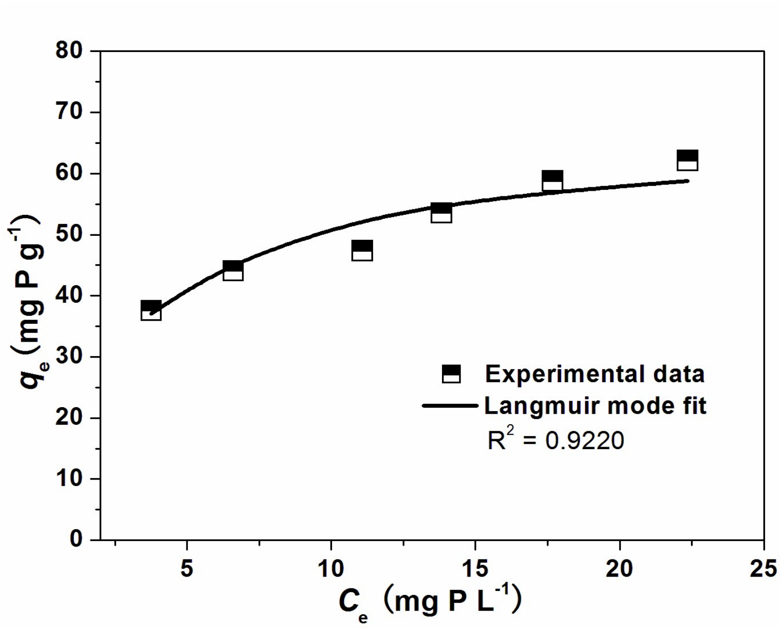


Fig. S1. Phosphate adsorption isotherm of AL-PEI-La in the ice-water bath at 273 K

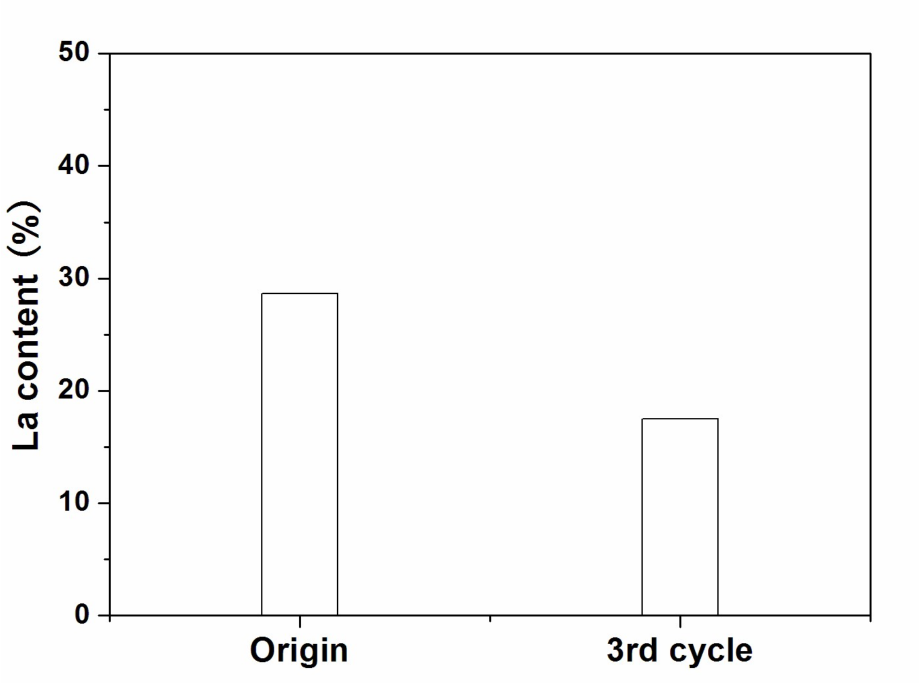


Fig. S2. The lanthanum content of AL-PEI-La origin AL-PEI-La and AL-PEI-LA after 3 cycles

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

| $C_o$ (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 isotherm constans | | | Freundlich isotherm constans | | |
|---|---|---|---|---|---|---|---|
| | | b (L $mg^{-1}$) | $q_m$ (mg $g^{-1}$) | $R^2$ | $K_f$ | n | $R^2$ |
| AL-PEI-La | 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 | | |
|---|---|---|---|
| | $\Delta G^0$ (kJ mol$^{-1}$) | $\Delta H^0$ (kJ mol$^{-1}$) | $\Delta S^0$ (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 |