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Supporting Information

Chemical Synthesis, Characterization and Theoretical Investigations of Stannite Phase $CuZn_2AlS_4$ Nanocrystals

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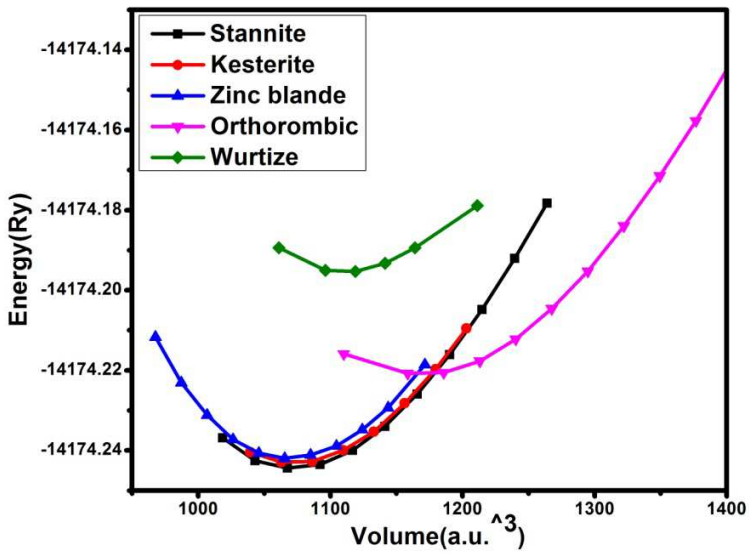
Table S1: Equilibrium total energy of various possible crystal structures of CZAS nanocrystals. (Simulation: Wien2k code).

Structures of $CuZn_2AlS_4$	**Equilibrium total energy**
Wurtzite : $P6_3mc$, space group no. 186	-14147.19545
Zinc blende: F4-3m, space group no.216	-14147.24191
Orthorhombic : $Pmn2_1$, space group no.31	-14147.22109
Kesterite : I-4, space group no.82	-14174.243161
Stannite: I-42m, space group no. 121	**-14174.244553**

Table S2: The optimized atomic positions for stannite $CuZn_2AlS_4$.

Elements	Wyckoff	x/a	y/b	z/c
Cu	2a	0	0	0
Zn	4d	0	0.5	0.25
Al	2b	0	0	0.5
S	8i	0.2537	0.2537	0.1205

Figure S1: Volume vs. Total energy for $CuZn_2AlS_4$.



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