

Synthesis, Structure, and Optical Properties of $K_{2.4}Ga_{2.4}M_{1.6}Q_8$ ($M=Si, Ge$; $Q= S, Se$) Crystals and Glasses

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Table S1. EDS elements ratio of the four compounds.

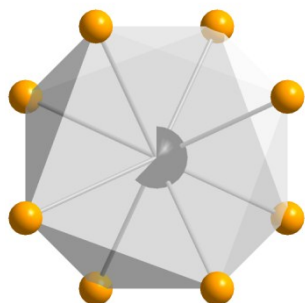
Compound	$K_{2.4}Ga_{2.4}Si_{1.6}S_8$	$K_{2.4}Ga_{2.4}Ge_{0.6}S_8$	$K_{2.4}Ga_{2.4}Si_{1.6}Se_8$	$K_{2.4}Ga_{2.4}Ge_{1.6}Se_8$
K (%)	16.8	17.5	17.2	16.6
Ga (%)	18.5	17.2	17.0	18.5
M' (%)	11.0	8.7	8.3	10.3
Q (%)	53.7	56.69	57.5	54.5

Table S2. Crystallographic data of $K_{2/3}Ga_{2/3}Ge_{1/3}Se_2$.

Formula	$K_{2/3}Ga_{2/3}Ge_{1/3}Se_2$
Space group	Pccn
Unit cell	$a=8.1208 \text{ \AA}$ $b=8.1208 \text{ \AA}$ $c=18.6240 \text{ \AA}$
Volume	1228.20 \AA^3
Z	12

Table S3. Atomic coordinates and for $K_{2/3}Ga_{2/3}Ge_{1/3}Se_2$.

Compounds	Ato	Wykoff	x/a	y/b	z/c	sof.
$K_{2/3}Ga_{2/3}Ge_{1/3}Se_2$	Se1	8e	0.90828	0.40828	0.08333	1.0
	Se2	8e	1.09172	0.90828	0.08333	1.0
	Se3	8e	0.90828	1.09172	0.25000	1.0
	Ga4	4d	3/4	1/4	1/6	1.0
	Ga5	4d	3/4	1/4	1/2	1.0
	Ge6	4d	1/4	3/4	1/6	1.0
	K7	4c	1/4	1/4	1/6	0.62
	K8	4c	1/4	1/4	1/2	0.62

Figure S1. Schematic diagram of $[KSe_{8/2}]$ square antiprism. Black: K; yellow: Se. Void of the black ball represents K vacancy.**Figure S2.** The PXRD patterns of powder samples of $K_{2.4}Ga_{2.4}Si_{1.6}S_8$ and $K_{2.4}Ga_{2.4}Si_{1.6}Se_8$. The black bars correspond to the theoretical patterns of $K_{2.4}Ga_{2.4}Si_{1.6}Se_8$.

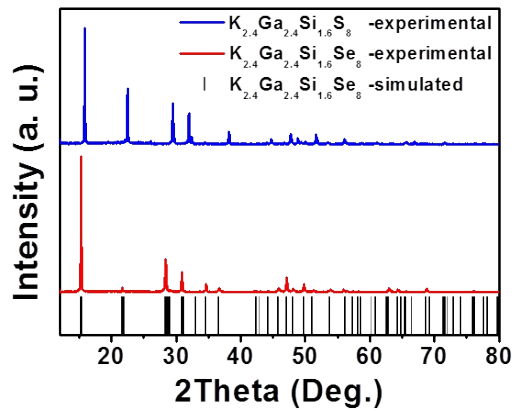


Figure S3. The PXRD patterns of powder samples recrystallized from $K_{2.4}Ga_{2.4}Ge_{1.6}S_8$ and $K_{2.4}Ga_{2.4}Ge_{1.6}Se_8$ glass at 600 °C for 5 hours. The black bars correspond to the theoretical patterns of $K_{2.4}Ga_{2.4}Ge_{1.6}Se_8$.

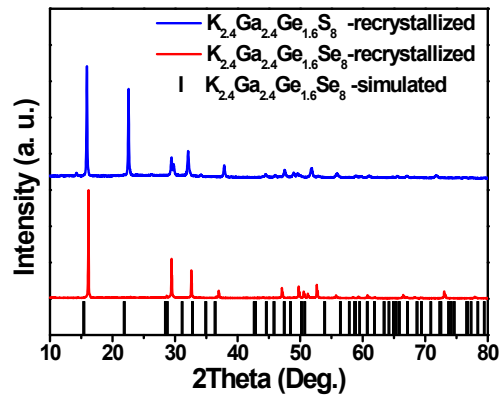


Figure S4. UV-Vis absorbance spectra of $K_{2.4}Ga_{2.4}Ge_{1.6}Q_4$ ($Q=S, Se$) powder and glass samples.

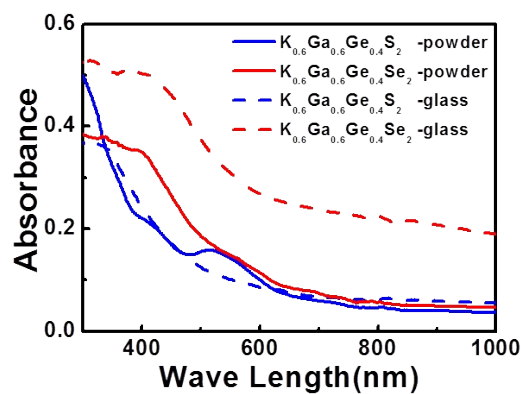


Figure S5. Infrared transmission spectra of $K_{2.4}Ga_{2.4}Ge_{1.6}Q_8$ ($Q=S, Se$) glasses.

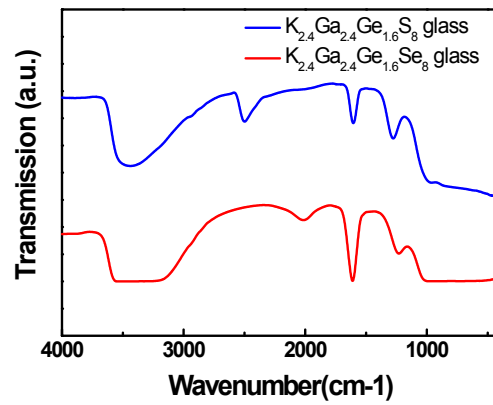


Figure S6. DTA curve of $K_{2.4}Ga_{2.4}Ge_{1.6}S_8$ glass.

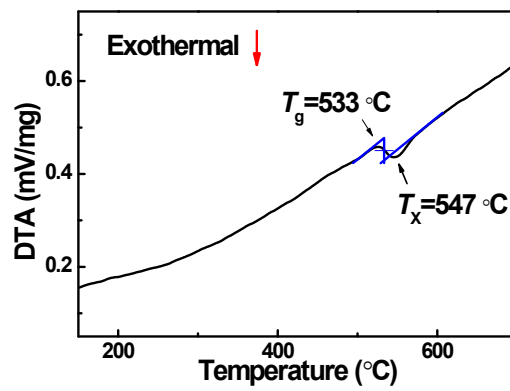


Figure S7. (a) Electronic-band structure of $KGaSe_2$. (b) Total DOS of $KGaSe_2$. (c-d) Partial DOS of Ga and Se in $KGaSe_2$. Partial DOS of K are too low and omitted here.

