Supporting information for: $Cr_{2.37}Ga_3Se_8$: A Quasi-Two-Dimensional Magnetic Semiconductor

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Content

Table S1. Bonds length (Å) in $Cr_{2.37}Ga_3Se_8$ at room temperature

	Se1	**Se2**	**Se3**	**Se4**	**Se5**	**Se6**
Ga1	2.370(2)	2.425(2)		2.368(3)	2.423(2)	
Ga2	2.377(3)×2		2.401(3)		2.442(3)	
Cr1		2.524(3)×2, 2.559(3)×2	2.588(3)			2.513(3)
Cr2		2.549(1)×2	2.615(3)×2			2.500(3)×2
Cr3	2.701(2)×4			2.727(2)×2		

Table S2. Anisotropic thermal displacements for $Cr_{2.37}Ga_3Se_8$ at room temperature

Atom	**U11**	**U22**	**U33**	**U23**	**U13**	**U12**
Se1	0.0109(4)	0.0181(5)	0.0217(5)	-0.0105(4)	0.0042(3)	0.0001(4)
Se2	0.0091(4)	0.0068(4)	0.0082(4)	-0.0005(3)	0.0042(3)	-0.0004(3)
Se3	0.0091(4)	0.0074(5)	0.0070(6)	0	0.0028(4)	0
Se4	0.0402(8)	0.0083(6)	0.0262(8)	0	0.0254(7)	0
Se5	0.0093(7)	0.0064(5)	0.0116(6)	0	0.0045(4)	0
Se6	0.0098(5)	0.0077(5)	0.0096(6)	0	0.0036(4)	0
Ga1	0.0171(5)	0.0132(5)	0.0158(5)	0.0028(4)	0.0081(4)	0.0011(4)
Ga2	0.0132(6)	0.0119(6)	0.0110(7)	0	0.0028(5)	0
Cr1	0.0084(8)	0.0063(8)	0.0104(9)	0	0.0041(7)	0
Cr2	0.0089(8)	0.0068(9)	0.0083(9)	0	0.0042(7)	0
Cr3	0.009(2)	0.009(2)	0.007(2)	0	0.0003(14)	0

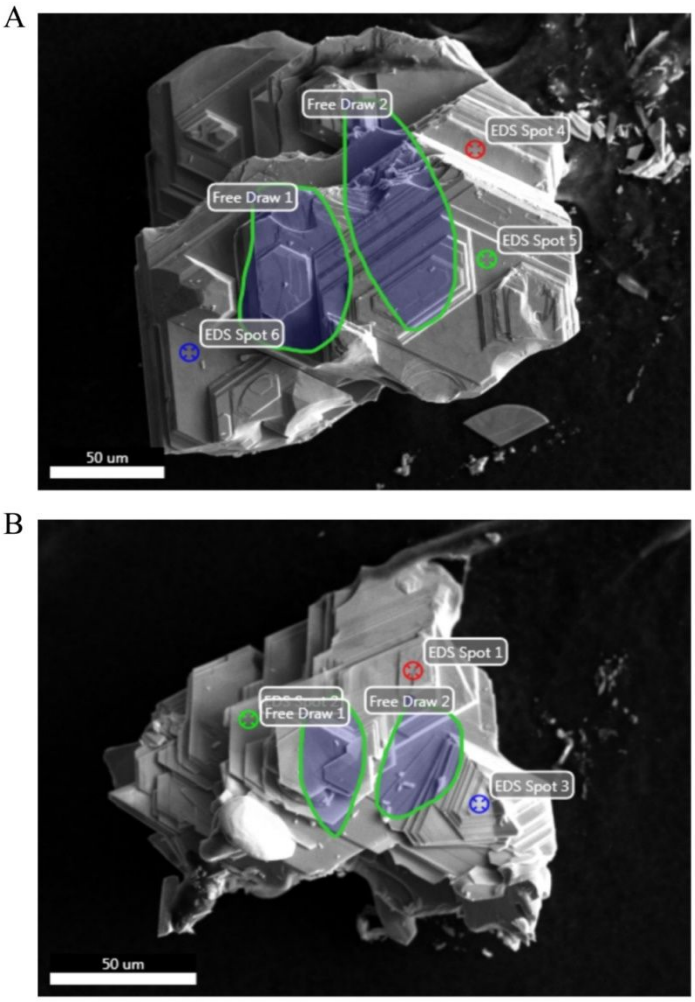

Figure S1. Two pieces of $Cr_{2.37}Ga_3Se_8$ sample are used to obtain energy dispersive spectrum. Three points and two areas in each sample are focused to get spectrum. Results of element ratio are displaying in ***Table S3***.

Table S3. Element ratio of $Cr_{2.37}Ga_3Se_8$ sample from energy dispersive spectrum

	Areas	**Cr**	**Ga**	**Se**
Sample A	Free Draw 1	2.38(3)	2.95(5)	8.00(8)
	Free Draw 2	2.39(5)	3.05(5)	8.00(9)
	EDS Spot 4	2.36(3)	2.95(5)	8.00(9)
	EDS Spot 5	2.39(1)	3.10(2)	8.00(3)
	EDS Spot 6	2.36(1)	3.05(2)	8.00(4)
Sample B	Free Draw 1	2.34(5)	2.99(7)	8.00(7)
	Free Draw 2	2.35(6)	3.02(4)	8.0(1)
	EDS Spot 1	2.31(5)	2.93(6)	8.00(5)
	EDS Spot 2	2.36(3)	3.00(8)	8.0(1)
	EDS Spot 3	2.39(4)	3.05(5)	8.00(4)

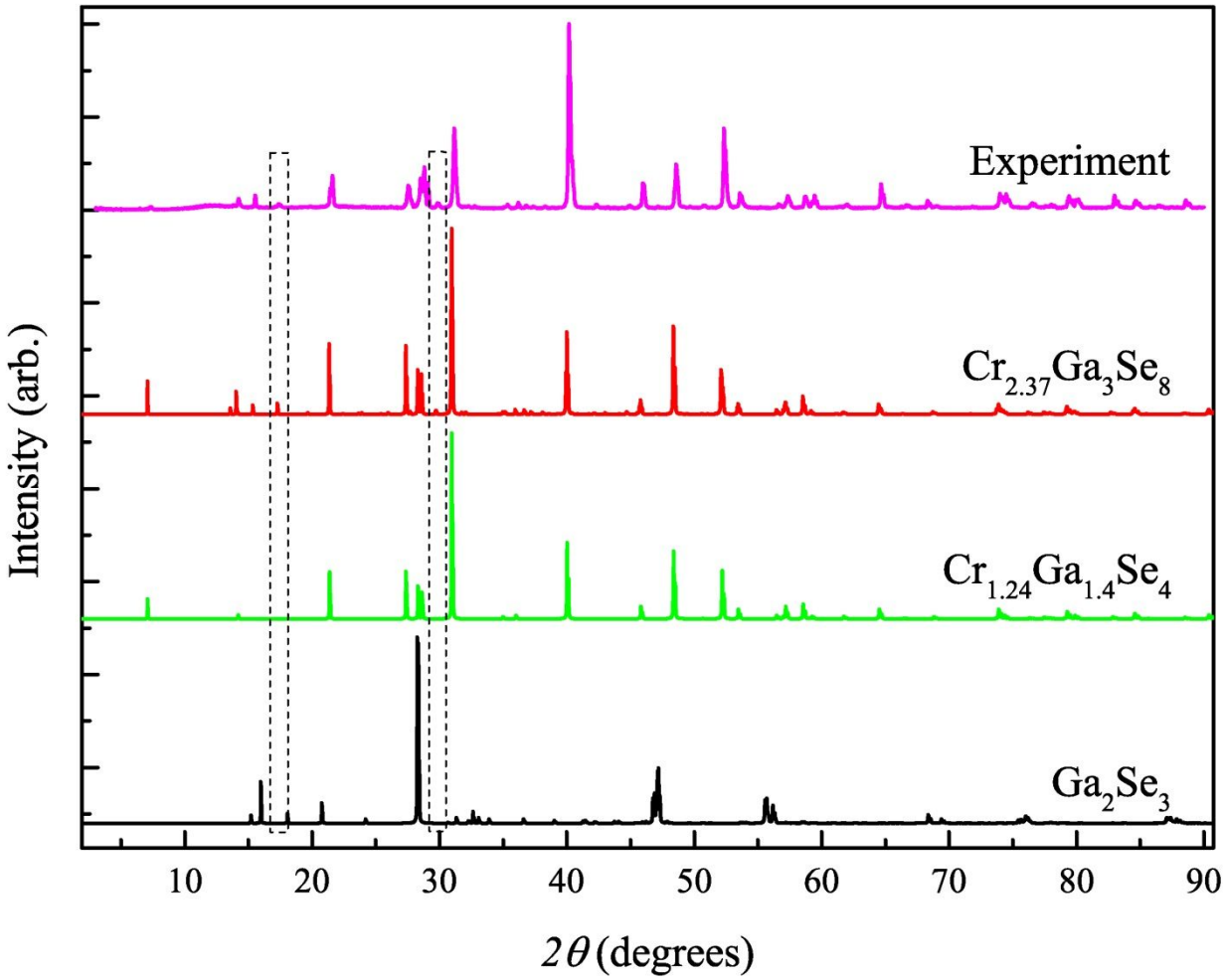

Figure S2. Compared with experiment curve, calculated X-ray diffraction patterns using different crystal structures represent by $Cr_{2.37}Ga_3Se_8$ (monoclinic structure) and $Cr_{1.24}Ga_{1.4}Se_4$ (hexagonal structure) are clearly different in 2θ range around 17° and 29.5°, emphasized by dashed box. Importantly, these peaks in experiment pattern do not come from Ga_2Se_3 impurity.

Table S4. Lattice parameters for LeBail refinement in $Cr_{2.37}Ga_3Se_8$ powder X-ray diffraction

***a*(Å)**	***b*(Å)**	***c*(Å)**	***α***	***β***	***γ***
12.9711(4)	7.5269(2)	13.9813(4)	90º	117.281(1)º	90º

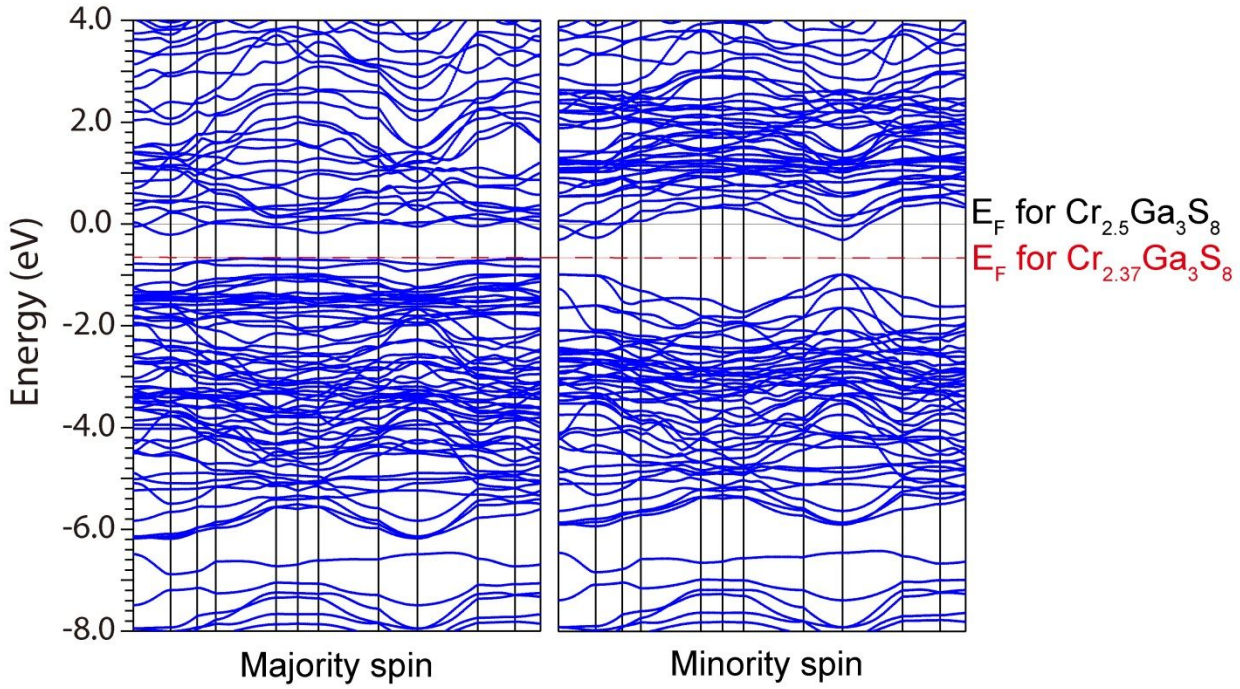

Figure S3. Band structure of $Cr_{2.5}Ga_3Se_8$ with spin polarization. Due to Cr vacancy on 2*b* site, Fermi level of $Cr_{2.37}Ga_3Se_8$ should be shifted to the red dash line.