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Supporting Information

Synthesis of $Cu_2ZnxSnySe_{1+x+2y}$ Nanocrystals with Wurtzite-Derived Structure

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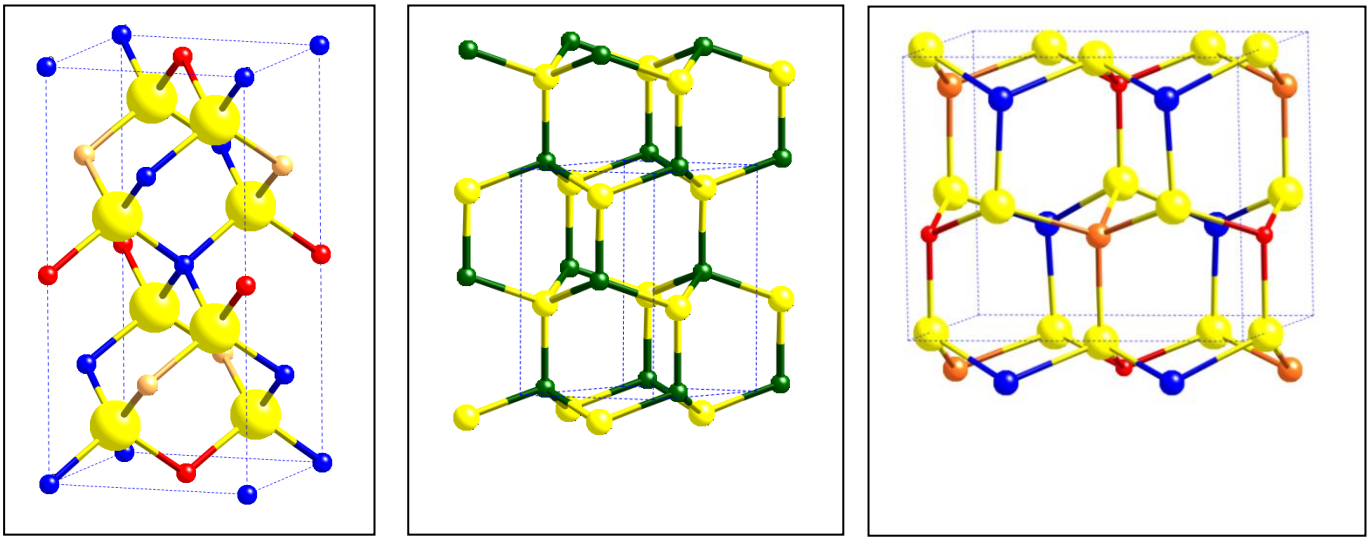
Simulation diffraction pattern of kesterite type, wurtzite type and wurtz-stannite type CZTSe

Crystal structures



kesterite type structure wurtzite type structure wurtz-stannite type structure

Figure. S1 Schematic representation of the unit cells of kesterite type, wurtzite type and wurtz-stannite type CZTSe (blue – Cu; orange – Zn; red – Sn; yellow – Se; green – random distribution of Cu,Zn and Sn)

Crystal structure data

Molecular formula	structure type	crystal system	space group
$Cu_2ZnSnSe_4$	kesterite	tetragonal	$I\bar{4}2d$

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$Cu_2ZnSnSe_4$	wurtzite	hexagonal	$P6_3mc$
$Cu_2ZnSnSe_4$	wurtz-stannite	orthorhombic	$Pmn2_1$

Table S0: Atomic coordinates related to the kesterite type structure (8g is an (x,y,z) position, nevertheless x and y are very similar)

Atom	Wyckhoff position	x	y	z
Cu	2a	0	0	0
Cu	2c	0	1/2	1/4
Zn	2d	1/2	0	1/4
Sn	2b	1/2	1/2	1
Se	8g	0.2587	0.2587	0.3714

Table S1: Atomic coordinates related to the wurtzite type structure (2b is the (1/3,2/3,z) position)

Atom	Wyckhoff position	x	y	z
Se	2b	1/3	2/3	3/8
Zn	2b	1/3	2/3	1.00
Cu	2b	1/3	2/3	1.00
Sn	2b	1/3	2/3	1.00

Chen et al. [1] have shown that the kesterite structure of CZTSe can be derived from zinc-blende type ZnSe by substituting Zn^{2+} atoms with Cu^{+}, Zn^{2+} and Sn^{4+}. Hereby we simulated diffraction pattern from the wurtzite ZnSe by replacing Zn^{2+} atomic position with Cu^{+}, Zn^{2+} and Sn^{4+}. The atomic ratio of Cu:Zn:Sn is 50:25:25.

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Table S2: Atomic coordinates related to the wurtz-stannite type structure (4b is the general position (x,y,z); 2a is the position (0,y,z)). The structure is based on Cu_2ZnSiS_4 (ICSD-261267). The given values result from the Rietveld analysis.

Atom	Wyckhoff position	x	y	z
Cu	4b	0.7524	0.6780	0.1790
Zn	2a	0.00	0.8448	2/3
Sn	2a	0.00	0.1773	0.1697
Se	2a	0.00	0.86280	0.0635
Se	2a	0.00	0.1913	0.5144
Se	4b	0.7290	0.6645	0.5508

Reference

(1) S. Chen, A. Walsh, Y. Luo, J.-H. Yang, X. Gong, S.-H. Wei, *Phys. Rev B,* 2010, **82**, 1.