Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Electronic Supplementary Information

Phase Selective Synthesis of Metastable Orthorhombic Cu_2ZnSnS_4

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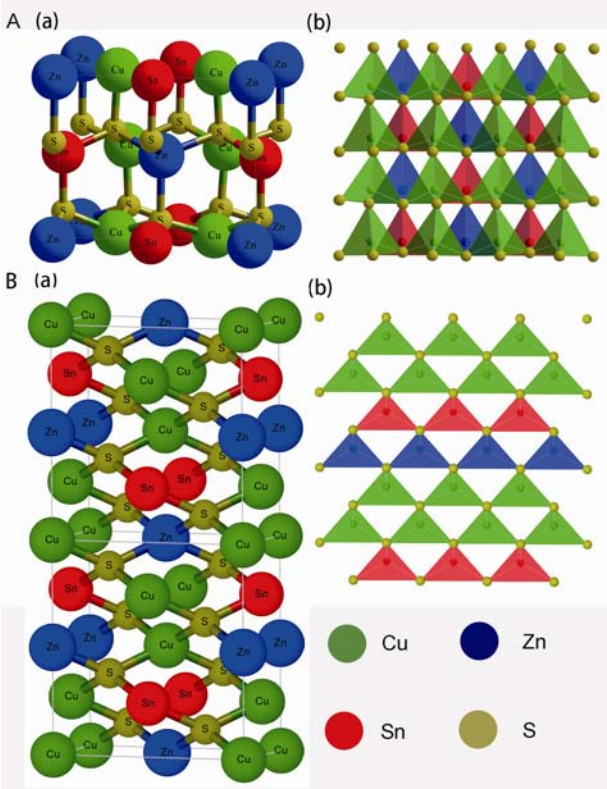

Figure S1 Crystal structures of orthorhombic CZTS (A) and kesterite CZTS (B).

Molecular	Cu_2ZnSnS_4
Crystal system	Orthorhombic
Space group	$Pmn2_1$
Number of formula units per unit cell	2
a (nm)	0.75385
b (nm)	0.64304
c (nm)	0.62038
Cell volume (nm^3)	0.30073
Number of atoms in the cell	16

Table S1 Crystal Data of the orthorhombic CZTS.

Atom	x/a	y/b	z/c
Cu	0.2504	0.3270	0
Zn	0	0.8411	0.9971
Sn	0	0.1786	0.4982
S1	0.2335	0.3420	0.3688
S2	0	0.2068	0.864
S3	0	0.8480	0.398

Table S2 Atomic coordinates for the Cu2ZnSnS4 compound.[1]

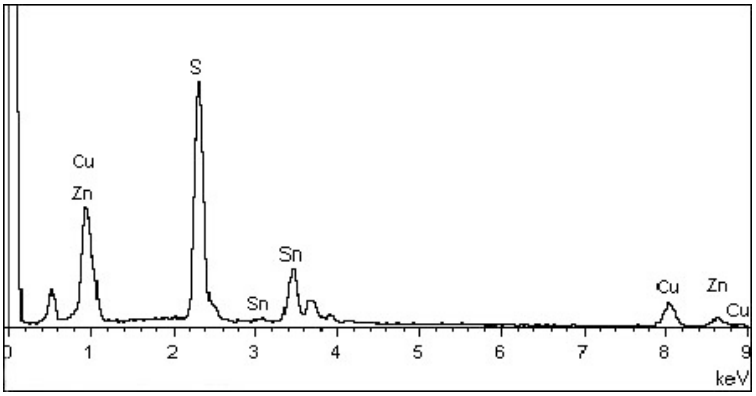

Figure S2. Spectrum of the Energy Dispersive X-ray Spectroscopy (EDS) of wurtzite-stannite CZTS nanocrystals.

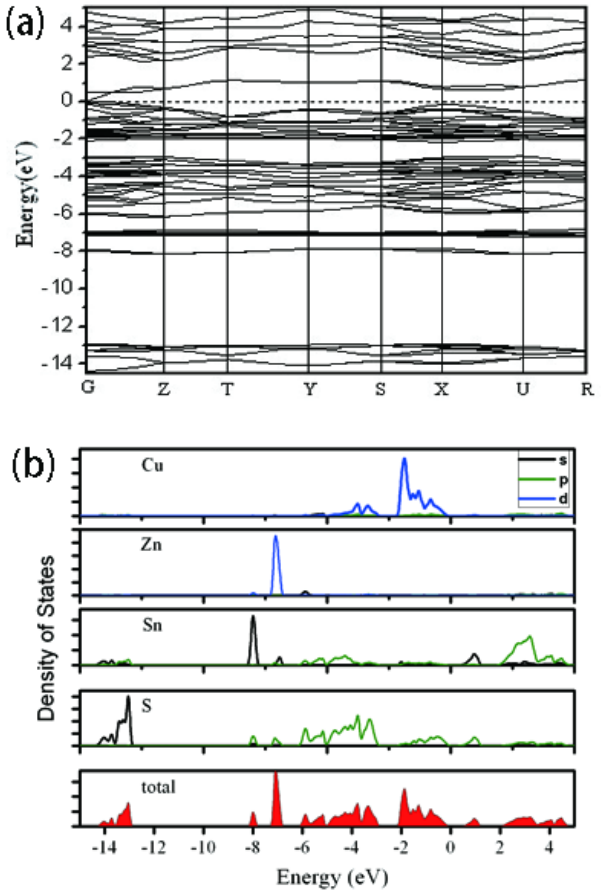

Figure S3. (a) Band structures of as-synthesized orthorhombic CZTS. (b) DOS and PDOS of orthorhombic CZTS.

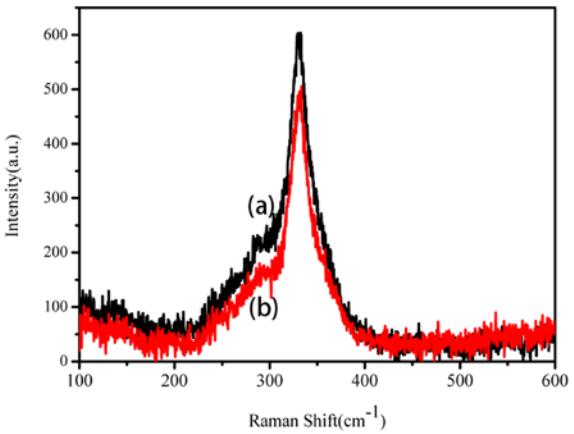

Figure S4. Raman spectra of orthorhombic CZTS synthesized in ultrapure water (a) and the mixed solvent of ultrapure water and ethylendiamine (b).

1. O. V. Parasyuka, Y. E. Romanyukb and I. D. Olekseyuka, *Journal of Crystal Growth*, 2005, 275, 4.