

Electronic Supplementary Information (ESI)

Cu_{2-x}Se nanooctahedra: controllable synthesis and optoelectronic properties

Wenliang Wang,^{a,b,c,d} Li Zhang,^{a,b,c,d} Guihuan Chen,^{a,b,c,d} Jun Jiang,^{a,b,c,d} Tao Ding,^{a,b,c,d} Jian Zuo^a and Qing Yang^{*a,b,c,d}

^a Hefei National Laboratory of Physical Sciences at the Microscale, University of Science and Technology of China (USTC), Hefei 230026, Anhui, P. R. China.

^b Department of Chemistry, USTC, Hefei 230026, Anhui, P. R. China.

^c Laboratory of Nanomaterials for Energy Conversion, USTC, Hefei 230026, Anhui, P. R. China.

^d Synergetic Innovation Center of Quantum Information & Quantum Physics, USTC, Hefei 230026, P. R. China

* Corresponding author. E-mail: qyoung@ustc.edu.cn; Fax: +86-551-63606266; Tel: +86-551-63600243.

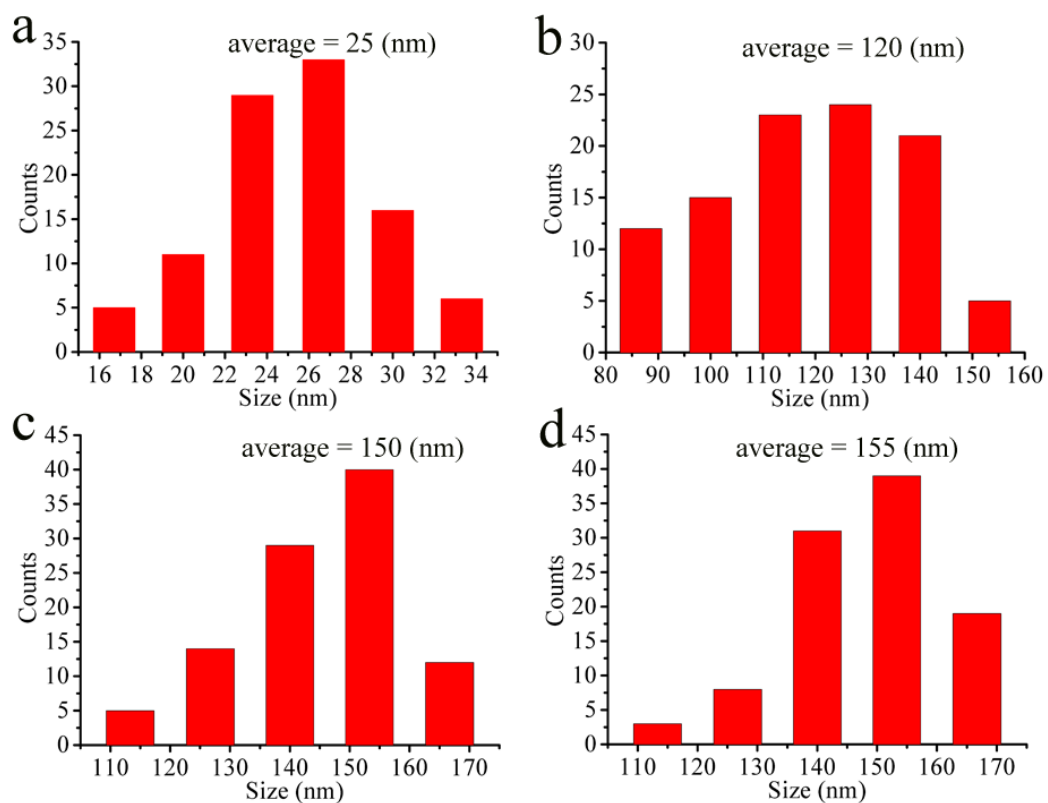


Fig. S1. Size distribution of the Cu_{2-x}Se NCs synthesized by injection of 1.0 mL ODE containing 0.1 mmol Ph_2Se_2 into 6 mL ODE and 0.5 mL OAm with 0.2 mmol CuCl at 270 °C with different reaction time: (a) 30 sec, (b) 5 min, (c) 45 min, and (d) 60min.

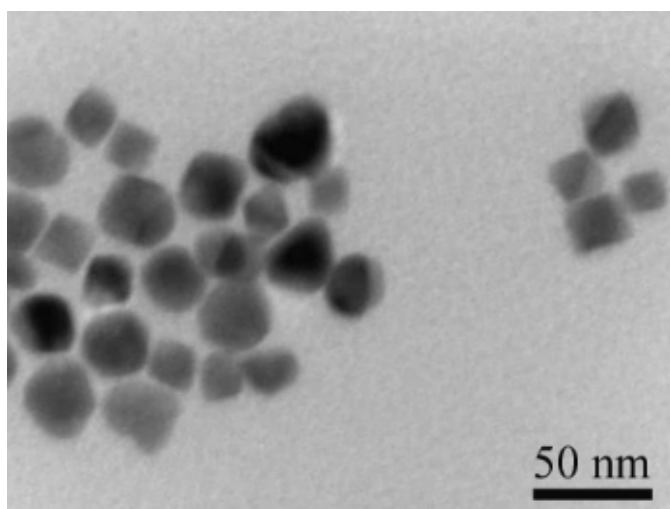


Fig. S2. TEM image of the products prepared at 270 °C in ODE (7.0 mL) and OAm (0.5 mL) for 30 sec.

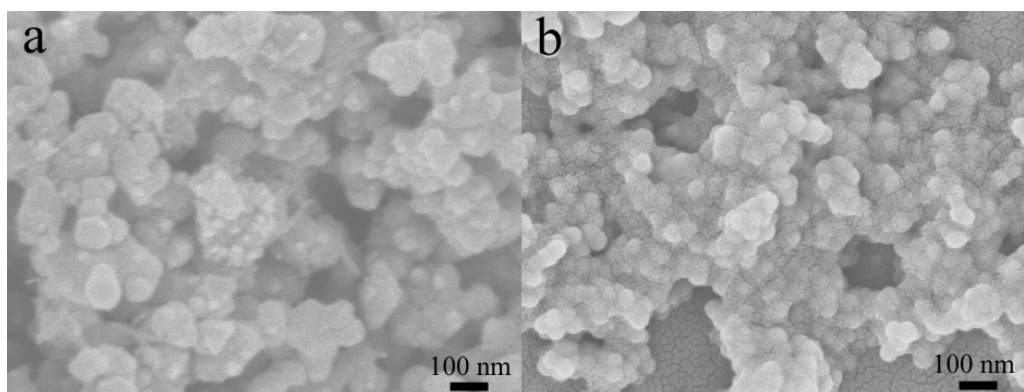


Fig. S3. SEM images of the products prepared at 270 °C for 30 min in (a) pure ODE (7.5 mL), and (b) pure OAm (7.5 mL), respectively.

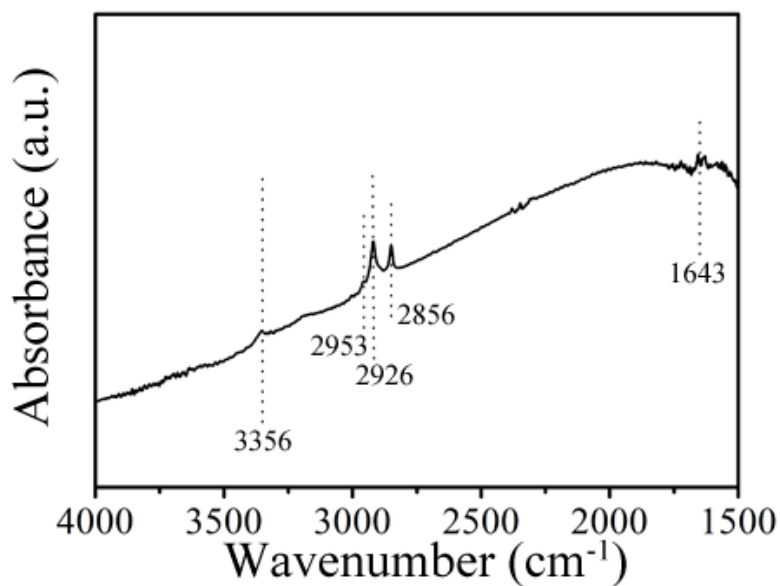


Fig. S4. ATR-FTIR spectrum for the as-synthesized octahedral Cu_{2-x}Se NCs.

ATR-FTIR is demonstrated to further characterize the capping agent binding to the surface of the as-synthesized octahedral Cu_{2-x}Se NCs obtained in a mixture media of ODE (7.0 mL) with OAm (0.5 mL). In Fig. S4, the absorbance bands at 2856, 2926 and 2953 cm^{-1} can be assigned to the C–H stretching modes.¹ The IR absorbance band at 3356 cm^{-1} is attributed to the stretching mode of N–H bond. Moreover, a small band peak at 1643 cm^{-1} is observed, revealing the existence of OAm on the Cu_{2-x}Se NCs surface as well.^{2,3} Therefore, it is suggested that the capping effect of the media, especially OAm, promotes the growth of the Cu_{2-x}Se NCs with well-defined octahedral shapes.

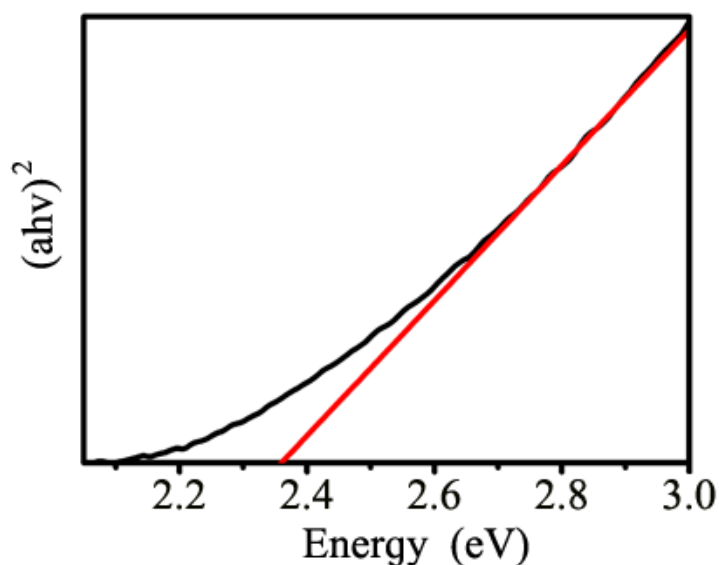


Fig. S5. Plot the direct band gap of the octahedral Cu_{2-x}Se NCs derived from UV-vis-NIR absorption spectrum.

Supplementary References

1. P. J. Thistlethwaite and M. S. Hook, *Langmuir*, 2000, **16**, 4993-4998.
2. X. Lu, H.-Y. Tuan, J. Chen, Z.-Y. Li, B. A. Korgel and Y. Xia, *J. Am. Chem. Soc.*, 2007, **129**, 1733-1742.
3. G. Shao, G. Chen, W. Yang, T. Ding, J. Zuo and Q. Yang, *Langmuir*, 2014, **30**, 2863-2872.