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Supplementary Information

Phase-Selective Hydrothermal Synthesis of Cu_2ZnSnS_4 Nanocrystals: The Effect of Sulphur Precursor

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The XRD patterns of Cu_2ZnSnS_4 (CZTS) with wurtzite structures were simulated using Visualization System for Electronic and Structural Analysis (VESTA) and CCDC Mercury 3.0 softwares. The crystal data of the wurtzite-kesterite CZTS is listed in Table S1. The crystal structure representation is shown in Figure S1.

Powder x-ray diffraction patterns of CZTS_TAA were analysed using the Total Pattern Analysis Solutions (TOPAS) version 4.1 software. The Rietveld method was employed. The included CuKa5 emission profile was used. The background was modelled with a 5th order Chebyshev and also a One_on_X function. The profile was fitted using a PV-TCHZ (modified Thomson-Cox-Hastings pseudo-Voigt) function for each phase (refined terms were U, V, W and X). The Simple_Axial_Model macro was used to model axial divergence. Other refined parameters included sample displacement, lattice parameters, and scale factors. Phase ratios were calculated assuming no amorphous/non-diffracting material.

Table S1: Crystal data of the wurtzite-kesterite CZTS

Formula	Cu_2ZnSnS_4
Crystal system	Monoclinic
Space group	Pc
Unit cell dimensions	a = 7.7077 Å; b = 6.6630 Å; c = 6.3482 Å
Cell volume	0.3260 nm^3
Number of formula units per unit cell	2
Number of atoms in the cell	16

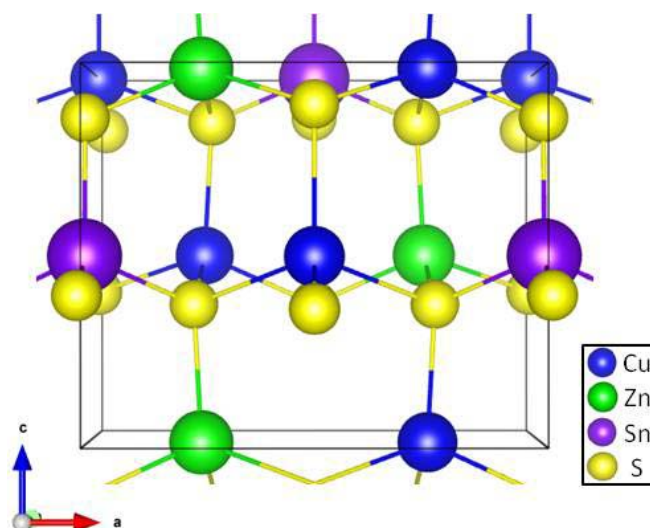

Fig. S1 Crystal structure of wurtzite Cu_2ZnSnS_4.

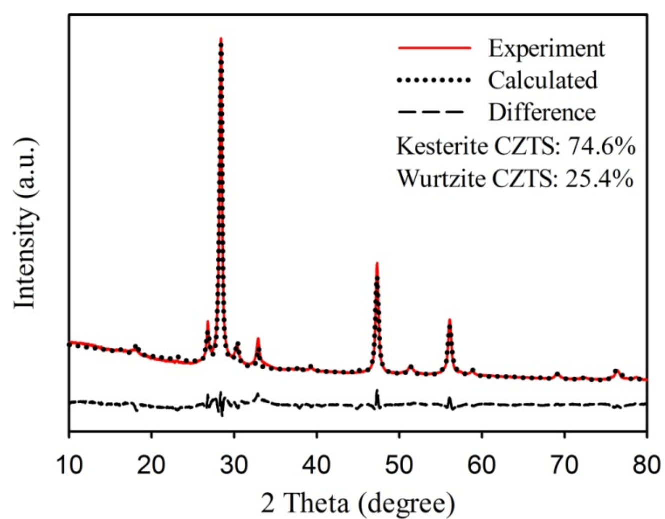

Fig. S2 Relative abundance of kesterite and wurtzite phase in CZTS_TAA based on refined experimental XRD data (goodness-of-fit indicator, S (= R_{wp}/R_e) = 4.87). The lower black line with few spikes indicates the standard deviation of the calculated XRD data compared to the experimental data.