

## Supporting Information:

### **Synthesis and high pressure transformation of metastable wurtzite structured CuGaS<sub>2</sub> nanocrystals**

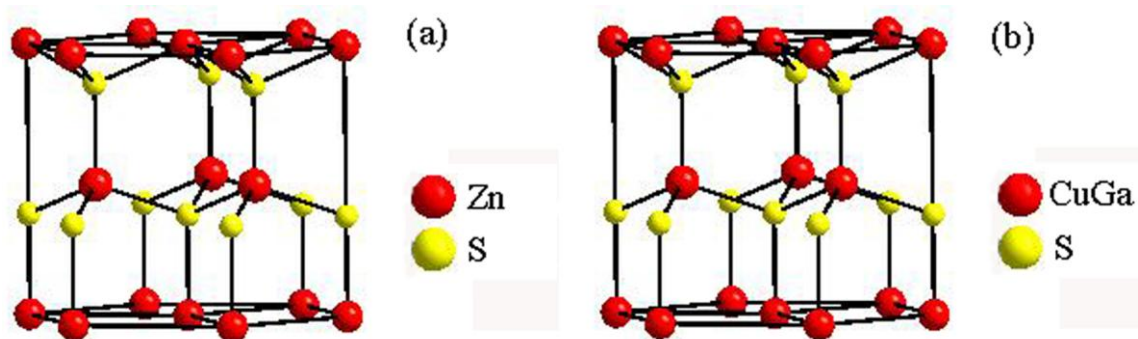
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**Figure S1.** Crystal structures of (a) wurtzite ZnS and (b) wurtzite CuGaS<sub>2</sub>.

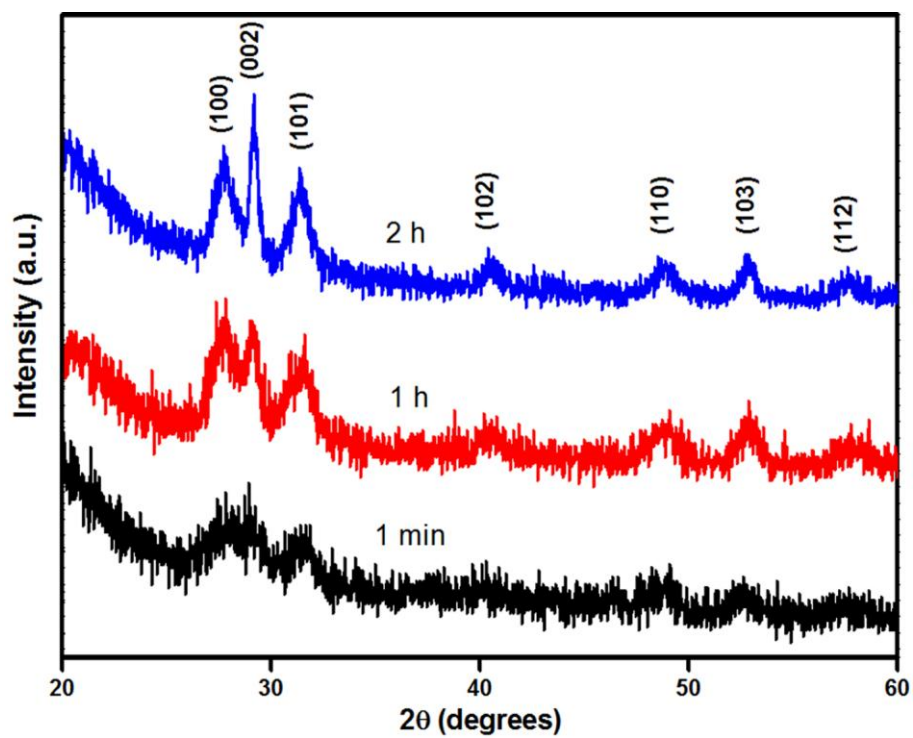
The crystal structure of CuGaS<sub>2</sub> nanocrystals can be represented by the wurtzite structured ZnS, where Cu and Ga occupy the same Zn positions with the occupation probability of Cu or Ga on every Zn positions was 50%.

#### Crystal data

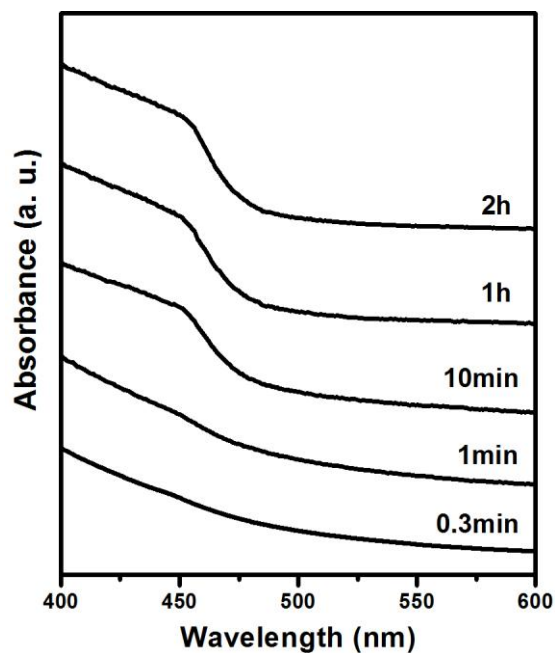
Formula	CuGaS <sub>2</sub>
Crystal system	Wurtzite
Space group	<i>P</i> 6 <sub>3</sub> <i>mc</i> (No. 186)
Lattice parameter:	$a=b= 3.71(6) \text{ \AA}$ , $c= 6.14(2) \text{ \AA}$

#### Atomic coordinates

	x/a	y/b	z/c
atomic positions for S:	1/3	2/3	0.375
	2/3	1/3	0.875
atomic positions for Cu :	2/3	1/3	0.5
atomic positions for Ga :	1/3	2/3	0

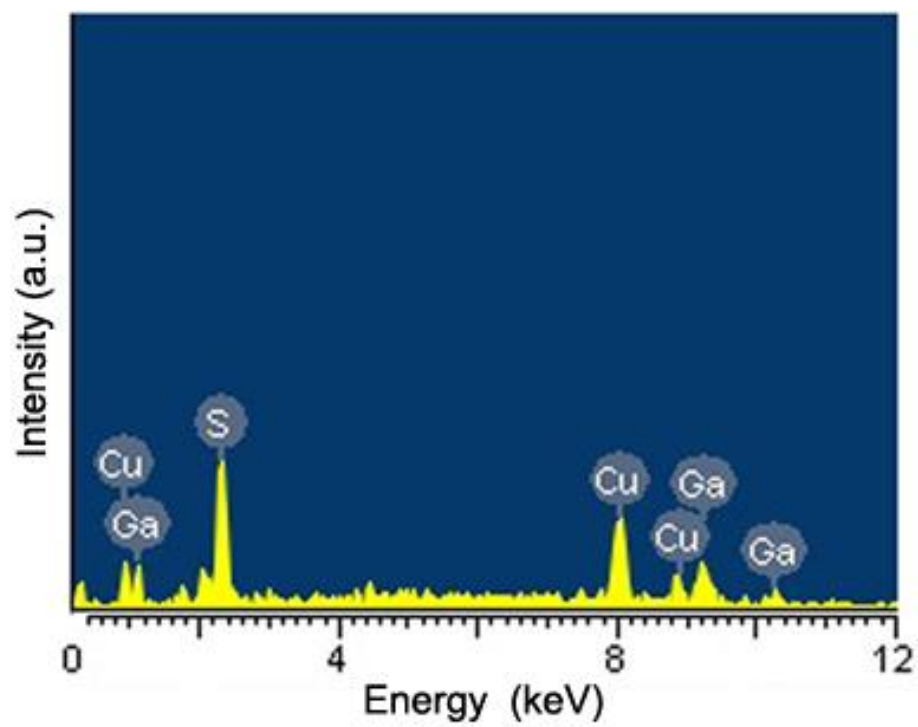


**Figure S2.** XRD patterns of the CuGaS<sub>2</sub> nanocrystals synthesized at different time.

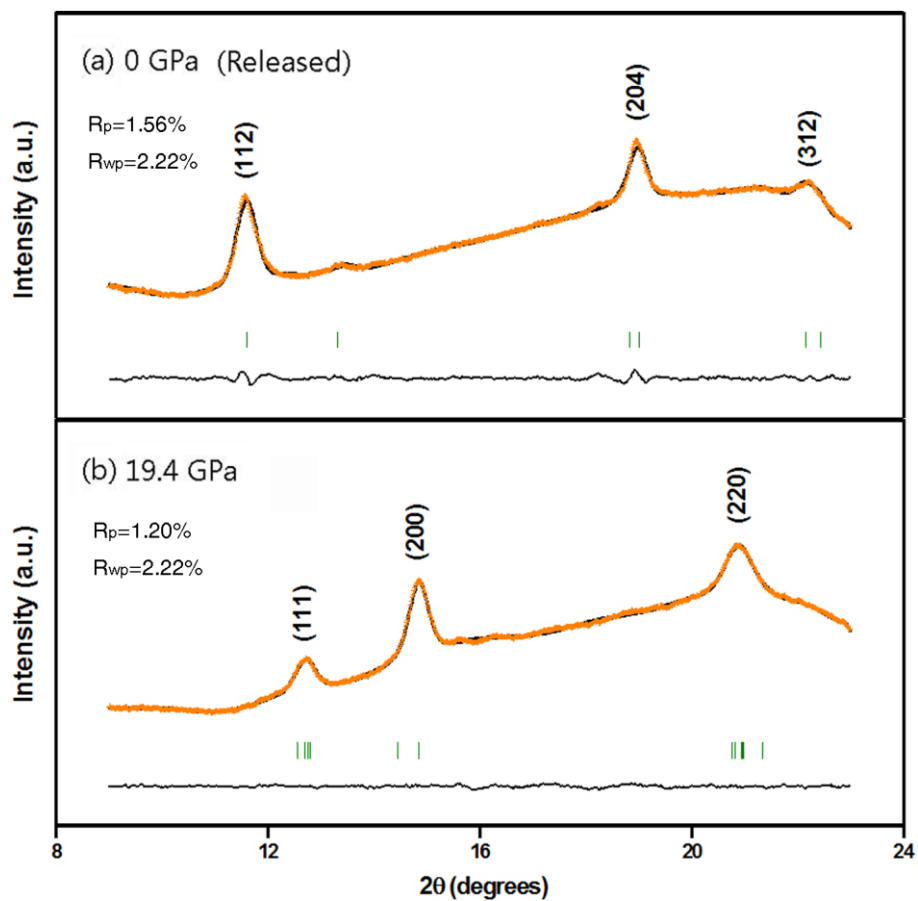


**Figure S3.** Temporal evolution of the UV-Vis absorption of the CuGaS<sub>2</sub> nanocrystals.

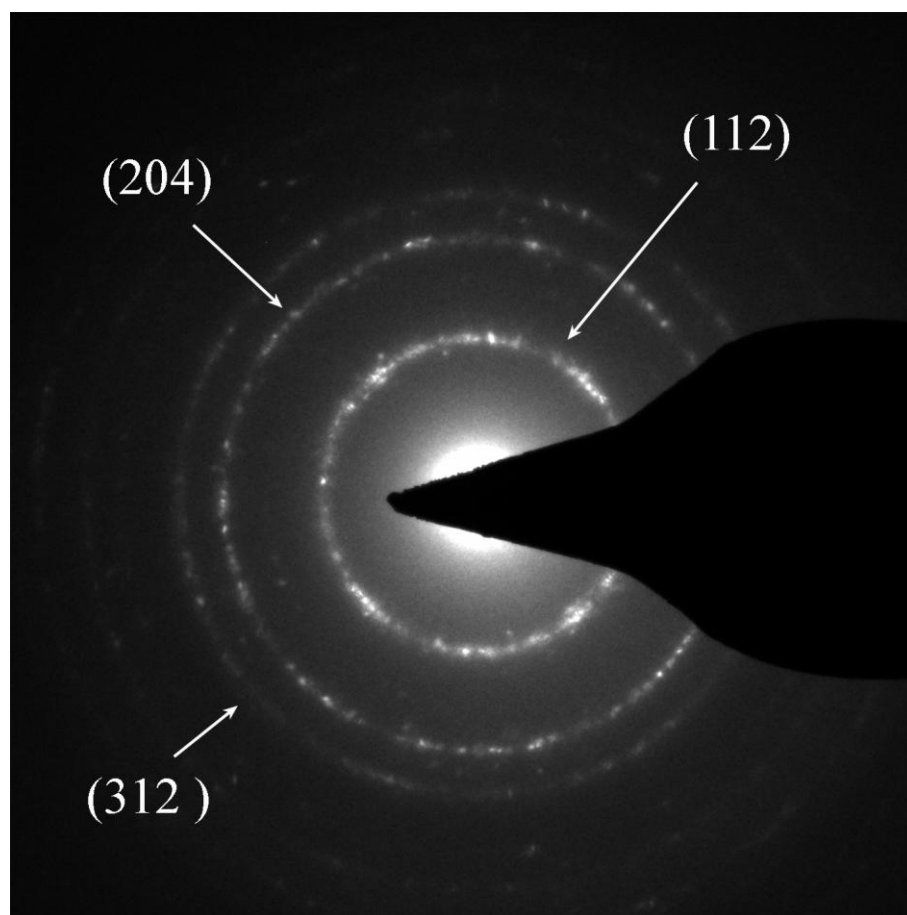
Figure S3 showed the temporal evolution of the UV-Vis absorption of the as-prepared CuGaS<sub>2</sub> nanocrystals taken at different time intervals. It was observed that no nanocrystals formed before 240°C, and then nanocrystals with an absorption peak started to form.



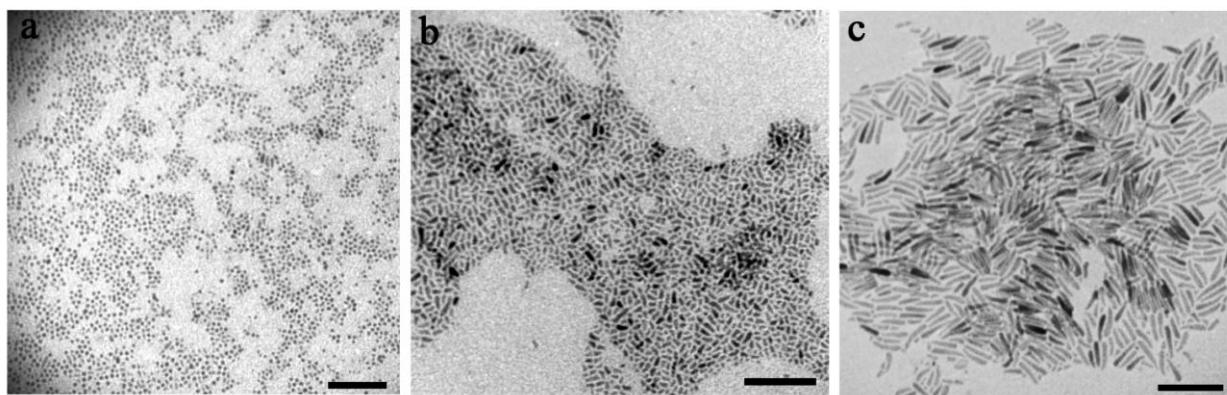
**Figure S4.** EDX spectrum of a sample of CuGaS<sub>2</sub> nanocrystals.



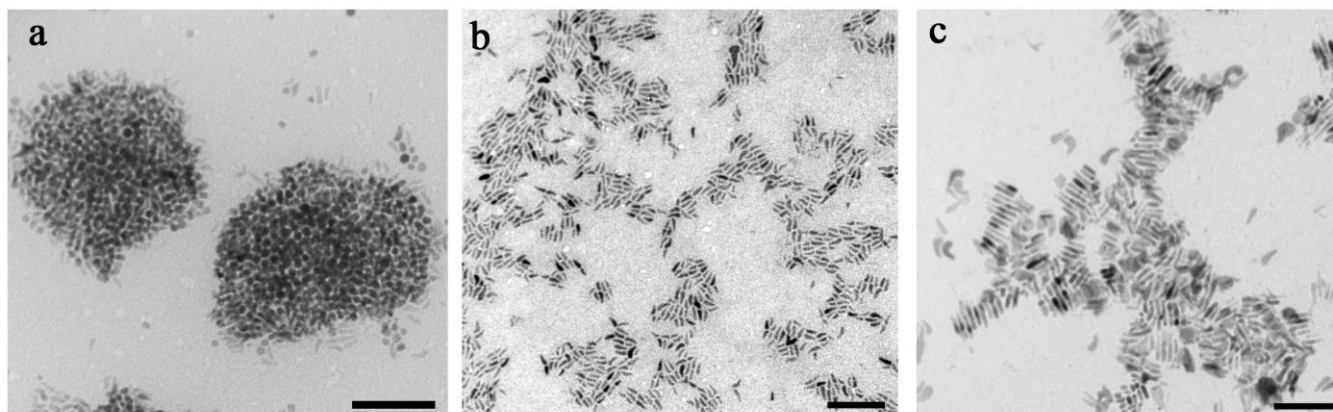
**Figure S5.** Experimental (orange cross) and refined (black solid line) XRD patterns for (a) chalcopyrite structure CuGaS<sub>2</sub> nanocrystals after decompression and (b) rock salt structure CuGaS<sub>2</sub> nanocrystals at 19.4 GPa



**Figure S6.** The selected area electron diffraction of decompressed samples.



**Figure S7.** TEM images of CuGaS<sub>2</sub> nanocrystals synthesized at 240 °C for different reaction times. (a) 1min, (b) 1h, and (c) 2 h. All scale bars represent 100 nm.



**Figure S8.** TEM images of CuGaS<sub>2</sub> nanocrystals synthesized at 240 °C for 1h with different reaction parameters. All scale bars represent 100 nm. Corresponding parameter see below.

Figure S8	DDT/ml	OA/ml	OLA/ml
(a)	0.25	0.25	
(b)	0.30	0.10	0.10
(c)	0.25		0.25



