Solution-based Synthesis of Wurtzite Cu_2ZnSnS_4 Nanoleaves Introduced by α-Cu_2S Nanocrystals as Catalyst

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Crystal data (Wurtzite)

Formula	ZnS	Cu_2ZnSnS_4
Space group	$P6_3mc$	$P6_3mc$
Lattice parameter (a)	3.800(0) Å	3.832(6) Å
Lattice parameter (c)	6.230(0) Å	6.327(6) Å

Atomic positions:

	x	y	z
S	**1/3**	**2/3**	**0.375**
	2/3	**1/3**	**0.875**
Cu/Zn/Sn	**1/3**	**2/3**	**0**
	2/3	**1/3**	**1/2**

Wurtzite Cu_2ZnSnS_4 can be obtained by partial replacing Zn sites in wurtzite ZnS using Cu and Sn atoms, which occupy the same positions. Among three atoms, the occupancy of Cu atoms is constant 50%, Zn and Sn atoms have the same values for 25%, respectively.

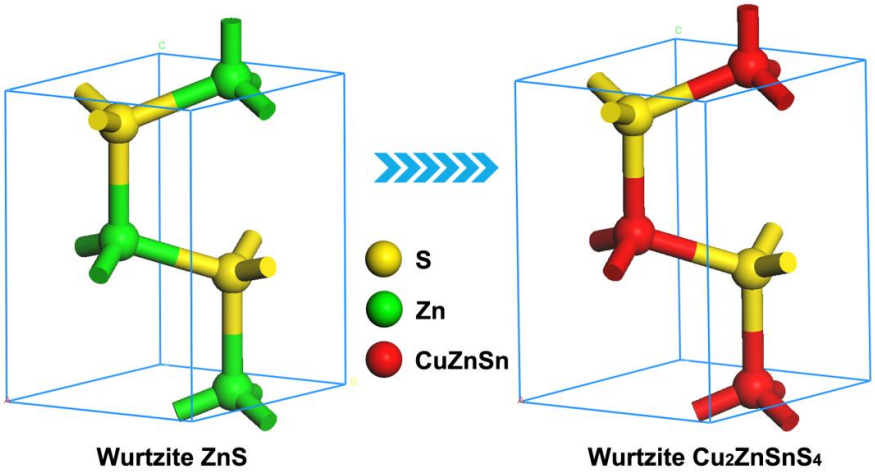

Figure S1. Crystal structure of wurtzite ZnS and Cu_2ZnSnS_4.

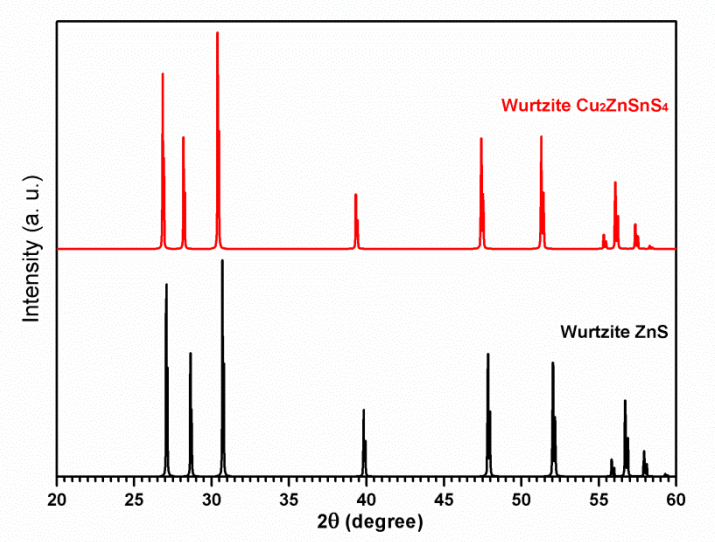

Figure S2. The XRD patterns of wurtzite ZnS and Cu_2ZnSnS_4. The XRD pattern of ZnS is obtained according to the JCPDS Card, No. 75-1534; and the XRD pattern of Cu_2ZnSnS_4 is simulated by CrystalMaker and CrystalDiffract software.

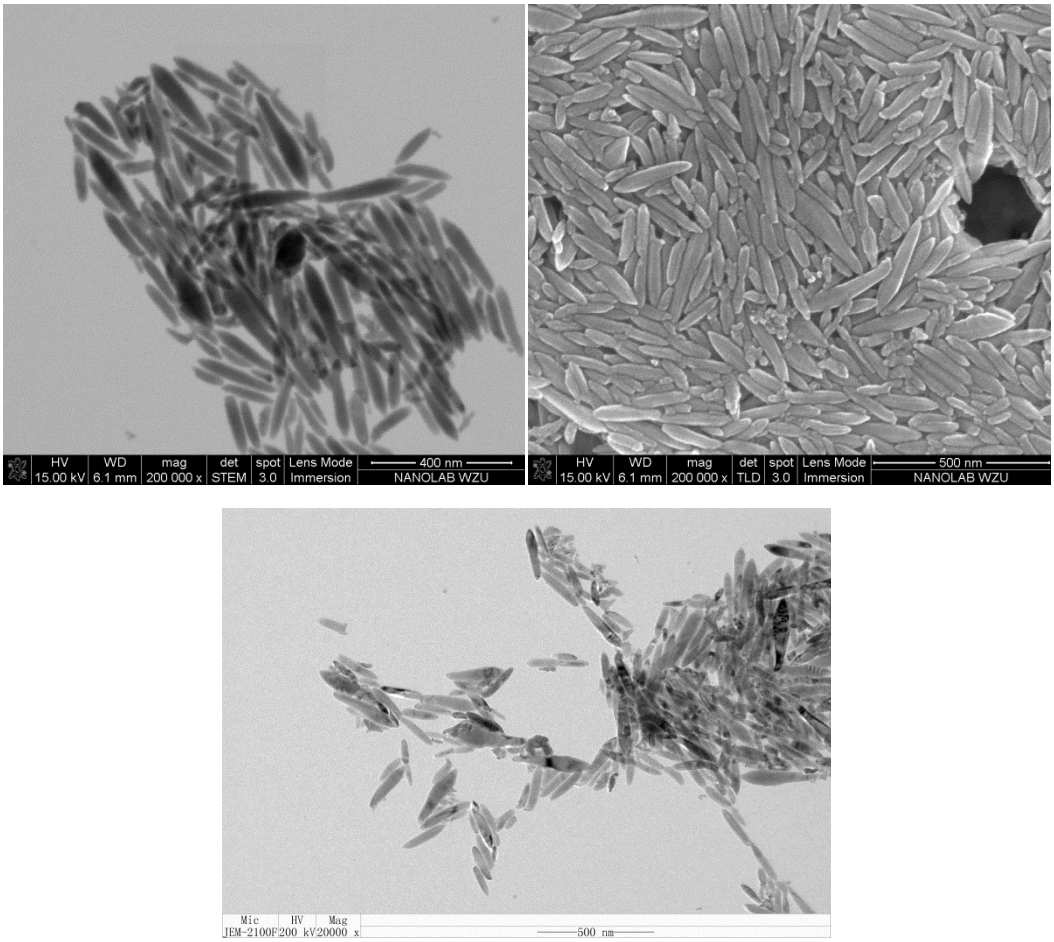

Figure S3. STEM and SEM images of Cu_2ZnSnS_4 nanomaterials prepared at the presence of octadecene.

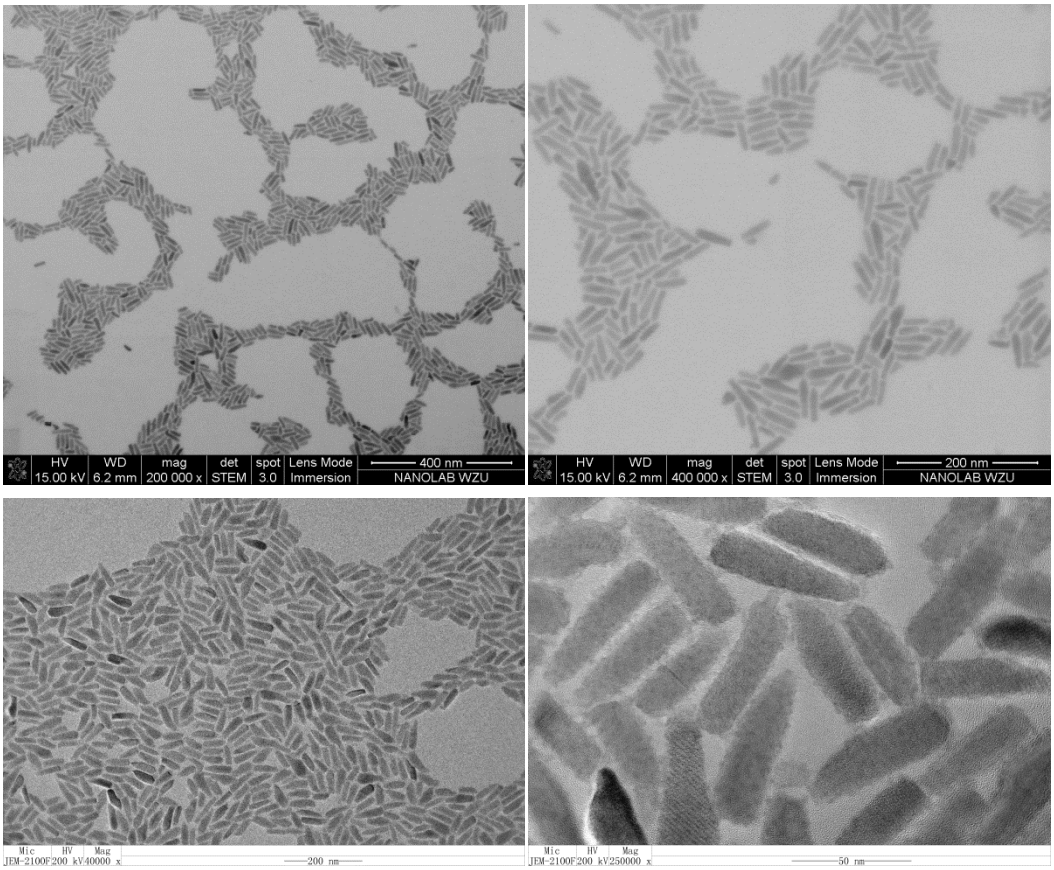

Figure S4. STEM and TEM images of Cu_2ZnSnS_4 nanomaterials prepared at the presence of OLA, OA, and DT.

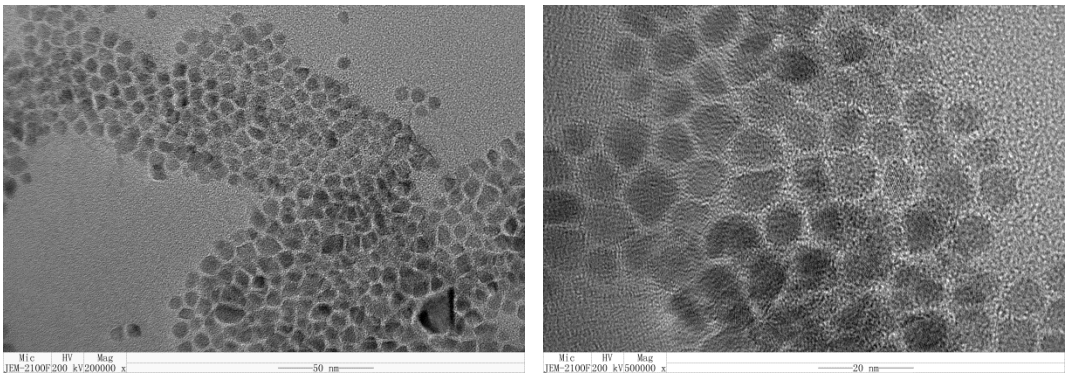

Figure S5. TEM images of Cu_2ZnSnS_4 nanomaterials prepared at the presence of OLA and DT.

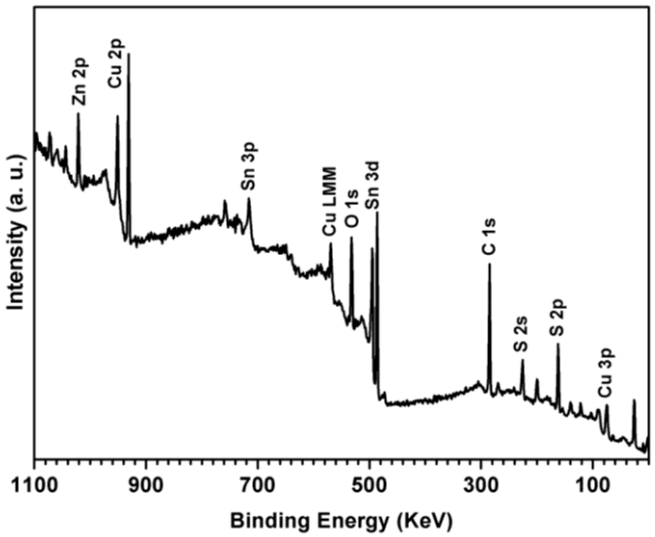

Figure S6. The survey spectrum of Cu_2ZnSnS_4 nanoleaves.

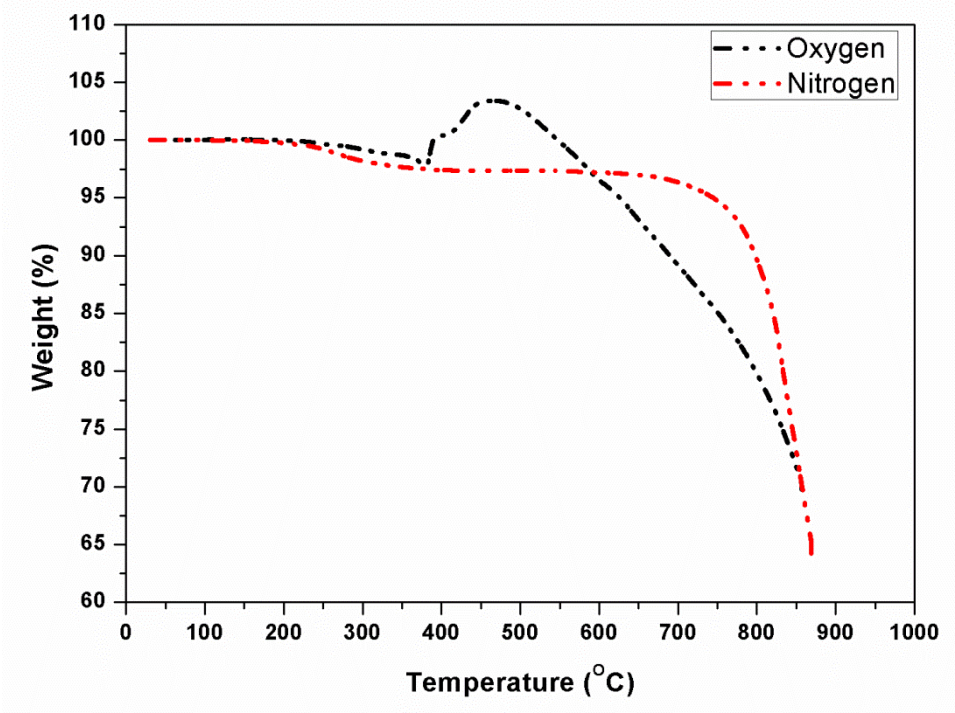

Figure S7. TGA curves of the as-synthesized CZTS nanoleaves. The first weight loss at about 250 ^{O}C under oxygen flow is attributed to the loss of attached ligands, the weight gain is attributed to the oxidation during the oxygen circumstance. While, the weight loss at about 250 ^{O}C under nitrogen flow is attributed to the loss of attached ligands,