

### **Supplementary information**

#### **Economical synthesis of MOF from CHNS analyzer waste CuO and PET bottles for congo red sequestration: A pathway towards dual mitigation**

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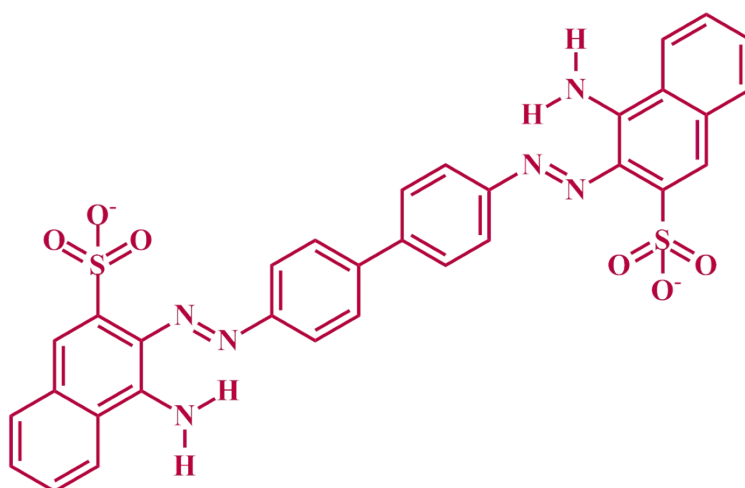
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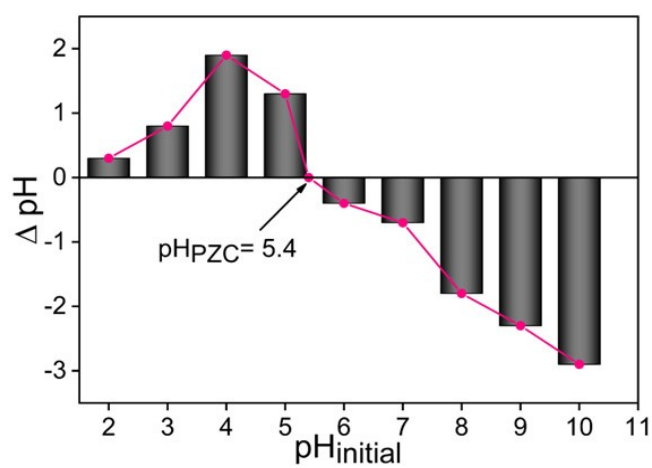
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### Supplementary information



**Fig. S1:** Structure of Congo red (anionic form).



**Fig. S2.** Point zero charge graph of Cu-PTA-MOF.

## Supplementary information

### **Text S1: Kinetics model for Adsorption.**

The linear equations of the kinetics model employed in the study are following:

$$\ln(Q_e - Q_t) = \ln Q_e - k_1 t \quad (\text{Pseudo-first-order}) \quad (\text{S1})$$

$$\frac{t}{Q_t} = \frac{1}{K_2 Q_e^2} + \frac{t}{Q_e} \quad (\text{Pseudo-second-order}) \quad (\text{S2})$$

where  $t$  (min) is contact time,  $Q_e$  and  $Q_t$  are the adsorption amounts (mg/g) at equilibrium and time  $t$  respectively. Here  $k_1$  ( $\text{min}^{-1}$ ) and  $k_2$  ( $\text{g} \cdot \text{mg}^{-1} \cdot \text{min}^{-1}$ ) denote the rate constants of the pseudo-first-order and the pseudo-second-order respectively.

### **Text S2: Adsorption isotherm models**

The linear equations for the adsorption isotherms employed in the study are outlined below:

$$\frac{C_e}{Q_e} = \frac{1}{K_L Q_m} + \frac{C_e}{Q_m} \quad (\text{Langmuir adsorption isotherm}) \quad (\text{S4})$$

$$\ln Q_e = \ln K_F + \frac{1}{n} \ln C_e \quad (\text{Freundlich adsorption isotherm}) \quad (\text{S5})$$

$$Q_e = \frac{RT}{b_T} \ln K_T + \frac{RT}{b_T} \ln C_e \quad (\text{Temkin adsorption isotherm}) \quad (\text{S6})$$

$$\ln\left(\frac{C_e}{Q_e}\right) = B \ln C_e - \ln A \quad (\text{Redlich-Peterson adsorption isotherm}) \quad (\text{S7})$$

where  $C_o$  and  $C_e$  denote initial and equilibrium concentrations of CR (mg/L),  $Q_e$  is the extent of the CR adsorbed at the stage of equilibrium (mg/g),  $Q_m$  denotes the optimum adsorption capacity (mg/g),  $K_L$ ,  $K_F$  and  $K_T$  signify Langmuir, Freundlich and Temkin isotherm constants (L/mg) respectively.  $n$  and  $b_T$  indicate the adsorption intensity and heat of adsorption (J/mol), respectively.  $R$  stands for the universal gas constant ( $8.314 \text{ J/mol} \times \text{K}$ ) and  $T$  (K) is the temperature.  $A$  is Redlich-Peterson isotherm constant (L/mg) and  $B$  is R-P parameter.

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### **Text S3: Thermodynamic parameters**

The equation of thermodynamics parameters employed in the study are given below:

$$\Delta G^\circ = -RT \ln K_L^\circ \quad (\text{S8})$$

$$\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ \quad (\text{S9})$$

$$\ln K_L^\circ = \frac{-\Delta H^\circ}{RT} + \frac{\Delta S^\circ}{R} \quad (\text{S10})$$

Considering the adsorption isotherm model, the dimensionless thermodynamic equilibrium constant was determined using the following equation:

$$K_L = \frac{(1000 \times K_L \times \text{molecular weight of adsorbate}) \times [\text{adsorbate}]^0}{\gamma}$$

where  $\gamma$  is the activity coefficient (dimensionless),  $K_L^\circ$  is the thermodynamic equilibrium constant (dimensionless),  $[\text{Adsorbate}]^0$  is the standard adsorbate concentration ( $\text{mol L}^{-1}$ ) and  $T$  (K) is the temperature, and  $R$  ( $8.314 \text{ J/mol} \times \text{K}$ ) is the universal gas constant.  $K_L$  is the fitted adsorption isotherm constant (Langmuir, Freundlich, Temkin and Redlich-Peterson).