

Supporting Information for:

Bandgap Regulation and Doping Modification of Ga_{2-x}Cr_xSe₃ Nanosheets

**Huan Yang^{a,b}, Yue Wu^{a,b}, Huirong Li^{a,b}, Yiwen Zhang^{a,b}, Linmei Gao^{a,b}, Lanfang Wang^{a,b}
and Fang Wang^{a,b,*}**

*^a School of Chemistry and Materials Science of Shanxi Normal University & Key Laboratory of
Magnetic Molecules and /Magnetic Information Materials of Ministry of Education, Taiyuan
030032, China.*

*^b Research Institute of Materials Science of Shanxi Normal University & Collaborative Innovation
Center for Advanced Permanent Magnetic Materials and Technology of Ministry of Education,
Taiyuan 030032, China.*

*E-mail: wf_0716@163.com (F. Wang).

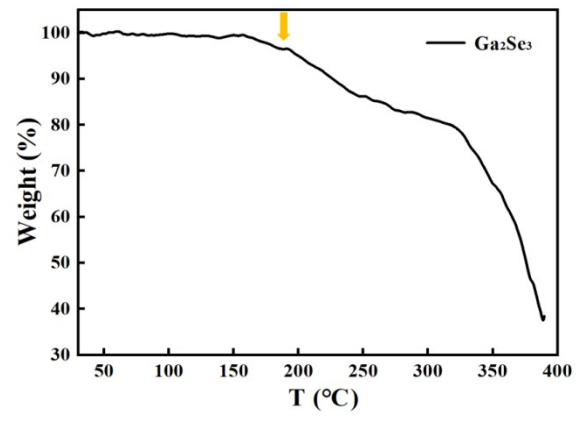


Fig. S1. Thermogravimetric analysis of Ga₂Se₃ nanoparticles.

Table S1. Unit cell parameters and unit cell volumes of Ga₂Se₃ and Ga₂Se₃ after annealing at different temperatures.

Sample	Ga ₂ Se ₃	150 °C	200 °C	250 °C	300 °C
lattice Constant a (Å)	5.4290	5.4678	5.4832	5.4668	5.4783
Unit cell volume V (Å) ³	160.01	163.47	164.86	163.38	164.41
ΔV (Å) ³		3.46	4.85	3.37	4.40

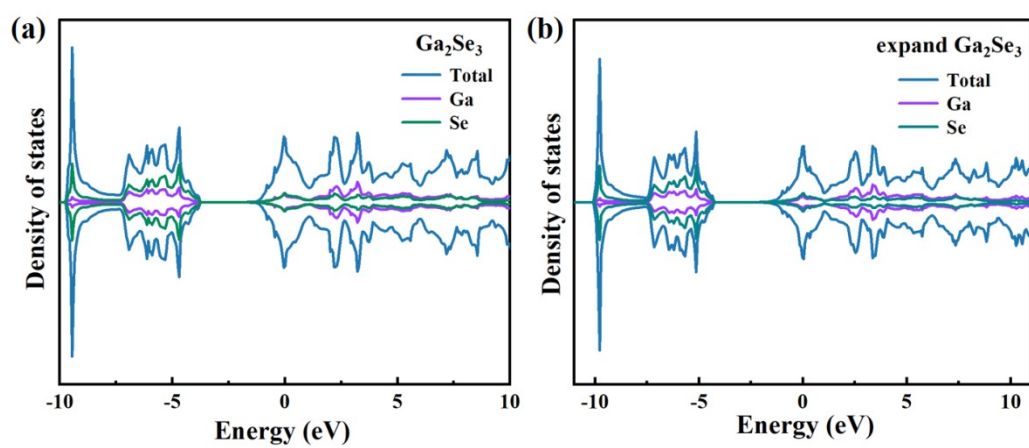


Fig. S2. Calculated DOS plots of Ga_2Se_3 and *expand* Ga_2Se_3 using HSE06 functional.

Table S2. Unit cell parameters and unit cell volumes of the $\text{Ga}_{2-x}\text{Cr}_x\text{Se}_3$ ($0 \leq x \leq 0.6$) nanosheets with different Cr contents

Sample	x = 0	x = 0.2	x = 0.4	x = 0.6
2θ ($^\circ$)	27.94	28.03	28.37	28.67
lattice Constant a (\AA)	5.4290	5.4239	5.4083	5.3935
Unit cell volume V (\AA^3)	160.01	159.56	158.20	156.90
ΔV (\AA^3)		0.45	1.82	3.11

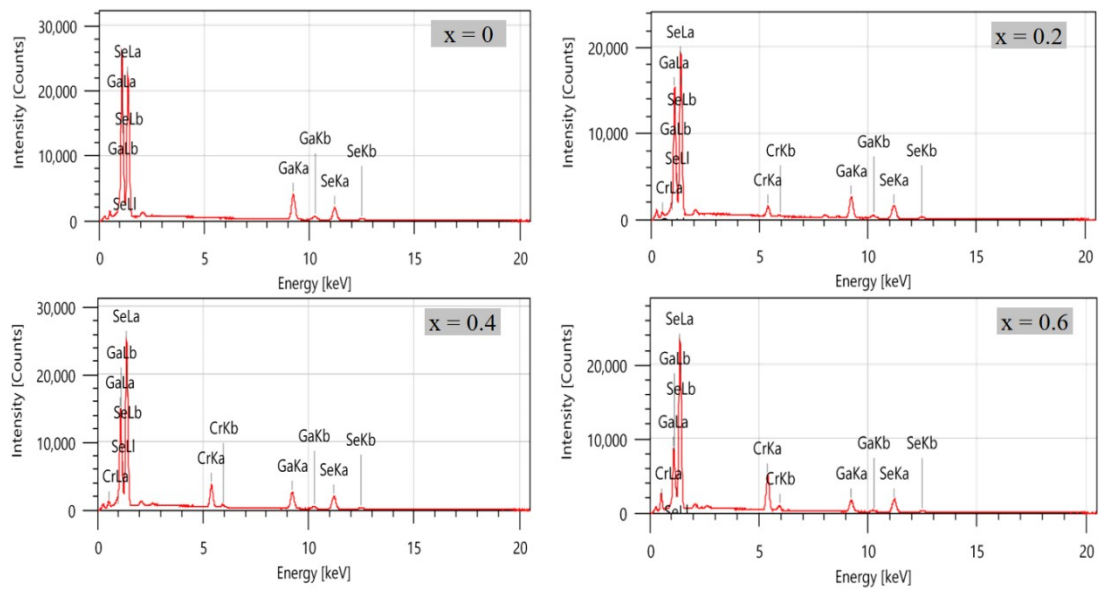


Fig. S3. EDX spectra of $\text{Ga}_{2-x}\text{Cr}_x\text{Se}_3$ ($0 \leq x \leq 0.6$) with different Cr concentrations.

Table S3. The content of Ga, Cr, Se elements in different Cr doping content (x).

Cr doping content (x)	Ga (at.%)	Cr (at.%)	Se (at.%)	(Ga+Cr)/Se
x = 0	41.75	0	58.25	41.75/58.25
x = 0.2	34.29	5.28	60.43	39.57/60.43
x = 0.4	27.46	12.30	60.24	39.76/60.24
x = 0.6	20.15	20.16	59.69	40.31/59.69

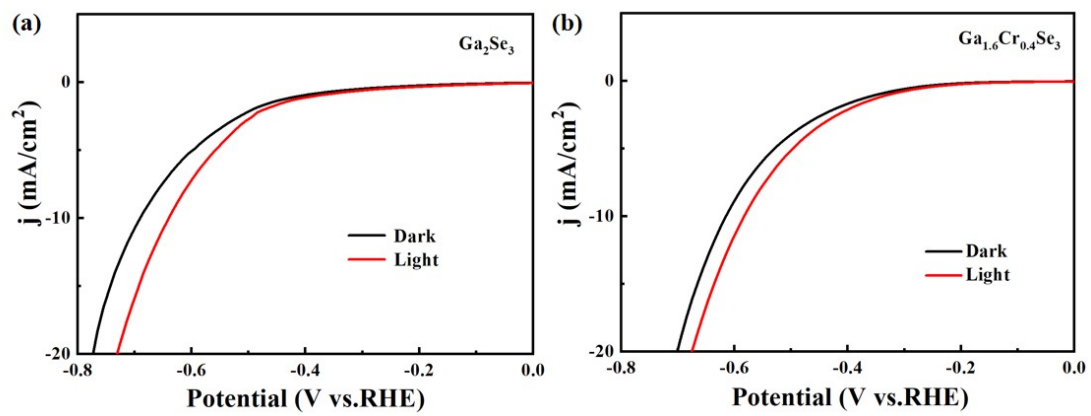


Fig. S4. LSV curves of Ga_2Se_3 and $\text{Ga}_{1.6}\text{Cr}_{0.4}\text{Se}_3$ samples under light and dark conditions.

Table S4. BET surface areas and pore properties of Ga₂Se₃ nanoparticles and Ga_{1.6}Cr_{0.4}Se₃ nanosheets.

Sample	BET surface area (m ² g ⁻¹)	Pore volume (cm ³ g ⁻¹)	Pore size (nm)
Ga ₂ Se ₃	7.9437	0.0594	18.8341
Ga _{1.6} Cr _{0.4} Se ₃	39.1334	0.1837	12.1886