SUPPORTING INFORMATION

Cu-deficient plasmonic $Cu_{2-x}S$ nanocrystals induced tunable photocatalytic activities

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SUPPORTING CALCULATIONS

Theoretical calculation of $Cu_{2-x}S$ NCs free carrier concentration is following: The carrier density can be calculated based on the Mie-Drude model, in which the relationship between the LSPR frequency (ω_{sp}) and the bulk plasma oscillation frequency (ω_p) can be expressed as follows:

$$\omega_{sp} = \sqrt{\frac{\omega_p^2}{1 + \frac{1 - L_j}{L_j}\varepsilon_m} - \gamma^2} \qquad (1)$$

where L_j is a shape-dependent geometrical factor, which can be obtained based on the aspect ratios of nanodisks [1]. ε_m is the dielectric constant of the solvent, and ε_m = 2.28 is available for the solvent TCE. γ represents the FWHM of the plasmon resonance band on the energy scale, which can be obtained by fitting the absorption band based on a Gaussian function. ω_p is the bulk plasmon oscillation frequency with the above expression. Herein, the geometrical factor L_j is calculated to be 0.33–0.43 for different nanodisks with variable aspect ratios. Thus ω_p can be calculated to be 2.05–2.44 eV for different $Cu_{2-x}S$ NCs on the basis of the above expression (1). To calculate the free carrier density (N_h), the following equation is applied:

$$\omega_p = \sqrt{\frac{N_h e^2}{\varepsilon_0 m_h}} \qquad (2)$$

where e is the electron charge, ε_0 is the free space permittivity, and m_h is the hole effective mass, $m_h = 0.8m_0$. From the above equation (eqn (2)), the carrier density N_h can be estimated to be 2.50~3.50*10^{21} cm^{-3} for a series of $Cu_{2-x}S$ NCs synthesized by using different injection volume of S-OA solution, which are summarized in Table 1.

SUPPLEMENTARY DATA

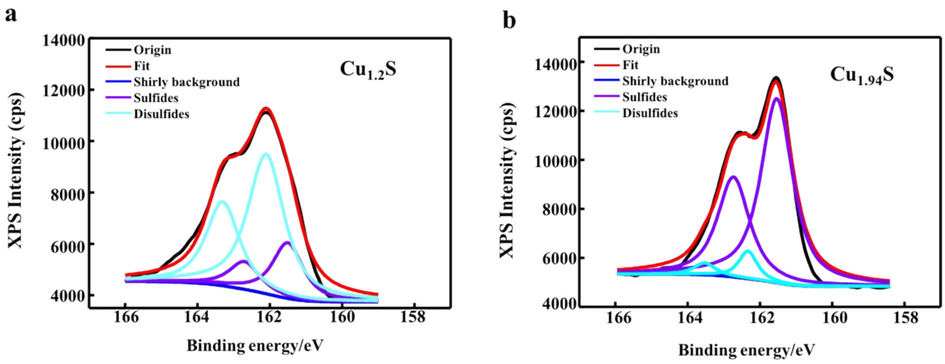

Fig. 1 XPS spectra of the $Cu_{2-x}S$ NCs synthesized by using different volume of S-OA solution: (a) $Cu_{1.2}S$ and (b) $Cu_{1.94}S$.

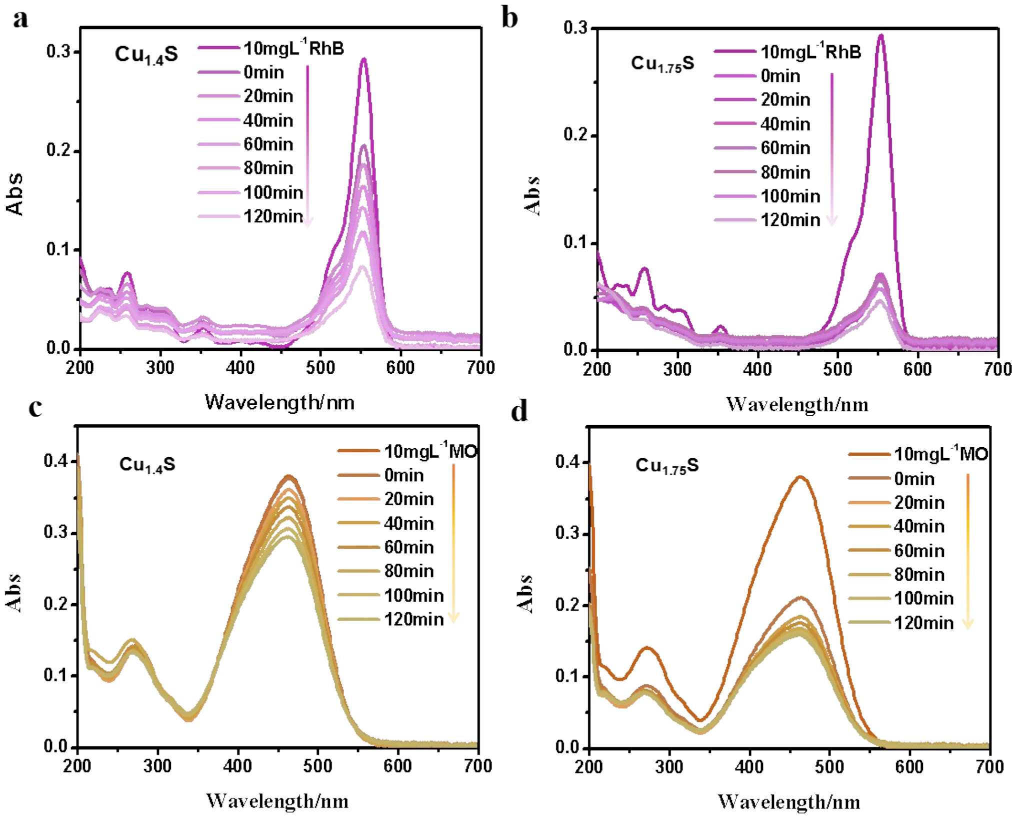

Fig. S2 UV-visible spectra change of (a,b) RhB, (c,d) MO with $Cu_{1.4}S$, $Cu_{1.75}S$ NCs as photocatalysts under UV irradiation, respectively.

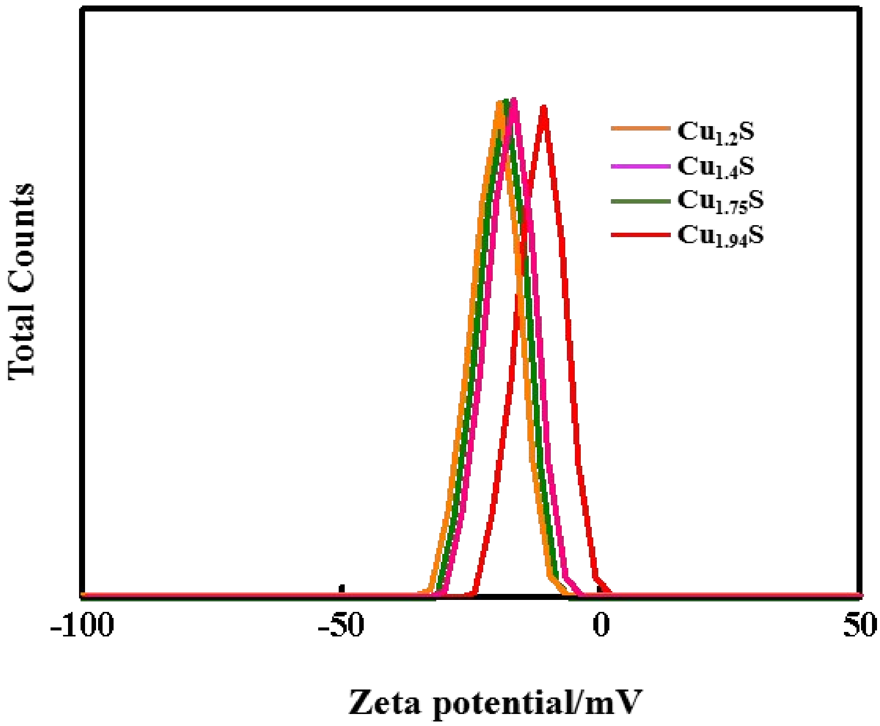

Fig. S3 Zeta potential of $Cu_{2-x}S$ NCs at pH 7.0.

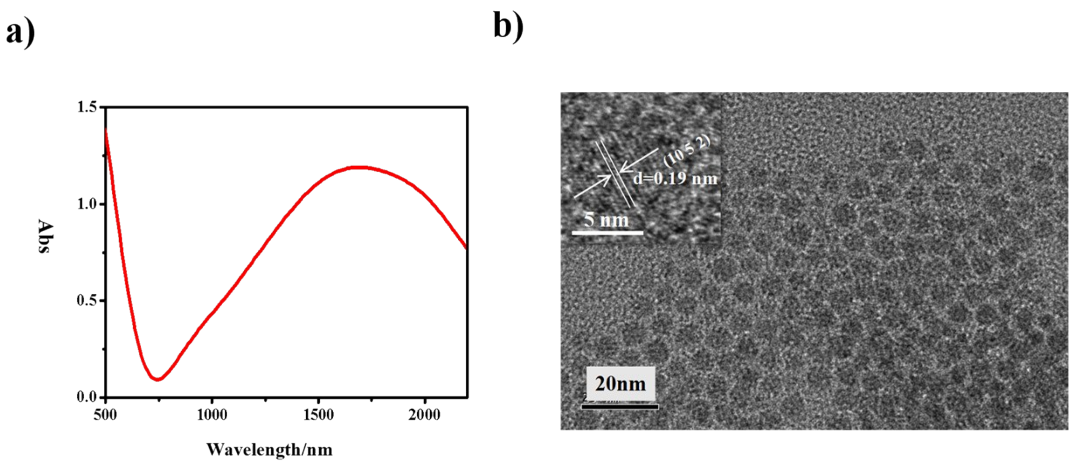

Fig. S4 a) NIR LSPR absorption spectra of the $Cu_{1.94}S$ NCs; b) TEM images of $Cu_{1.94}S$ nanostructures. Inset: higher magnification of individual $Cu_{1.94}S$ NCs.

REFERENCES

1 D. X. Zhu, A. W. Tang, H. H. Ye, M. Wang, C. H. Yangand F. Teng, J. Mater. Chem. C, 3（2015）6686–6691.