

Supplementary Information for:

Porous organic polymers marry with chelating agents: A facile strategy to develop effective and multi-purpose absorbents for wastewater treatment

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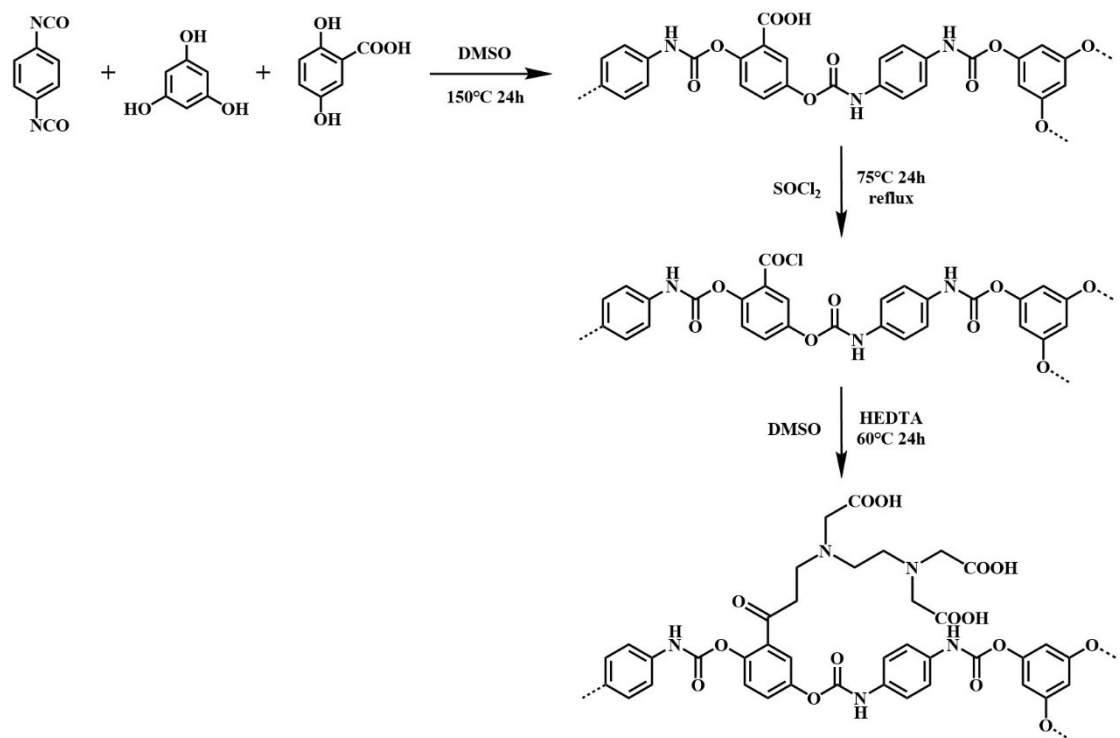


Fig. S1 Preparation progress of CPOP-HEDTA

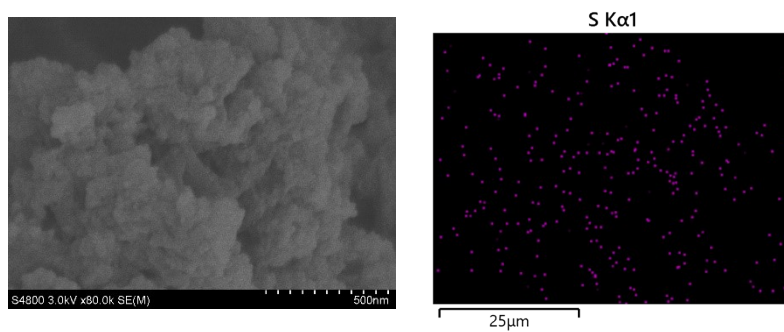


Fig. S2 SEM and elemental mapping image of Sulfur in CPOP-HEDTA before adsorption.

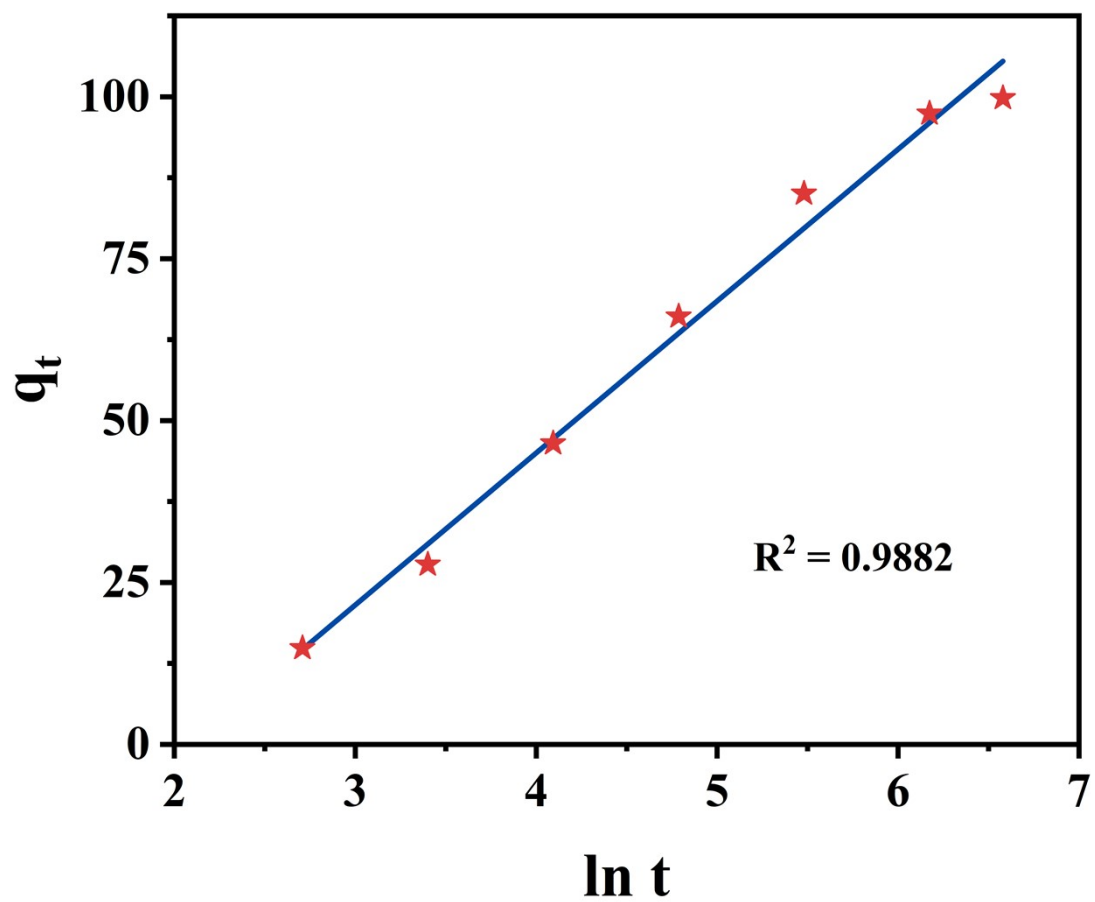


Fig. S3 Elovich model for MB adsorption by CPOP-HEDTA

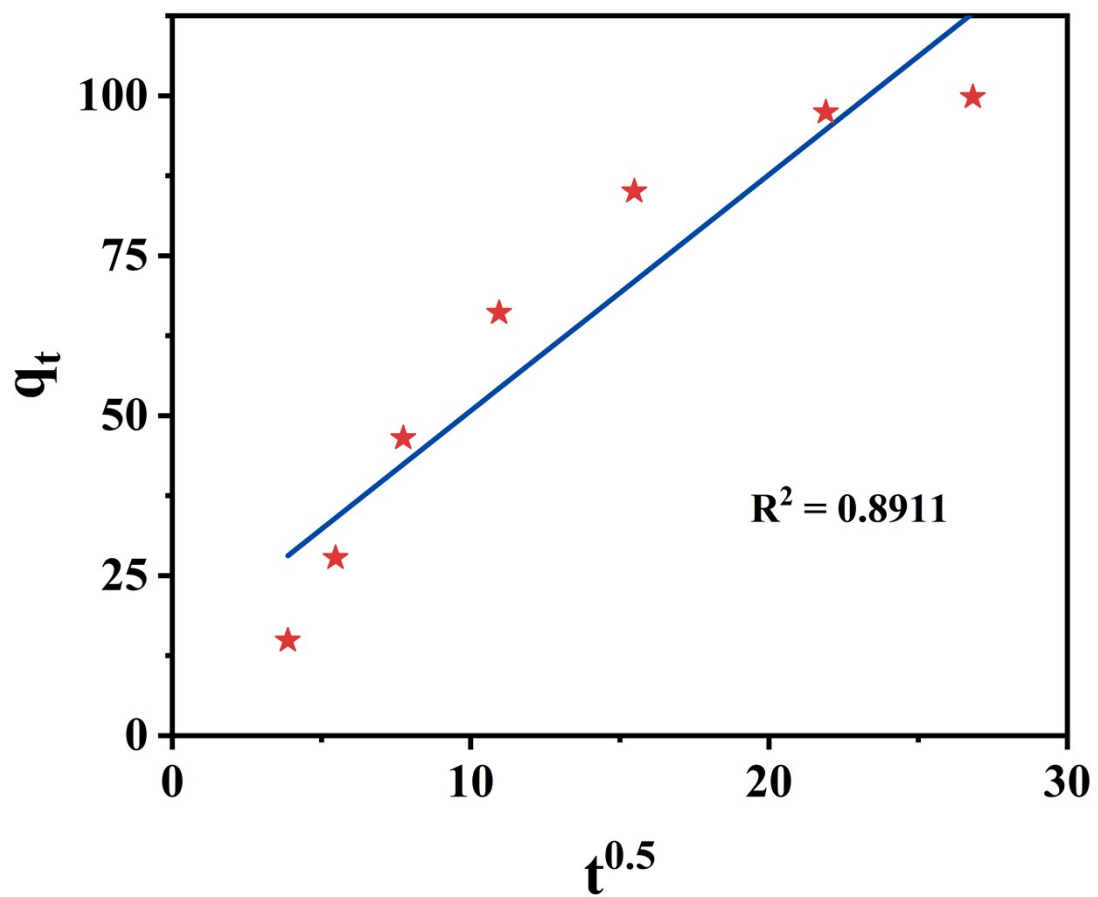


Fig. S4 Intraparticle diffusion model for MB adsorption by CPOP-HEDTA

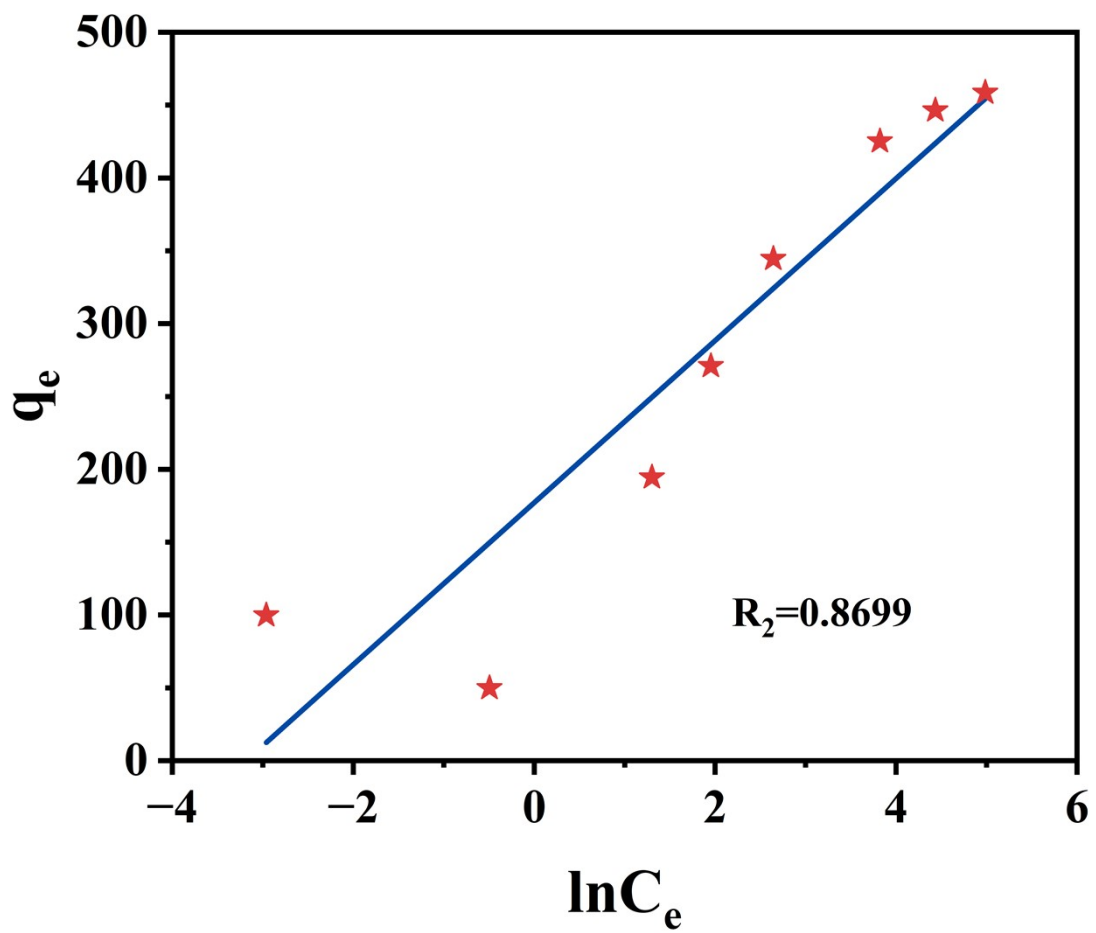


Fig. S5 Tempkin isotherm for MB adsorption by CPOP-HEDTA

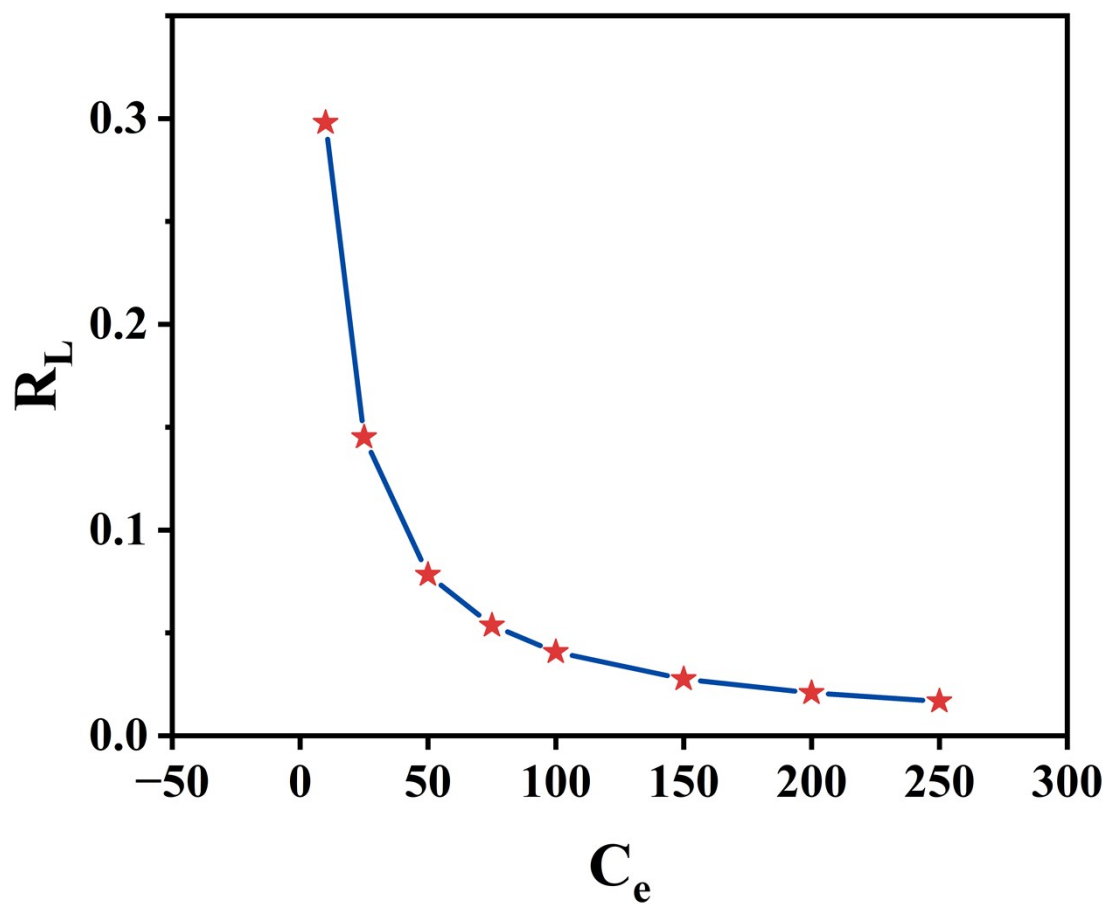
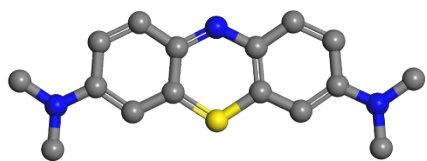
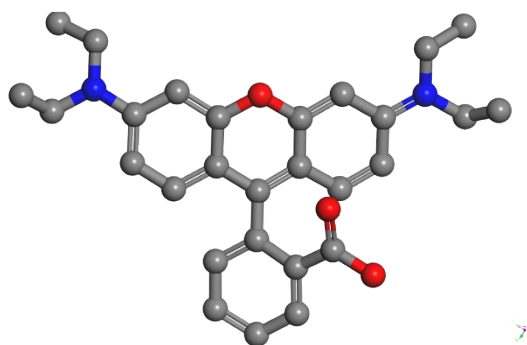


Fig. S6 R_L with distinct initial concentrations for MB adsorption by CPOP-HEDTA

(A)



(B)



(C)

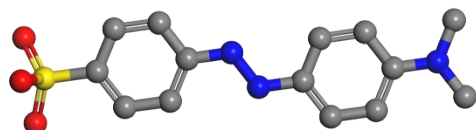


Fig. S7 Ball-and-stick molecule model of (A) methylene blue (B) rhodamine B (C) methyl orange

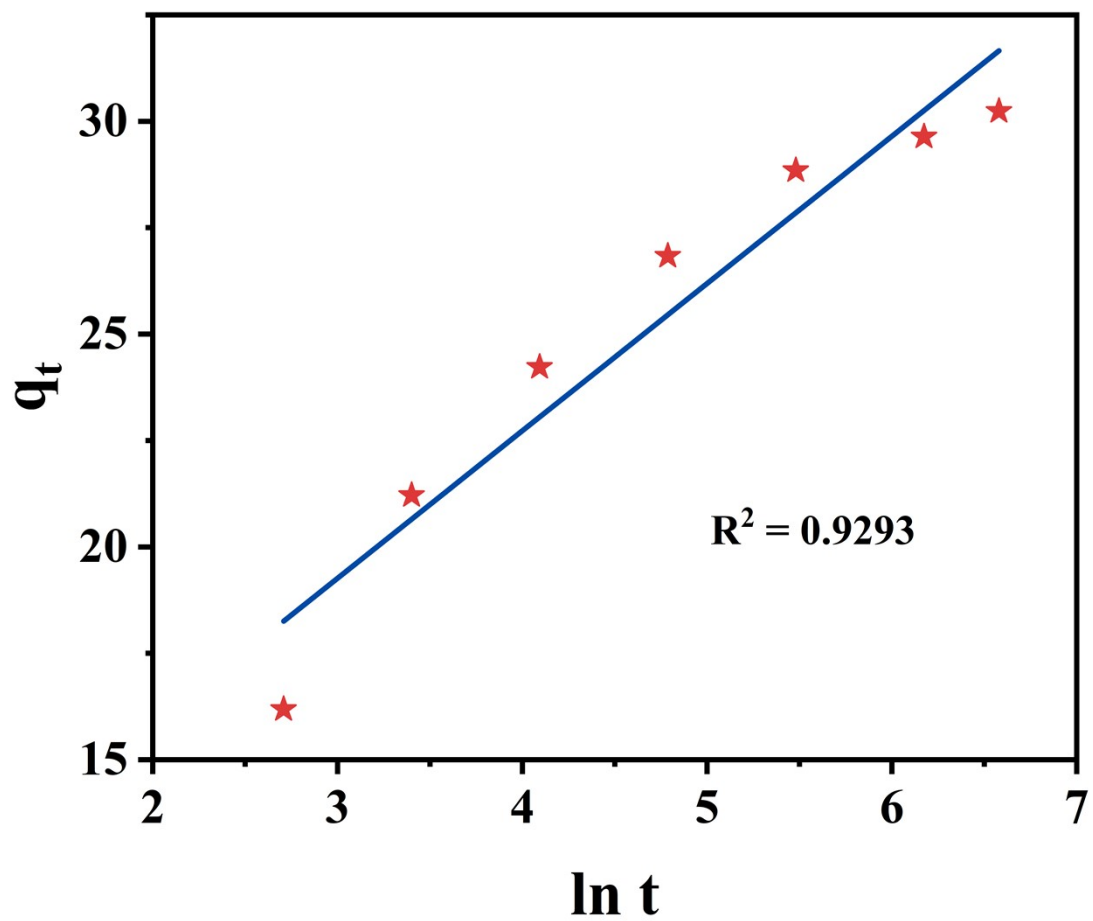


Fig. S8 Elovich model for Fe^{3+} adsorption by CPOP-HEDTA

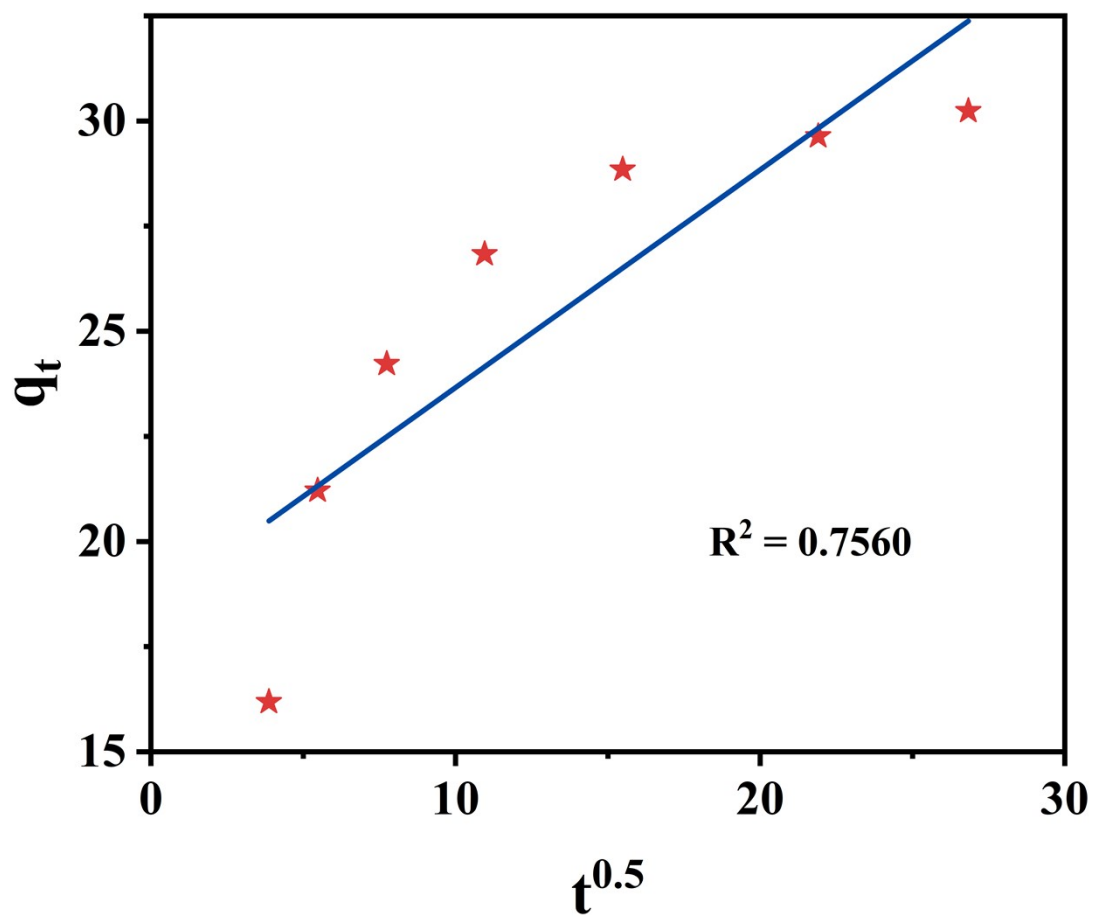


Fig. S9 Intraparticle diffusion model for Fe^{3+} adsorption by CPOP-HEDTA

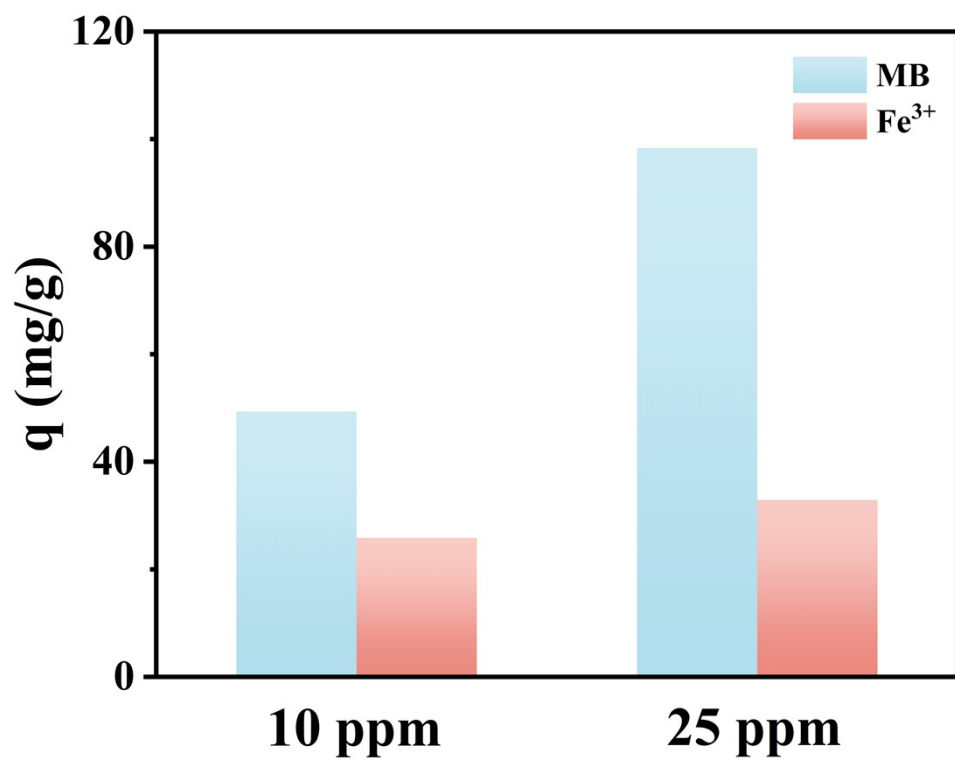


Fig. S10 Synchronous adsorption capacities of MB and Fe³⁺ on CPOP-HEDTA

The adsorption kinetics models were described as follows:

Pseudo-first-order kinetics model: $\ln(q_e - q_t) = \ln q_e - k_1 t$ (Equation.S2)

Pseudo-second-order kinetics model: $\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$ (Equation.S3)

Elovich kinetics model: $q_t = \frac{1}{\beta} \ln(\alpha\beta) + \frac{1}{\beta} \ln t$ (Equation.S3)

Intraparticle diffusion kinetics model: $q_t = k_i t^{0.5} + C_i$ (Equation.S4)

Where, q_t (mg/g) and q_e (mg/g) are the adsorption capacity at a given time and at equilibrium respectively. k_1 (min^{-1}) and k_2 ($\text{g mg}^{-1} \text{min}^{-1}$) are the rate constants of pseudo-first-order and pseudo-second-order kinetics respectively. α ($\text{mg g}^{-1} \text{min}^{-1}$) is the initial adsorption rate in the chemisorption. β (g/mg) is a parameter that demonstrates the relation between the degree of surface coverage and activation energy in the chemisorption. k_i ($\text{mg g}^{-1} \text{min}^{-0.5}$) is the constant of intraparticle diffusion. C_i is the constant of boundary layer affects and the adsorption kinetics is controlled by intraparticle diffusion diminutively when $C_i = 0$.

The adsorption isotherms were described as follows:

Langmuir isotherm: $\frac{C_e}{q_e} = \frac{1}{k_L q_m} + \frac{C_e}{q_m}$ (Equation.S5)

$R_L = \frac{1}{1 + k_L C_0}$ (Equation.S6)

Freundlich isotherm: $\ln q_e = \ln k_F + \frac{1}{n} \ln C_e$ (Equation.S7)

Tempkin isotherm: $q_e = \beta \ln k_T + \beta \ln C_e$ (Equation.S8)

(Equation.S8)

$\beta = \frac{RT}{b}$ (Equation.S9)

Where, q_m (mg/g) is the theoretical maximum adsorption capacity and k_L is the constant energy relevant to the heat of adsorption calculated by Langmuir isotherms. C_e (mg/L) is the absorbate concentration in the liquid phase at equilibrium. q_e (mg/g) is the adsorption capacity at equilibrium. R_L is an essential separation factor of Langmuir isotherm defined as **Equation S6** showed. The value of R_L illustrates the type of isotherm, $R_L > 1$ is unfavorable, $R_L = 1$ is linear, $1 > R_L > 0$ is favorable and $R_L = 0$ is irreversible.

k_F (mg/g) (L/mg)^{1/n} represents the adsorption capacity while n represents the intensity of adsorption in Freundlich theory and the favorability of the adsorption.

When $n > 1$, the adsorption process is favorable and heterogeneous. β represents the heat of adsorption expressed in **Equation S9** and b is the energy constant in Tempkin isotherm. R is $8.314 \text{ J/(K}\cdot\text{mol)}$ and T is absolute temperature. k_T is a constant of Tempkin isotherm.

The thermodynamics equations are as follows:

$$\text{Van't Hoff equation: } \ln K_c = \frac{\Delta S^0}{R} - \frac{\Delta H^0}{RT}$$

(Equation.S10)

$$K_c = \frac{q_e}{C_e} \quad \text{Equation.S11}$$

$$\Delta G^0 = -RT \ln K_c \quad \text{Equation.S12}$$

$$\text{Arrhenius equation: } k_2 = k_0 e^{-\frac{E_a}{RT}}$$

(Equation.S13)

Where, ΔS^0 ($\text{J mol}^{-1} \text{ K}^{-1}$) is entropy change and ΔH^0 (J/mol) is enthalpy change. R is $8.314 \text{ J/(K}\cdot\text{mol)}$ and T is absolute temperature. K_c (L/g) is standard thermodynamic equilibrium constant expressed in **equation S11**, where C_e (mg/L) is the adsorbate concentration in the liquid phase at equilibrium and q_e (mg/g) is the adsorption capacity at equilibrium. ΔG^0 (J/mol) is Gibbs free energy change and can be calculated by **Equation S12**.