

Supplementary Material For
Dynamic isomers engaged fabrication of copper sulfide rattle-type structures and
their optoelectronic properties

Zhen Fang, ^{*a} Yufeng Liu,^a Qin Wang,^a Yueting Fan,^a Xiaowang Liu^a and
Weizhi Wang^a

^a Anhui Key Laboratory of Functional Molecular Solids, College of Chemistry and Materials Science, Anhui Normal University, Wuhu, 241000, P. R. China. E-mail: fzfsn@mail.ahnu.edu.cn; Fax: +86-553-3869302; Tel: +86-553-3937135.

1. XPS results

The XPS survey spectrum in **Fig. S1** reveals that the obtained sample consists of Cu and S. The binding energies of all spectra were corrected by referencing the C1s value of 284.6 eV. The high-resolution XPS spectra of Cu 2p and S 2p region are shown in figure 1b and 1c. The spectrum of the Cu 2p signal reveals that the binding energy of Cu 2p_{3/2} and Cu 2p_{1/2} is 932.5 eV and 952.2 eV. The sulfur 2p peaks are located at 162.7 eV, which are consistent with the 160-164 eV range expected for S in sulfide phase.¹

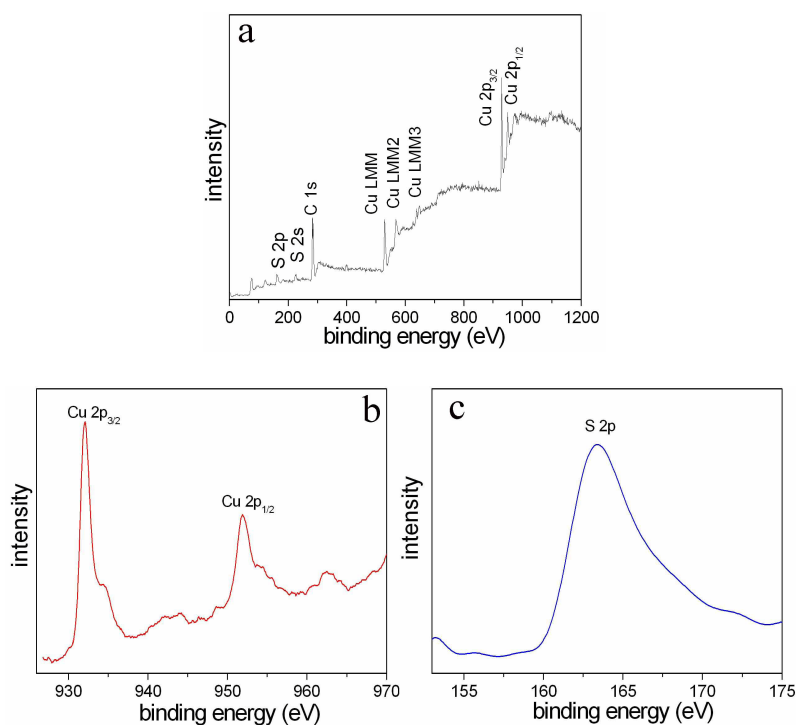


Fig. S1 (a) XPS survey spectrum; (b) and (c) high-resolution XPS spectra of Cu 2p and S 2s.

2. Size distribution

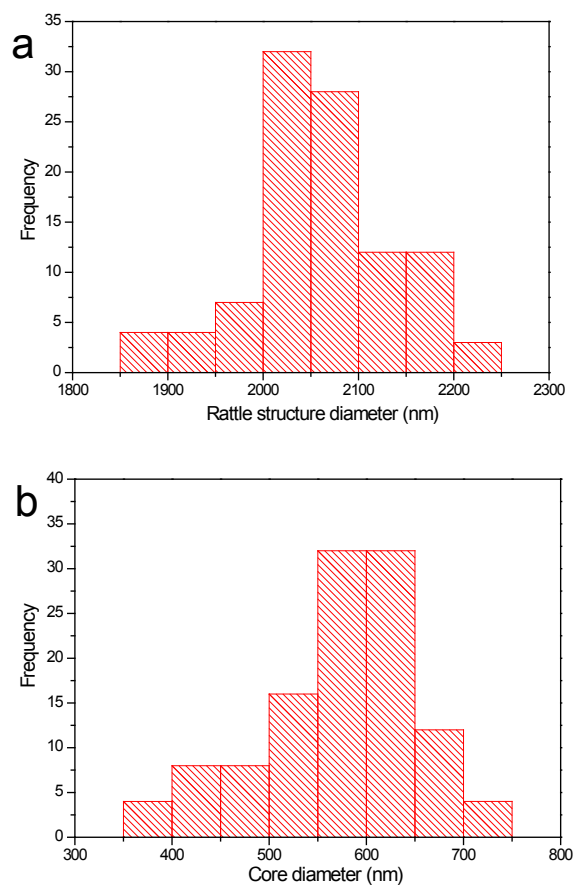


Fig. S2 Size distribution of (a) the rattle type structure and (b) the core.

3. The reaction between the centrifugated solution and Fe^{3+}

The centrifugated solution obtained at 6 hours turn into red for the formation of $[\text{Fe}(\text{SCN})_x]^{3-x}$ When Fe^{3+} was added into it

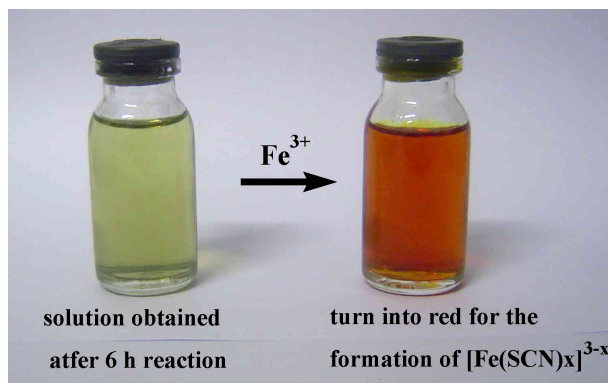


Fig. S3 Digital photo of the solution before and after Fe^{3+} added.

4. The effect of anions

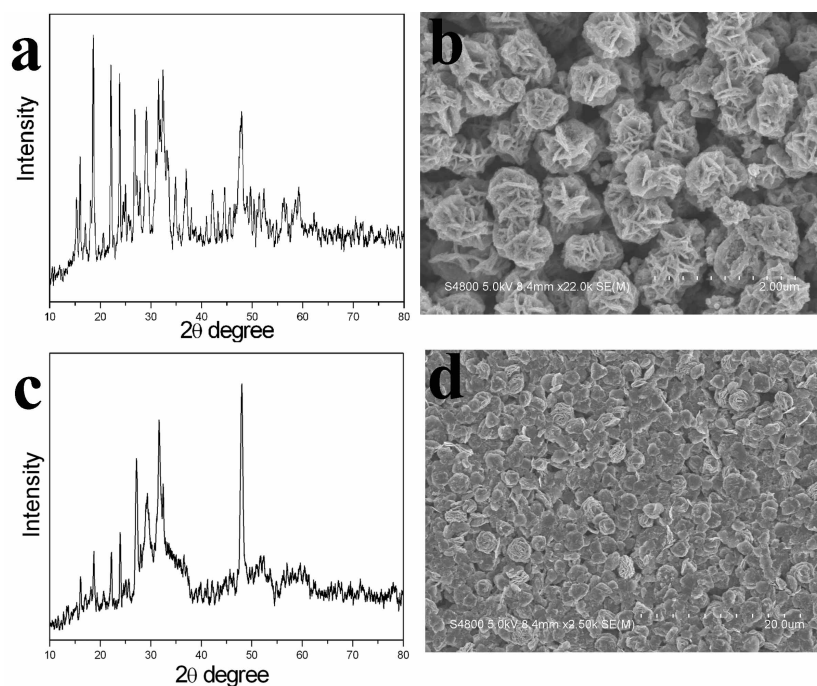


Fig. S4 XRD pattern and SEM image of intermediate obtained at 4 h with (a and b) CuSO_4 , (c and d) $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$.

5. SEM evolution process

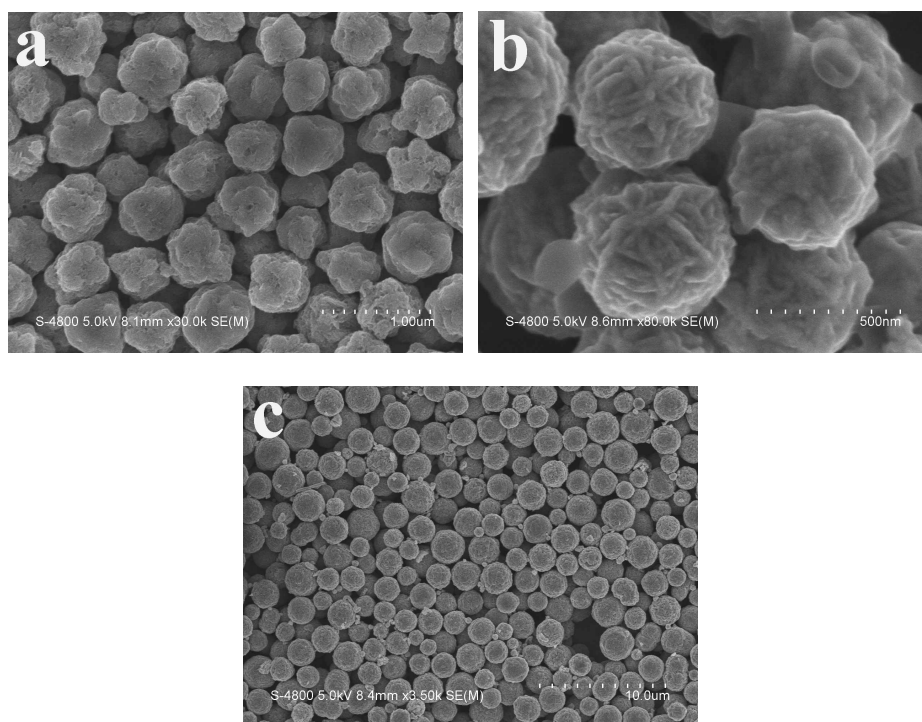


Fig. S5 SEM image of the evolution process of $\text{Cu}_{1.8}\text{S}$ RTS after (a) 1 h, (b) 6 h and (c) 1 day reaction.

6. Optoelectronic device

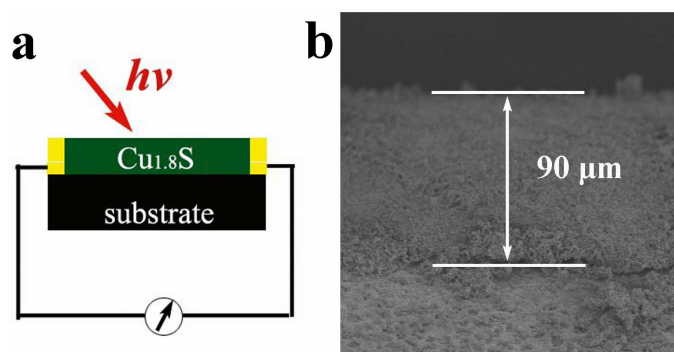


Fig. S6 (a) sketch map of setting for photocurrent measurement; (b) SEM image of the prepared $\text{Cu}_{1.8}\text{S}$ film.

References

1. Y. F. Liu, J. B. Cao, Y. Y. Wang, J. H. Zeng and Y. T. Qian. *Inorg. Chem. Commun.* 2002, **5**, 407–410.