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Synthesis of poly(hexachlorocyclotriphosphazene-co-phenolphthalein) microspheres with negative charges for the selective removal of cationic dyes

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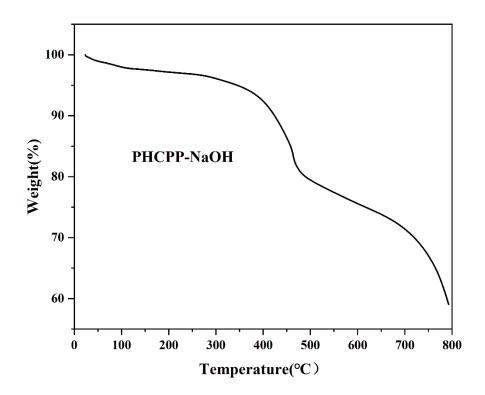


Figure S1. The thermogravimetric analysis curves of prepared PHCPP-NaOH.

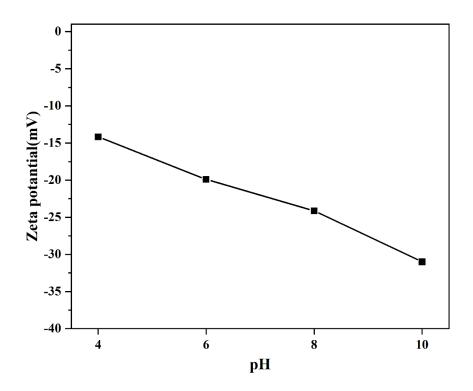


Figure S2. The zeta potential analysis curves of prepared PHCPP-NaOH.

The pseudo-first-order kinetic model (equation S1) and pseudo-second-order kinetic model (equation S2) to fit the experimental data.

$$\ln (q_e - q_t) = \ln (q_e) - k_1 t$$
equation S1
$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e} t$$
equation S2

Where $k_1 \pmod{1}$ and $k_2 \pmod{1}$ represent the rate constants for the pseudofirst-order kinetic model and pseudo-second-order kinetic model, respectively.

Weber's intraparticle diffusion model is an important tool for studying and applying mass transfer and reaction processes in porous media. It helps provide relevant information about different stages of the adsorption process, contributing to a deeper understanding of adsorption characteristics. The equation is expressed as follows equation S3:

$$q_t = K_{ji}t^{1/2} + c_i \qquad \text{equation S3}$$

Where K_{ji} represents the intraparticle diffusion rate constant, and c_i is the intercept of the linear portion of the equation.

The Langmuir adsorption isotherm model is a classic adsorption model used to describe the adsorption behavior of molecules on an adsorbent surface. The Langmuir model is based on a key assumption that adsorbed molecules on the surface can only form a single molecular layer. This implies that the adsorption sites on the adsorbent surface are limited, and once occupied, they are no longer available for the adsorption of other molecules. The equation for this model can be described as follows:

$$\frac{c_e}{q_e} = \frac{1}{k_L q_0} + \frac{c_e}{q_0}$$
 equation S4

Where k_L (L/mg) is the Langmuir constant and q_0 (mg/g) is the maximum monolayer adsorption capacity.

The Freundlich isotherm model is suitable for describing adsorption behavior on heterogeneous surfaces. Unlike the Langmuir model, the Freundlich model does not assume that the adsorbed molecules form a single monolayer on the surface. Instead, it allows for the formation of multiple layers of adsorption on the adsorbent surface, making it applicable to various adsorption systems. The equation is defined as:

$$\ln q_e = \ln k_F + \frac{1}{n} \ln c_e$$
 equation S5

The Freundlich constants, $k_{\rm F}$ (mg/g) and 1/n (with n as the unit of L/mg), correspond to the adsorption capacity and adsorption intensity, respectively, in the Freundlich isotherm model.

The enthalpy change (ΔH^0), entropy change (ΔS^0), and free energy change (ΔG) can be determined using the following equations:

$$\ln k_{d} = \frac{\Delta S^{0}}{R} - \frac{\Delta H^{0}}{RT}$$
equation S6

$$\Delta G^{0} = -RT \ln k_{d}$$
equation S7

$$k_{d} = \frac{q_{e}}{c_{e}}$$
equation S8

Where k_d (L/mol) is the Langmuir equilibrium constant, T (K) is the absolute temperature, R (8.314 (J/mol K)) is the gas constant.