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## Supporting information

## Synthesis and dye adsorption studies of $\{dibromo(1,1'-(1,2-ethanediyl)bis(3-methyl-imidazole-2-thione) dicopper(I)\}_n$ polymer and conversion it to CuO nanospheres for their photocatalytic and antibacterial applications

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| Compound 1  |            |              |           |              |            |
|-------------|------------|--------------|-----------|--------------|------------|
| Cu1-Br1     | 2.5337(8)  | Cu1-Br1'     | 2.5296(8) | Cu1-S1       | 2.3866(13) |
| Cu1-S1'     | 2.4066(13) |              |           |              |            |
| S1-Cu1-S1'  | 108.48(5)  | S1-Cu1-Br1   | 110.56(4) | S1-Cu1-Br1'  | 113.35(4)  |
| S1'-Cu1-Br1 | 111.57(4)  | S1'-Cu1-Br1' | 110.38(4) | Br1-Cu1-Br1' | 102.45(3)  |
| Compound 2  |            |              |           |              |            |
| Cu1-Br1     | 2.3507(5)  | Cu1-Br2      | 2.3891(5) | Cu1-Br3      | 2.3777(5)  |
| Br1-Cu1-Br2 | 123.30(2)  | Br1-Cu1-Br3  | 119.60(2) | Br2-Cu1-Br3  | 117.10(2)  |

Table S1. Selected bond lengths (Å) and bond angles (°) for compounds 1 and 2.



Figure S1. The PXRD patterns of **1** in simulated form (blue) and as-synthesized (black).



Figure S2. Color changes of the dye solutions of (a) the CR, (b) the AB, (c) the MG and (d) the VB and the precipitation 1 during adsorption process within 120 min.



Figure S3. The absorption curves vs. time for four selected dyes of (a) the CR, (b) the AB, (c) the MG and (d) the VB.



Figure S4. The emission spectra of the ebit (red) and 1 (blue) and when 1 was immersed in dye solutions of the AB (yellow), the CR (pink), the MG (orange) and the VB (green).



Figure S5. The IR spectra of the as-synthesized **1** (black) and when was immersed in dye solutions of the AB (blue), the CR (red), the MG (green) and the VB (purple).



Figure S6. The PXRD patterns of the as-synthesized **1** (black) and when was immersed in dye solutions of the CR (red), the AB (blue), the MG (green) and the VB (purple).



Figure S7. The adsorption kinetic curves of (a) Pseudo-first order, (b) Intraparticle diffusion, and (c) Elovich models for the AB dye.



Figure S8. The adsorption kinetic curves of (a) Pseudo-first order, (b) Intraparticle diffusion, and (c) Elovich models for the MG dye.



Figure S9. The adsorption kinetic curves of (a) Pseudo-first order, (b) Intraparticle diffusion, and (c) Elovich models for the AB dye.

![](_page_11_Figure_0.jpeg)

Figure S10. The adsorption kinetic curves of (a) Pseudo-first order, (b) Pseudo-second-order and (c) Intraparticle diffusion models for the CR dye.

Table S2. The kinetics parameters for adsorption of different dyes from aqueous solutions by polymer **1** at room temperature.

|                     |  |         | Par           | ameters          |                |
|---------------------|--|---------|---------------|------------------|----------------|
| Kinetic models      | Equations  | The dye | Adj. R-square | q <sub>e</sub>   | $K_1$          |
|                     | $1 \ k_1 \ 1$  | AB      | 0.638         | 0.653            | 5.420          |
| Daguda first andar  | $\frac{a}{a} = \frac{a}{a} \frac{t}{t} + \frac{a}{a}$  | MG      | 0.808         | 11.530           | 2.031          |
| Pseudo-mist order   | $q_t$ $q_e$ $q_e$  | VB      | 0.331         | 4.032            | -4.520         |
|                     |  | CR      | 0.269         | 1.118            | -6.688         |
|                     | t - 1 + t  |         | Adj. R-square | q <sub>e</sub>   | K <sub>2</sub> |
| Pseudo-second order | $\frac{\overline{q}_{t}}{q_{t}} - \frac{\overline{k_{2}q_{e}^{2}}}{k_{2}q_{e}^{2}} + \frac{\overline{q}_{e}}{q_{e}}$ | CR -    | 0.859         | 2.240            | 0.007          |
|                     |  |         | Adj. R-square | K <sub>dif</sub> | x <sub>i</sub> |
|                     |  | AB      | 0.616         | -0.325           | 3.430          |
| Intraparticle       | 1  | MG      | 0.851         | -2.029           | 17.378         |
| diffusion           | $q_t = k_{dif} t^2 + x_i$  | VB      | 0.869         | -1.038           | 13.468         |
| unfusion            |  | CR      | 0.907         | -1.050           | 10.847         |
|                     | lng h 1  |         | Adj. R-square | а                | b              |
| Elovich             | $q_t = \frac{lnu_e b_e}{lnt} + \frac{1}{lnt}lnt$   | AB      | 0.795         | 0.007            | -0.954         |
|                     | $b_e b_e$  | MG      | 0.964         | 0.000024         | -0.492         |
|                     |  | VB      | 0.777         | 0.00093          | -0.359         |

![](_page_13_Figure_0.jpeg)

Figure S11. The adsorption isotherm curves of (a) Freundlich and (b) Temkin models for the CR dye.

![](_page_14_Figure_0.jpeg)

Figure S12. The adsorption isotherm curves of (a) Langmuir and (b) Temkin models for the MG dye.

![](_page_15_Figure_0.jpeg)

Figure S13. The adsorption isotherm curves of (a) Langmuir and (b) Freundlich models for the AB dye.

![](_page_16_Figure_0.jpeg)

Figure S14. The adsorption isotherm curves of (a) Langmuir and (b) Freundlich models for the VB dye.

| Isotherm   |   |         | Pa            | rameters    |                           |
|------------|---|---------|---------------|-------------|---------------------------|
| models     | Equations                                     | The dye | Adj. R-square | $q_{\rm m}$ | $K_1$                     |
|            |   | AB      | 0.942         | 3.057       | 0.390                     |
| Lanomuir   | $\frac{c_e}{-} = \frac{1}{-} + \frac{c_e}{-}$ | MG      | 0.615         | -14.510     | 0.006                     |
| Dungmun    | $q_e  q_m k_l  q_m$                           | VB      | 0.851         | 1.237       | 0.707                     |
|            |   |         | Adj. R-square | n           | $\mathbf{k}_{\mathrm{f}}$ |
|            | 1   | AB      | 0.957         | -0.902      | 7.000                     |
| Freundlich | $logq_e = logk_f + -logc_e$                   | VB      | 0.939         | -0.189      | 1719.175                  |
|            | , n   | CR      | 0.915         | 3.099       | 3.074                     |
|            |   |         | Adj. R-square | $B_1$       | $\mathbf{k}_{\mathrm{t}}$ |
| Temkin     | $q_e = B_1 ln k_t + B_1 ln c_e$               | CR      | 0.924         | 4.146       | 29.100                    |
|            |   | MG      | 0.873         | 6.478       | 0.055                     |

Table S3. Evaluated model parameters of adsorption isotherms for different dyes by the polymer **1** at room temperature.

![](_page_18_Figure_0.jpeg)

Figure S15.The UV-Vis adsorption spectra of the Rhodamine B as a function of irradiation time for (a) the blank, (b) the as-synthesized CuO nanospheres, (c) the H<sub>2</sub>O<sub>2</sub> and (d) the commercial CuO with addition of H<sub>2</sub>O<sub>2</sub>.

![](_page_19_Figure_0.jpeg)

Figure S16. The adsorption kinetic curves for (a) Pseudo-first order, (b) Pseudo-second-order,(c) Intraparticle diffusion and (d) Elovich kinetic models in the photodegradation of the RhB solution by the CuO nanospheres.

| Kinetic models            | Equations   | Parameters       |          |
|---------------------------|---|------------------|----------|
|                           | $1 k_1 1$   | Adj. R-square    | 0.809    |
| Pseudo-first order model  | $\frac{1}{q_t} = \frac{1}{q_e t} + \frac{1}{q_e}$     | q <sub>e</sub>   | 0.604    |
|                           |   | $\mathbf{k}_1$   | -0.00036 |
|                           |   | Adj. R-square    | 0.115    |
| Pseudo-second order model | $\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$ | q <sub>e</sub>   | 1.495    |
|                           |   | K <sub>2</sub>   | 0.035    |
|                           |   | Adj. R-square    | 0.865    |
| Intraparticle             | $\frac{1}{2}$   | K <sub>dif</sub> | 0.955    |
| diffusion model           | $q_t = \kappa_{dif} t^2 + x_i$                        | X <sub>i</sub>   | -2.320   |
|                           | lng h   | Adj. R-square    | 0.935    |
| Elovich model             | $q_t = \frac{i n a_e b_e}{h} + \frac{1}{h} lnt$       | а                | 0.000012 |
|                           | ~e Se   | b                | 0.226    |

Table S4. The fitted kinetics parameters for photodegradation of the RhB solution by the CuO nanospheres.

![](_page_21_Picture_0.jpeg)

Figure S17. The SEM image of the commercial CuO.