

Supplementary Information for:

Easy-fabrication and low-cost carbamate-based Porous organic polymers for efficient removal of methylene blue

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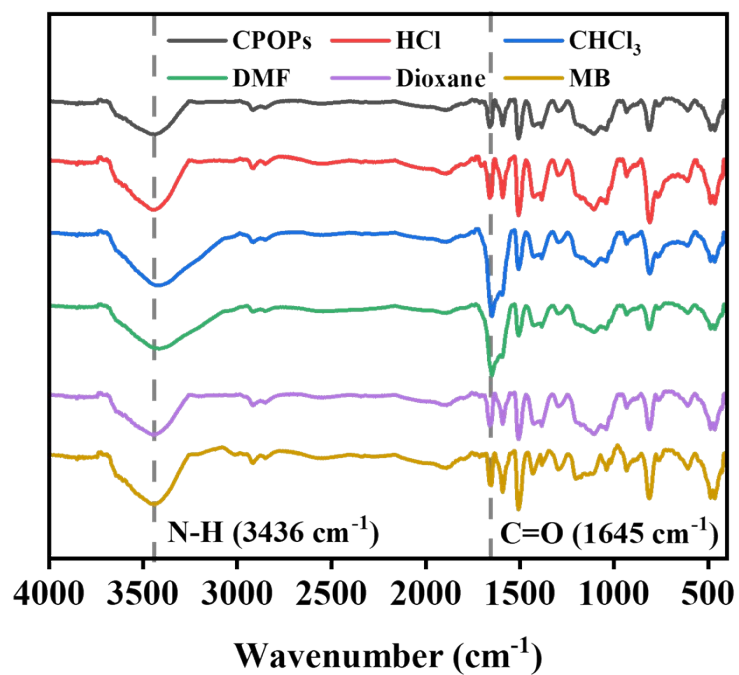


Fig. S1 FTIR spectra of CPOPs after treatment with HCl (pH=2), CHCl₃, *N,N*-Dimethylformamide (DMF), Dioxane and MB solution (after washing by ethanol) for 24h

Table S1 Elemental analysis of CPOPs

Element	C	O	H	N
Weight (%)	65.90	20.62	3.6	9.88

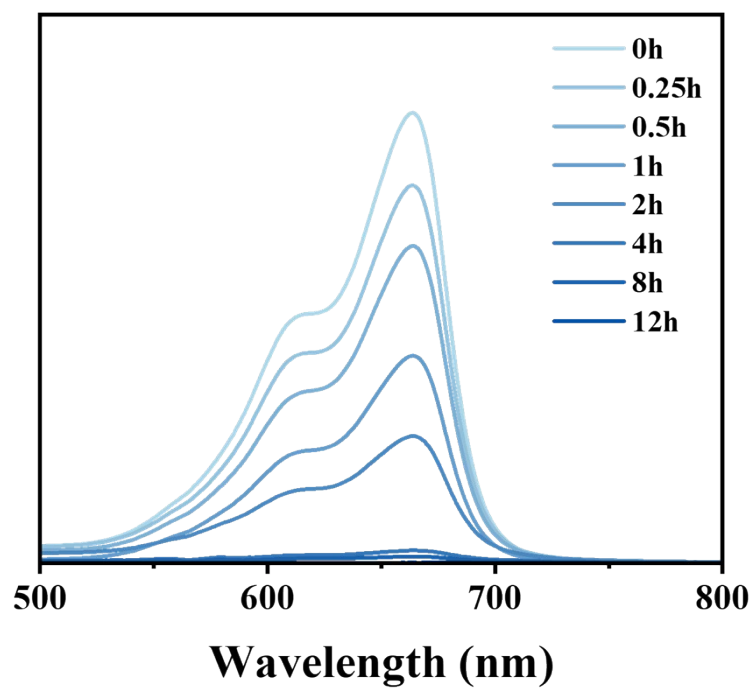


Fig. S2 UV-visible spectra of MB residue solution with the increase of absorption time

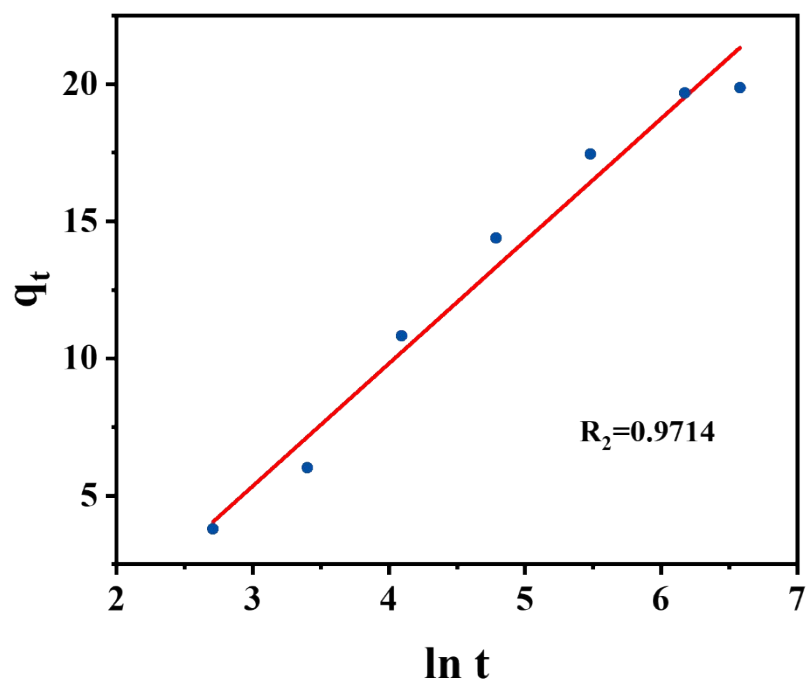


Fig. S3 Elovich model for MB adsorption by CPOPs

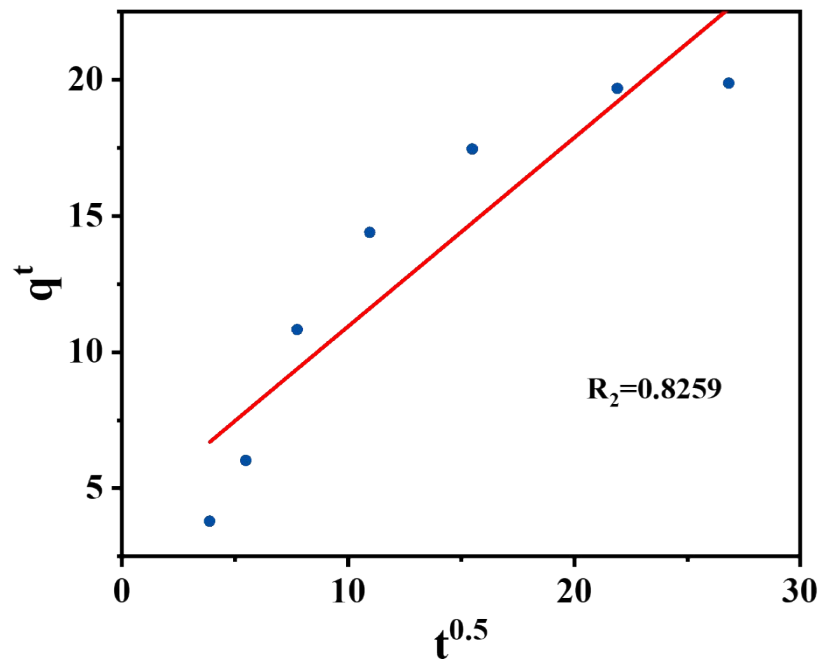


Fig. S4 Intraparticle diffusion model for MB adsorption by CPOPs

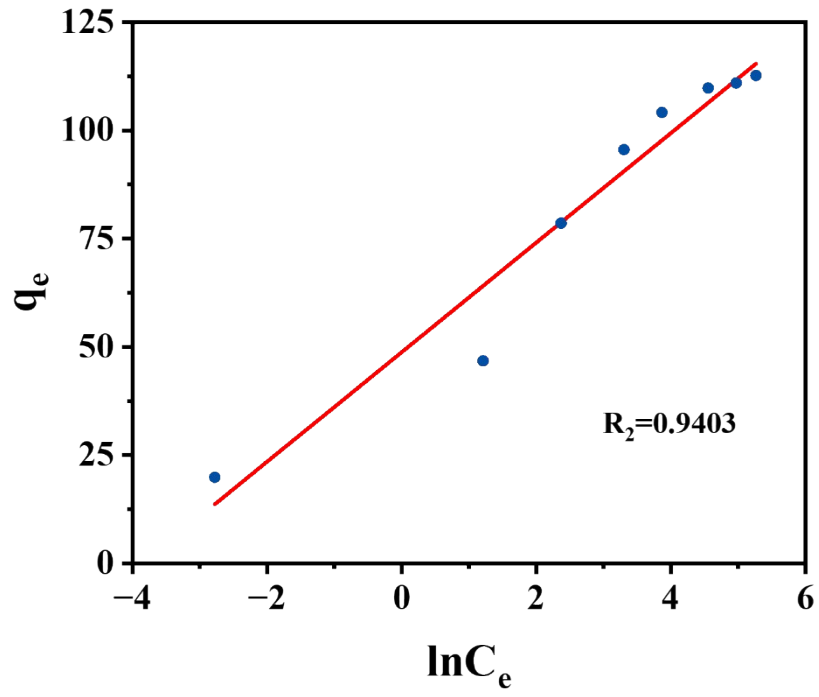


Fig. S5 Tempkin isotherm for MB adsorption by CPOPs

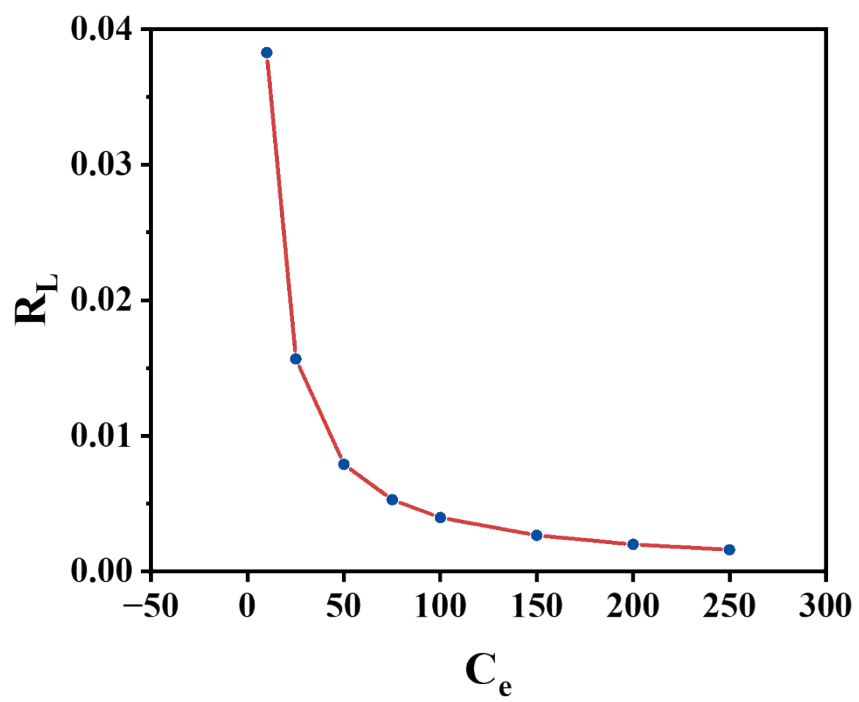


Fig. S6 R_L with distinct initial concentrations for MB adsorption by CPOPs

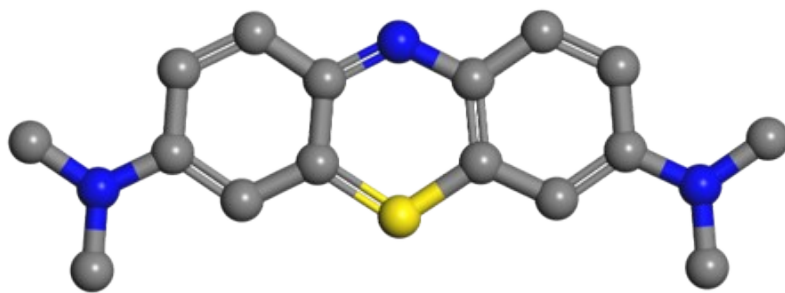


Fig. S7 Ball-and-stick molecule model of methylene blue

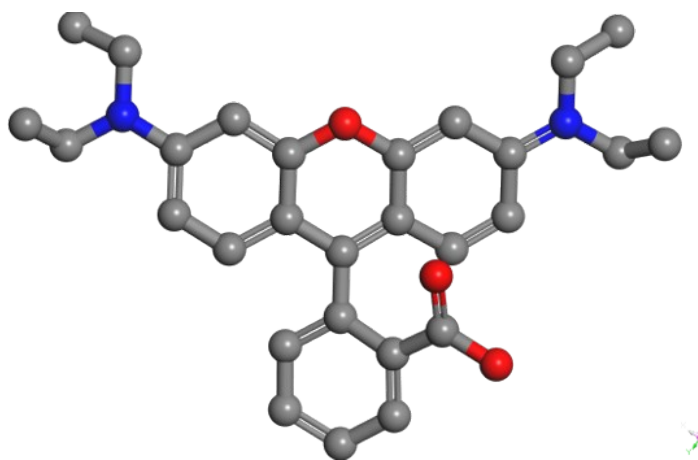


Fig. S8 Ball-and-stick molecule model of Rhodamine B

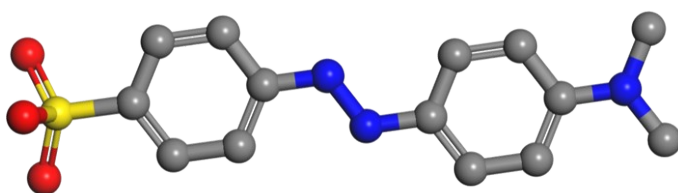


Fig. S9 Ball-and-stick molecule model of methyl orange

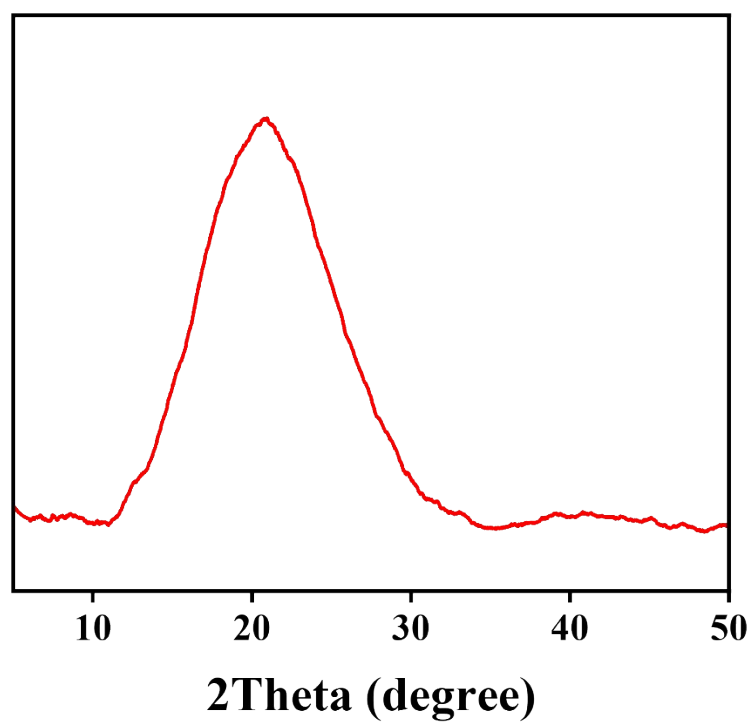


Fig. S10 XRD curve of CPOPs after MB adsorption

The adsorption kinetics models were described as follows:

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

Pseudo-second-order kinetics model: $\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$ * MERGEFORMAT (Equation.S2)

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

Intraparticle diffusion kinetics model: $q_t = k_i t^{0.5} + C_i$ * MERGEFORMAT (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: $\frac{C_e}{q_e} = \frac{1}{k_L q_m} + \frac{C_e}{q_m}$ * MERGEFORMAT

(Equation.S5)

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

Freundlich isotherm: $\ln q_e = \ln k_F + \frac{1}{n} \ln C_e$ * MERGEFORMAT

(Equation.S7)

Tempkin isotherm: $q_e = \beta \ln k_T + \beta C_e$ * MERGEFORMAT

(Equation.S8)

$\beta = \frac{RT}{b}$ * MERGEFORMAT (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**.