Electronic Supplementary Information (ESI)

Facile non-injection synthesis of high quality CZTS nanocrystals

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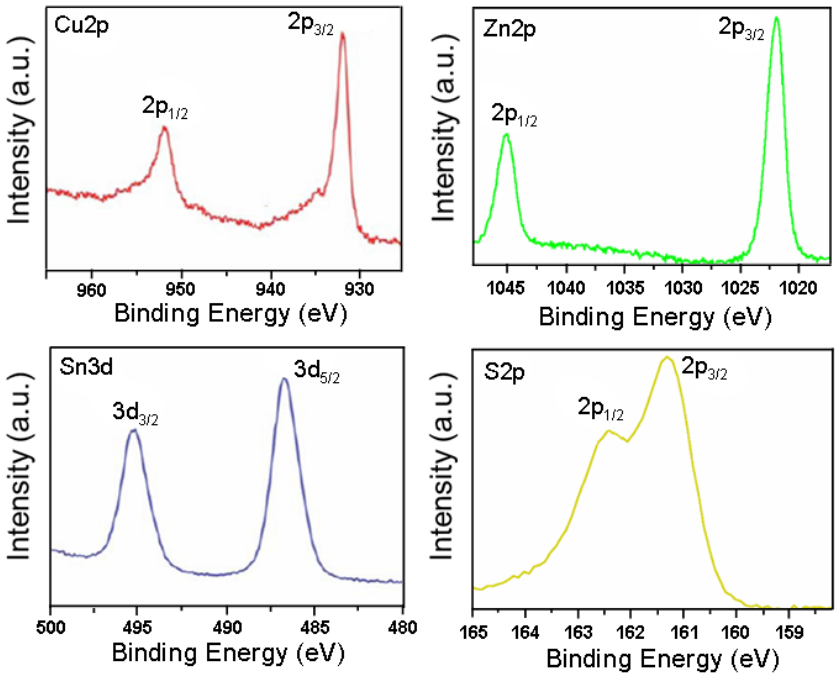

Fig. S1 XPS spectra of the four constituent elements of the CZTS nanocrystals

The copper 2p peaks located at 931.9and 952 eV show a peak splitting of 20.1 eV, suggesting Cu(I). The zinc 2p peaks at 1022 and 1045 eV show a peak separation of 23 eV, consistent with the standard splitting of 22.97 eV, indicative of zinc(II). The tin 3d peaks locate at 486.4 and 495 eV with a peak splitting of 8.6 eV, indicating Sn(IV). The sulfur $2p_{3/2}$ and $2p_{1/2}$ peaks in the spectra are located at 161.2 and 162.4 eV, which are consistent with the 160-164 eV range expected for S in sulfide phases.

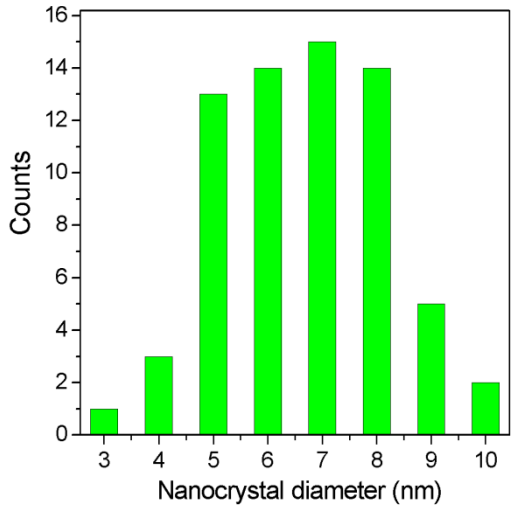

Fig. S2 Corresponding size distribution plot for the CZTS nanocrystals

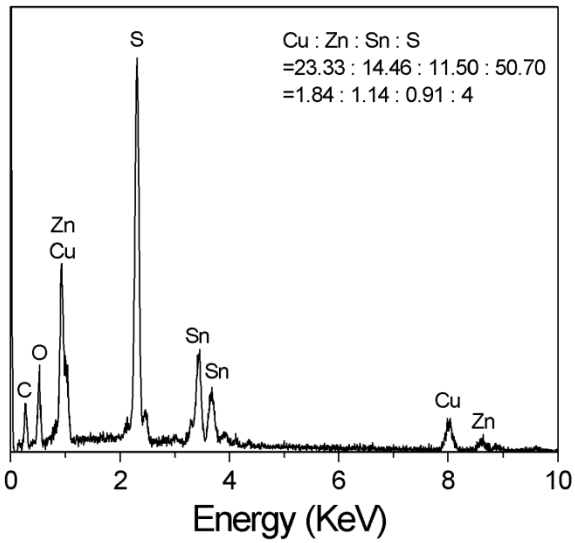

Fig. S3 EDS spectrum of the as-synthesized CZTS nanocrystals. The CZTS nanocrystals are slightly Cu, Sn poor and Zn rich with the metal composition of Zn/Sn=1.25 and Cu/(Zn+Sn)=0.90.

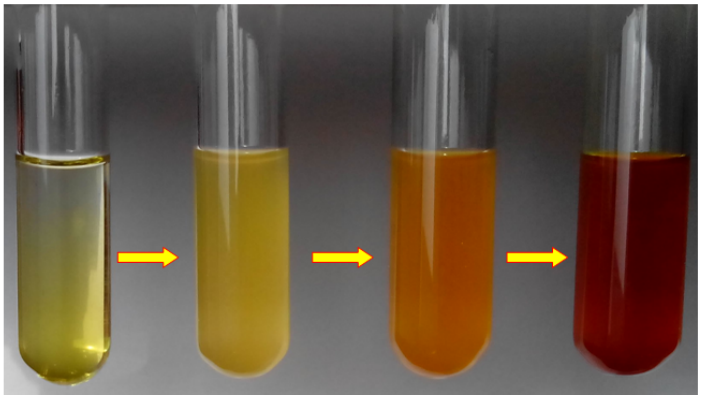

Fig. S4. Color changes from yellow to orange and then to red color in the preparation of the polysulfide precursor solution.

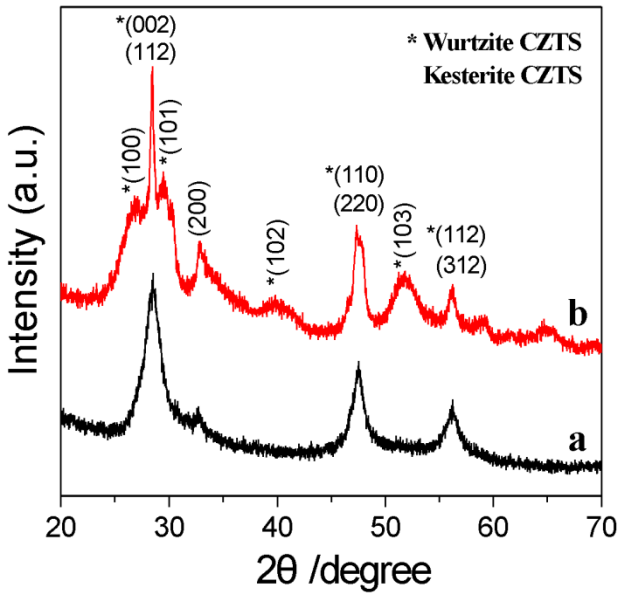

Fig. S5 XRD patterns of the obtained CZTS nanocrystals in (a) KTB ethanol solution, (b) NaOH ethanol solution.

When KTB was substituted for NaOH in our synthetic procedure, two coexisting CZTS phases (wurtzite and kesterite) were found. As shown in Fig. S4b, the major diffraction peaks can be indexed to kesterite CZTS and/or cation-disordered wurtzite CZTS proposed by Peng et al.[1] Because the arrangements of atoms in two crystal structures (kesterite and wurtzite) are basically similar, the three diffraction peaks at about 28°, 47°, and 56° for these two structures are almost at the same positions.[2] In other words, the diffraction peaks at about 28°, 47°, and 56° can be attributed to (112), (220), and (312) planes of kesterite CZTS or (002), (110), and (112) planes of wurtzite CZTS, respectively. The diffraction peaks that appeared at about 27°, 30°, 39°, and 52° are attributed to (100), (101), (102), and (103) planes of wurtzite CZTS. The diffraction peak at around 33°correspond to the characteristic (200) plane of kesterite CZTS.

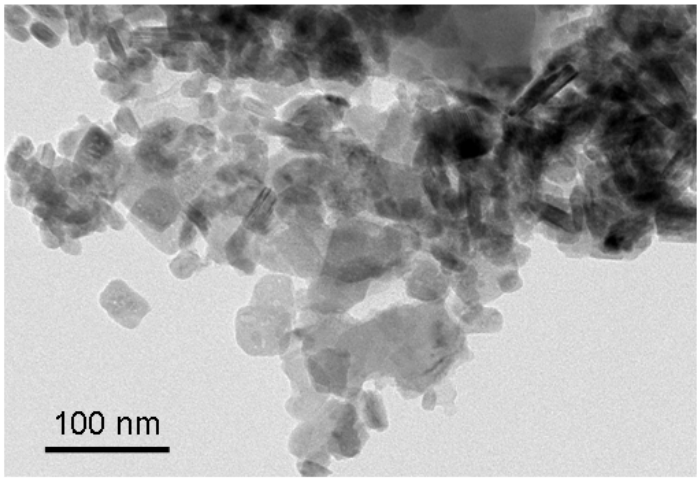

Fig. S6 TEM image of the CZTS nanocrystals obtained in NaOH ethanol solution.

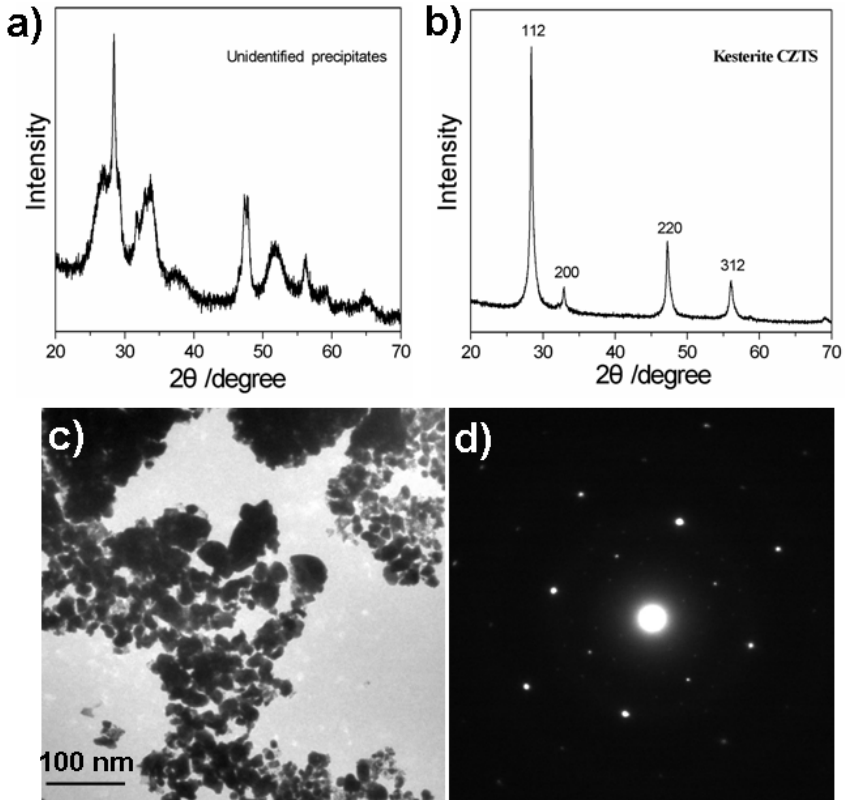

Fig. S7 XRD pattern of the obtained samples at heating temperature of (a) 200 °C and (b) 300 °C; TEM (c) and SAED (d) images of the CZTS nanocrystals obtained at heating temperature of 300 °C

References:

1. X. T. Lu, Z. B. Zhuang, Q. Peng, Y. D. Li, *Chem. Commun.*, 2011, **47**, 3141−3143.

2. H. C. Jiang, P. C. Dai, Z. Y. Feng, W. L. Fan, J. H. Zhan, *J. Mater. Chem.*, 2012, **22**, 7502−7506.