Supplementary Information (SI) for CrystEngComm.

Top-seeded solution growth and characterization of β-Ga_2O_3

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Table S1. Crystallographic Data and Structural Refinements for β-Ga_2O_3.

Empirical formula	Ga_2O_3
Formula weight	374.88
Temperature (K)	273
Crystal system	Monoclinic
Space group	*C*2/*m*
a (Å)	12.247(10)
b (Å)	3.044(2), β=103.866(4)°
c (Å)	5.813(5)
Volume(Å^3)	210.41(3)
Z	2
D_c (g cm^{-3})	5.917
μ (mm^{-1})	24.279
F(000)	334
Completeness to theta	99.6%
GOF on F^2	1.042
R_1, wR_2 (I >2σ(I))[a]	0.0221, 0.0513
R_1, wR_2 (all data)	0.0282, 0.0542
Largest diff. peak and hole (eÅ^{-3})	0.781 and -0.763

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$ and $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w F_o^4]^{1/2}$ for $F_o^2 > 2\sigma(F_o^2)$

Table S2. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2), bond valence sums (BVSs) for β-Ga_2O_3.

Atom	x/a	y/b	z/c	U(eq)	BVS
Ga1	0.40951(5)	0.5	0.70552(11)	0.0062(2)	2.92
Ga2	0.65866(5)	0	0.81391(11)	0.0061(2)	2.94
O1	0.3264(3)	0.5	0.9365(7)	0.0055(8)	1.93
O2	0.3354(4)	0.5	0.3910(8)	0.0090(8)	1.87
O3	0.4963(3)	0	0.7566(8)	0.0098(9)	2.06

Table S3. Selected Bond Distances (Å) and Angles (°) for β-Ga_2O_3.

Atom–Atom	Length [Å]	Atom–Atom–Atom	Angle [°]
Ga1-O2	1.836(5)	O3-Ga1-O1	106.08(14)
Ga1-O3	1.839(2)	O3-Ga2-O2#7	94.71(15)
Ga2-O3	1.936(4)	O3-Ga2-O1#4	169.43(17)

Ga2-O2#5	1.945(3)	O2#7-Ga2-O1#4	91.85(15)
Ga2-O1#6	2.080(3)	O2#5-Ga2-O1#8	171.80(18)
Ga1-O2	1.836(5)	O1#4-Ga2-O1#8	80.82(11)
Ga1-O3	1.839(2)	O2#5-Ga2-O1#6	81.06(13)
Ga2-O3	1.936(4)	O1#4-Ga2-O1#6	80.82(11)
Ga2-O2#5	1.945(3)	O2-Ga1-O3#2	106.82(16)
Ga2-O1#6	2.080(3)	O3#2-Ga1-O3	111.7(2)
Ga1-O2	1.836(5)	O3#2-Ga1-O1	106.08(14)
Ga1-O3	1.839(2)	O3-Ga2-O2#5	94.71(15)
Ga2-O3	1.936(4)	O2#5-Ga2-O2#7	103.0(2)
Ga2-O2#5	1.945(3)	O2#5-Ga2-O1#4	91.85(15)
Ga2-O1#6	2.080(3)	O3-Ga2-O1#8	92.02(14)
Ga1-O2	1.836(5)	O2#7-Ga2-O1#8	81.06(13)
Ga1-O3	1.839(2)	O3-Ga2-O1#6	92.02(14)
Ga2-O3	1.936(4)	O2#7-Ga2-O1#6	171.80(18)
Ga2-O2#5	1.945(3)	O1#8-Ga2-O1#6	94.04(16)
Ga2-O1#6	2.080(3)	O2-Ga1-O3	106.82(15)
O2-Ga1-O1	119.41(19)		

Symmetry transformations used to generate equivalent atoms:

#1 x, y-1, z #2 x, y+1, z #3 x-1/2, y+1/2, z #4 x+1/2, y-1/2, z

#5 -x+1, -y, -z+1 #6 -x+1, -y, -z+2 #7 -x+1, -y+1, -z+1 #8 -x+1, -y+1, -z+2

Table S4. The full-width at half maximum (FWHM) comparison of β-Ga_2O_3 by different methods.

Compound	Methods of crystal growth	FWHM	Ref.
β-Ga_2O_3	the floating zone technique (OFZ)	324″	[1]
β-Ga_2O_3	edge-defined film-fed growth (EFG)	90″	[2]
β-Ga_2O_3	OFZ	100″	[3]
β-Ga_2O_3	OFZ	108″	[4]
β-Ga_2O_3	Czochralski (CZ)	36″	[5]
β-Ga_2O_3	EFG	59.4″	[6]
β-Ga_2O_3	EFG	69.3″	[7]
β-Ga_2O_3	**TSSG**	**140.04″**	**This work**

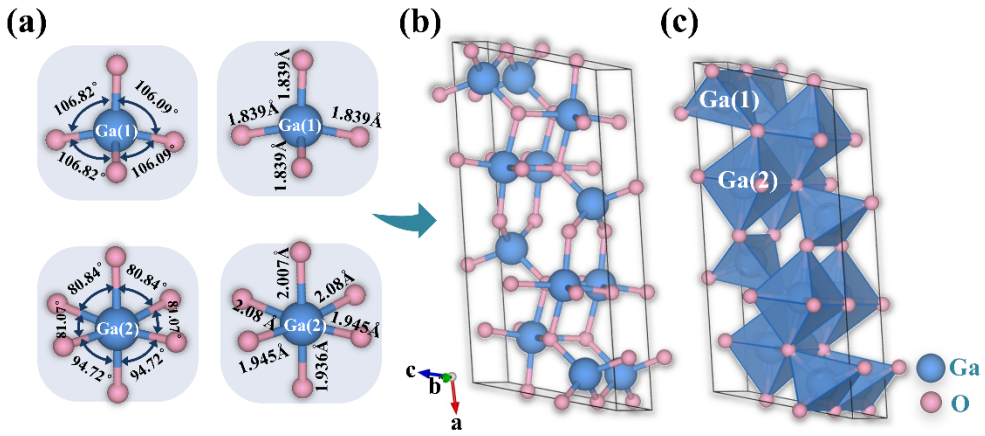


Fig. S1. (a) Complete coordination environment of cations in β-Ga_2O_3, (b) Ball-and-stick representation of the unit cell of β-Ga_2O_3 crystal structure along the b-axis, and (c) polyhedral representation of the β-Ga_2O_3 crystal structure.

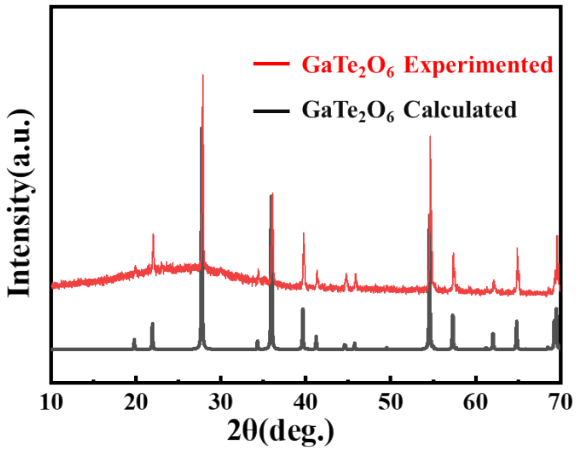
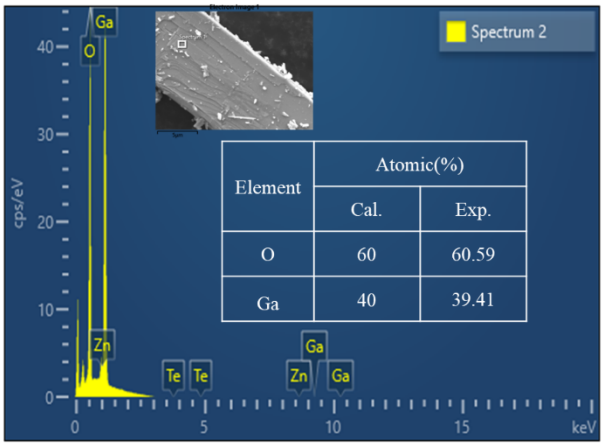


Fig. S2. The powder X-ray diffraction pattern of $GaTe_2O_6$ crystal (sticking on the rod).



Element	Atomic(%)	
	Cal.	Exp.
O	60	60.59
Ga	40	39.41

Fig. S3. The EDS spectra of β-Ga_2O_3 crystal.

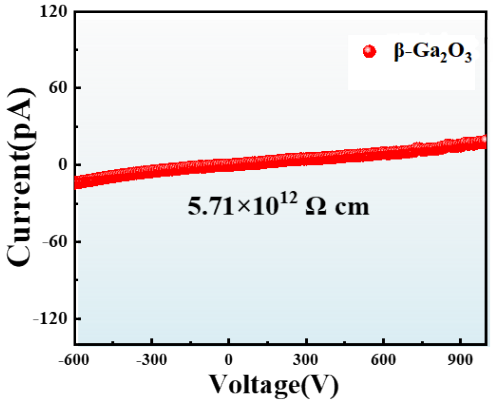


Fig. S4. I-V curves for resistivity measurements of β-Ga_2O_3 crystal.

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