Supporting Information for

One step synthesis of silane-capped copper clusters as sensitive optical probe and efficient catalyst for reversible color switching

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Quantum yield calculation. Both quinine sulfate dissolved in 0.1 M H_2SO_4 and rhodamine B in ethanol were employed as reference. The quantum yield (QY) of the as-prepared Cu CLs in THF was obtained by the following equation:

$$\frac{Q}{Q_r} = \frac{A_r}{A} \times \frac{I}{I_r} \times \frac{n^2}{n_r^2}$$

where A (A_r) is the absorbance at excitation wavelength, I (I_r) is the integrated fluorescence intensity, and n (n_r) is the solvent's refractive index of the as-prepared Cu CLs (reference fluorophores). The QYs reported for quinine sulfate and rhodamine b are 54 % and 69 % (excited at 365 nm), respectively.



Figure S1. ESI-MS spectrum of the as-synthesized Cu CLs in the low m/z range. Those specific charge peaks at 449.04, 472.03, 563.93, 607.92 are ascribed to $[Cu_4(SSiO_3C_6H_{14}) + H]^+$, $[Cu_4(SSiO_3C_6H_{15}) + Na]^+$, $[Cu_4(SSiO_3C_3H_{10})_2 + H]^+$ and $[Cu(SSiO_3C_6H_{15})_2(SSiO_3C_3H_9) + H]^+$, respectively, evincing that these Cu CLs are mainly composed of 4 atoms.



Figure S2. Comparison of experimental result (left) and isotope simulated pattern (right) for $Cu_4(SSiO_3C_6H_{15})_3$.



Figure S3. Comparison of experimental result (left) and isotope simulated pattern (right) for $Cu_5(SSiO_3C_6H_{15})_3$.



Figure S4. Emission spectrum of the as-synthesized Cu CLs in ethanol under excitation of 375 nm.



Figure S5. Excitation spectra of the as-synthesized Cu CLs for emissions at 410 nm (red curve) and 580 nm (blue curve). The peaks of these two bands are located at almost the same position, namely \sim 375 nm.



Figure S6. Fluorescence intensity evolution of the as-prepared Cu CLs under continuous UV irradiation at 365 nm.



Figure S7. FTIR spectra of the as-prepared Cu CLs and MPTS. No peaks at 2560 cm⁻¹ appearing in the Cu CLs' spectrum implies the absence of –SH bond.



Figure S8. XPS spectrum of Cu 2p from the sample without the satellite peak at 942 eV, which is ascribed to the characteristic peak of Cu (II). The BEs of Cu $2p_{1/2}$ and Cu $2p_{3/2}$ are 932.6 eV and 952.0 eV, respectively.



Figure S9. XPS spectrum of S 2p from the as-synthesized Cu CLs. The BE of S 2p is measured to be 162.7 eV, slightly higher than that of S from thiolates.



Figure S10. Mass spectrum of the as-obtained mixture after the synthetic process. The strong specific charge peak at 412.88 is assigned to [RSSR+Na]⁺.



Figure S11. Comparison of experimental result (left) and isotope simulated pattern (right) for (CuSR)₃.



Figure S12. Comparison of experimental result (left) and isotope simulated pattern (right) for (CuSR)₄.



Figure S13. Comparison of MPTS's fluorescence spectra before (black curve) and after (red curve) adding H_2O_2 .



Figure S14. The relationship between $ln(C_0/C)$ and reaction time t in the presence (black dots) and absence (red dots) of Cu CLs during the reduction of MB by NaBH₃CN. It can be seen that in the first 4 minutes these processes are ascribed to

pseudo-first order reactions.



Figure S15. UV-vis spectra of MB in the absence of Cu CLs. Red lines are absorption curves of MB solution before (dash line) and after (solid line) adding NaBH₃CN. Blue dash line: absorption curve of MB solution with NaBH₃CN after 30 minutes of UV irradiation at 365 nm.