

Electronic Supplementary Material (ESI) for Dalton Transactions.

This journal is © The Royal Society of Chemistry 2023

Co-Adsorption and Fenton-like oxidation in the efficient removal of methylene blue by MIL-88B@UiO-66 nanoflowers

Pingping Teng, Ying Liu, Zhongqiao Sun, Hao Meng, Yide Han and Xia Zhang*

Department of Chemistry, College of Sciences, Northeastern University, Shenyang 10819, P. R. China.

*Corresponding author

Email: xzhang@mail.neu.edu.cn (Prof. Zhang)

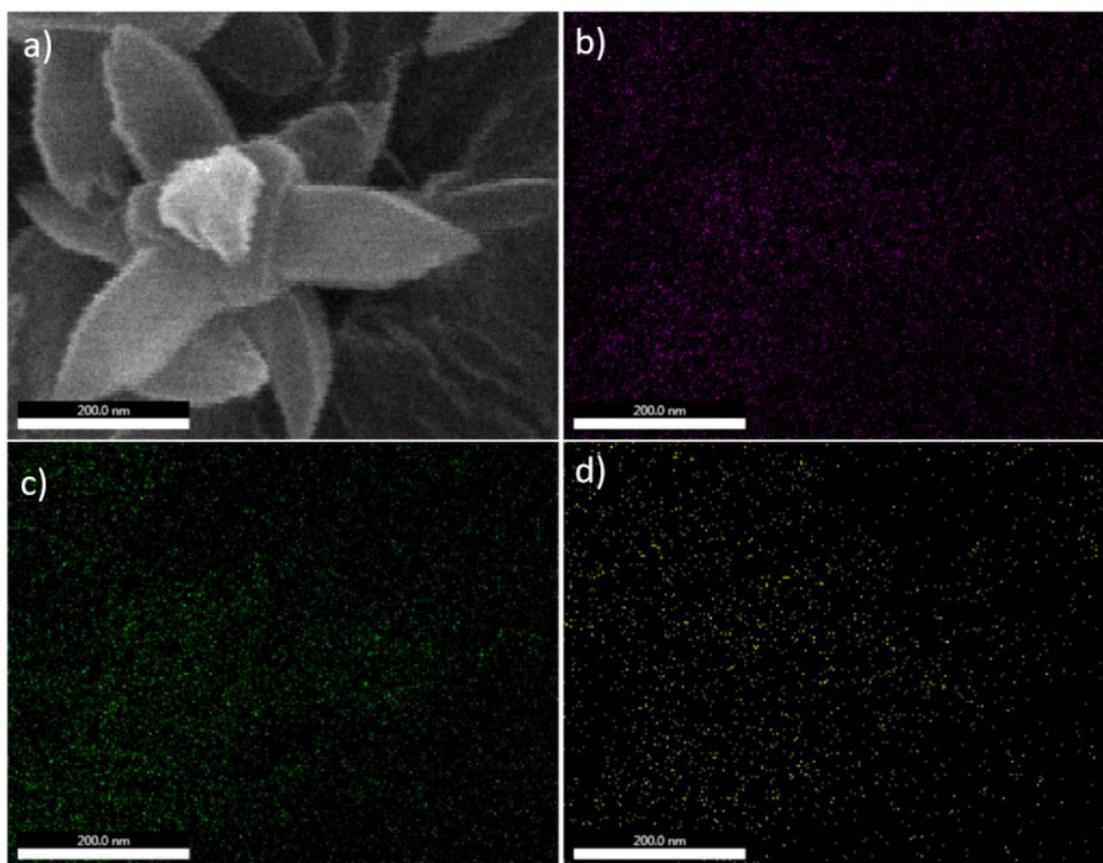


Fig. S1: (a) Scanning electron microscope image before EDS. The EDS mapping of MIL-88B@UiO-66 : (b) O; (c) Zr; (d) Fe.

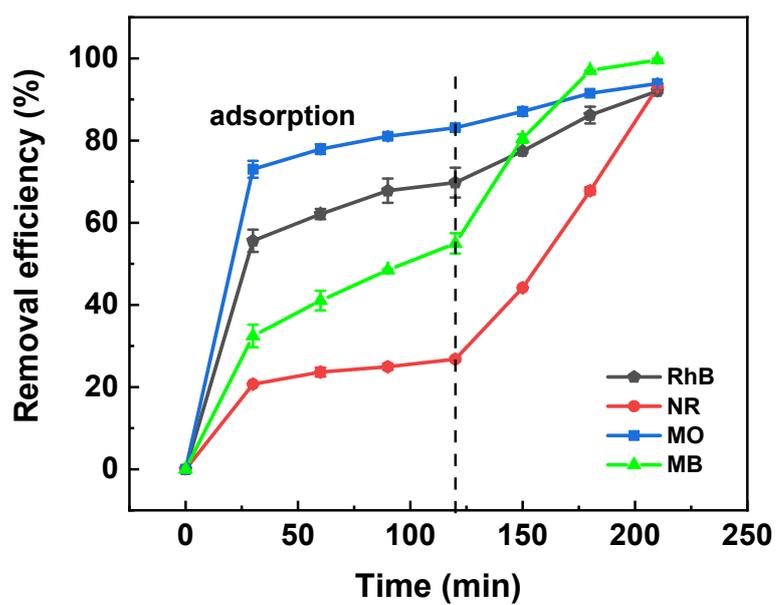


Fig. S2: Removal percentages of four dyes by MIL-88B@UiO-66.

The adsorption thermodynamics for the adsorption of MB on MIL-88B@UiO-66:

The adsorption equilibrium of MB by MIL-88B@UiO-66 at elevated temperatures with an initial concentration of 100 mg/L is shown in Fig. 7c. The adsorption thermodynamic parameters including standard Gibbs free energy (ΔG^θ), standard enthalpy change (ΔH^θ) and entropy change (ΔS^θ) can be calculated based on Eqs. (1) to (4).

$$\Delta G^\theta = -RT \ln K_D \quad (1)$$

$$\Delta G^\theta = \Delta H^\theta - T \Delta S^\theta \quad (2)$$

$$\ln K_D = -\frac{\Delta H^\theta}{RT} + \frac{\Delta S^\theta}{R} \quad (3)$$

$$K_D = \frac{q_e}{C_e} \quad (4)$$

In which, K_D is the partition coefficient of adsorption (L/mg); q_e and C_e are the adsorbed amounts (mg/g) of MB and the concentrations of MB in solution at equilibrium (mg/L), respectively; R is the gas constant (8.314 J/mol·K), and T is the absolute temperature (K). From Eq. (3), the standard enthalpy change and entropy change can be calculated using the slope and intercept of the line obtained by plotting $\ln K_D$ versus $1/T$ versus, and then standard Gibbs free energy is calculated by using Eq. (2).

Fig. S3 shows the variation of $\ln K_D$ upon with $1/T$, the equation of the curve is simulated as $Y = -2022.72 X + 5.33$. The thermodynamic parameters calculated from the fitting results are shown in Table S1. It can be concluded that the adsorption of MB by MIL-88B@UiO-66 is an endothermic and entropy increase process, and the standard Gibbs free energy is a little larger than 0 at the experimental temperature.

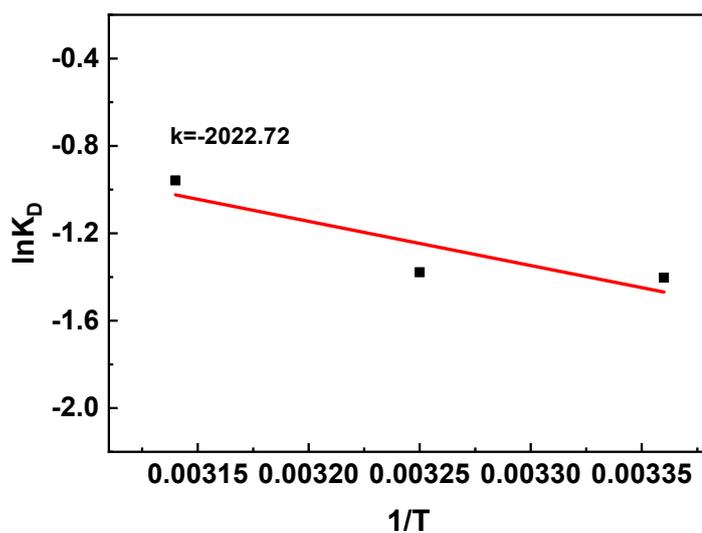


Fig. S3: Plotting curves of $\ln K_D$ versus $1/T$ for MB adsorption on MIL-88B@UiO-66.

Table S1: Thermodynamic parameters of MB adsorption by MIL-88B@UiO-66.

Adsorbents	Temperature /K	ΔH^θ (KJ· mol ⁻¹) 1)	ΔS^θ (J· mol ⁻¹ · K ⁻¹) 1)	ΔG^θ (KJ· mol ⁻¹) 1)
MIL-	298	16.817	44.294	3.617
88B@UiO-66	308			3.174
	318			2.732

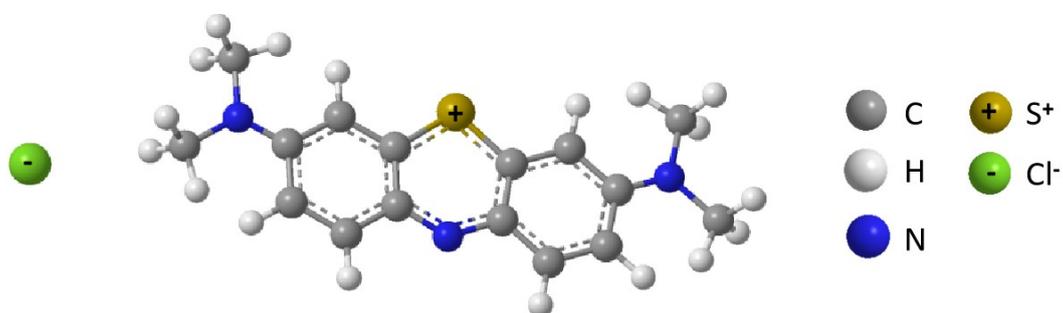


Fig. S4: Structure diagram of methylene blue.

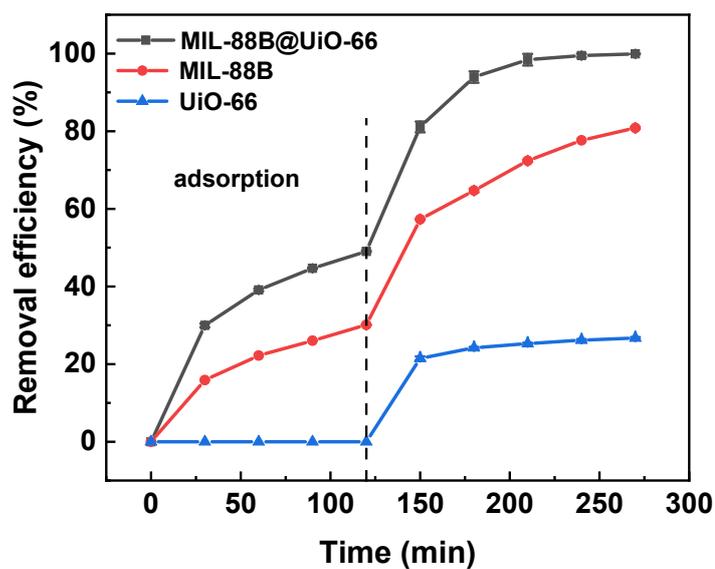


Fig. S5: Comparison of adsorption and Fenton-like catalytic properties of different MOFs. Reaction conditions: $m(\text{MOF})=80$ mg, $n(\text{H}_2\text{O}_2)=2 \times 10^{-6}$ mol, $C(\text{MB}) = 100.0$ mg/L, $V(\text{MB})=100$ mL, $T=25$ °C.