[Electronic Supplementary Information]

Ab Initio Insights into Radiation-Induced Defects and Band-Gap Evolution in α-, β-, and κ-Ga_2O_3

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(Dated: January 29, 2026)

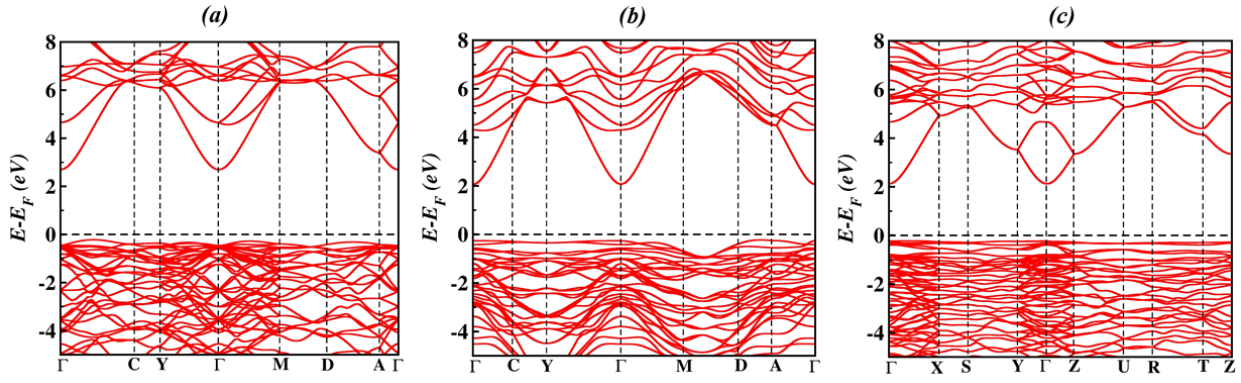

FIG. 1: The Electronic band structures at GGA PBE level of theory for (a) α-Ga_2O_3, (b) β-Ga_2O_3, and (c) κ-Ga_2O_3.

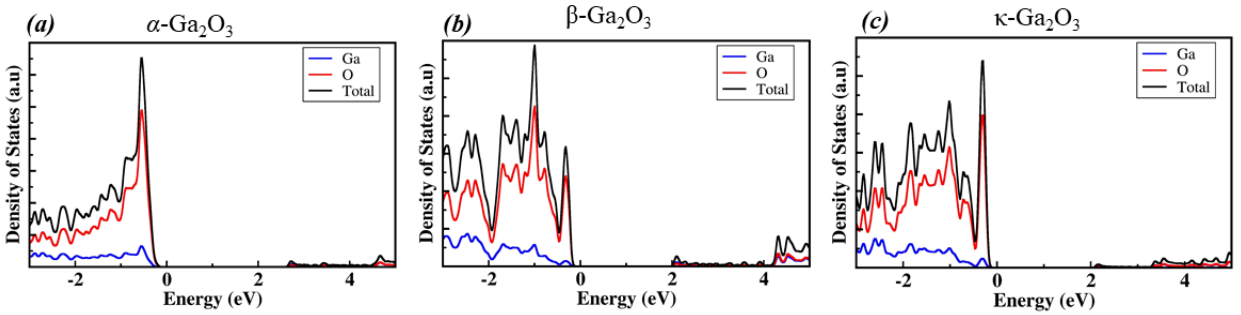

FIG. 2: The Partial Density of state at GGA PBE level of theory for (a) α-Ga_2O_3, (b) β-Ga_2O_3, and (c) κ-Ga_2O_3.

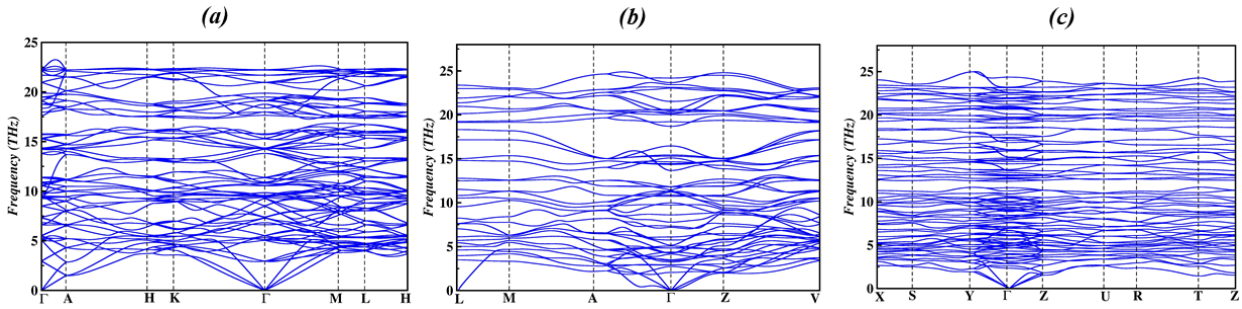

FIG. 3: The Obtained Phonon spectra for (a) α-Ga_2O_3, (b) β-Ga_2O_3, and (c) κ-Ga_2O_3.

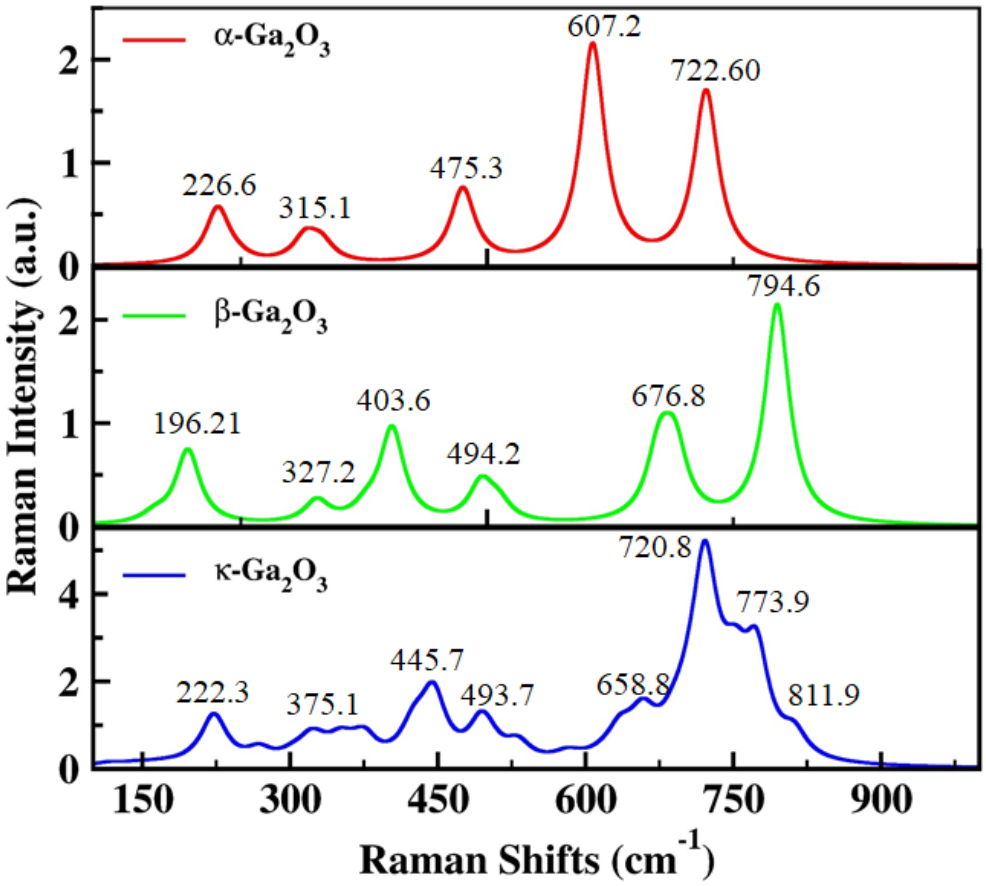

FIG. 4: Calculated Raman peaks for (a) α-Ga_2O_3, (b) β-Ga_2O_3, and (c) κ-Ga_2O_3.

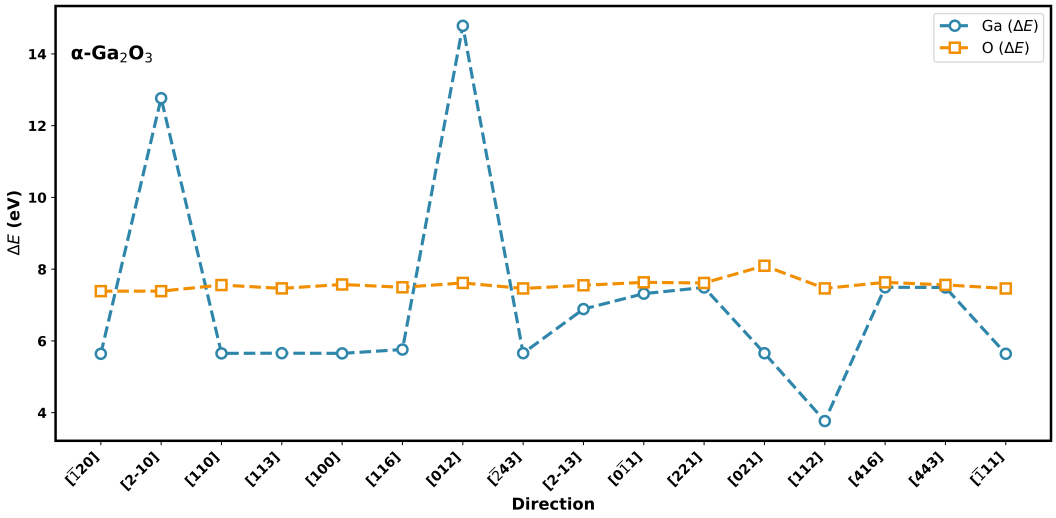

FIG. 5: Directional variation of formation energy difference (ΔE) for Ga and O PKAs in α-Ga_2O_3.

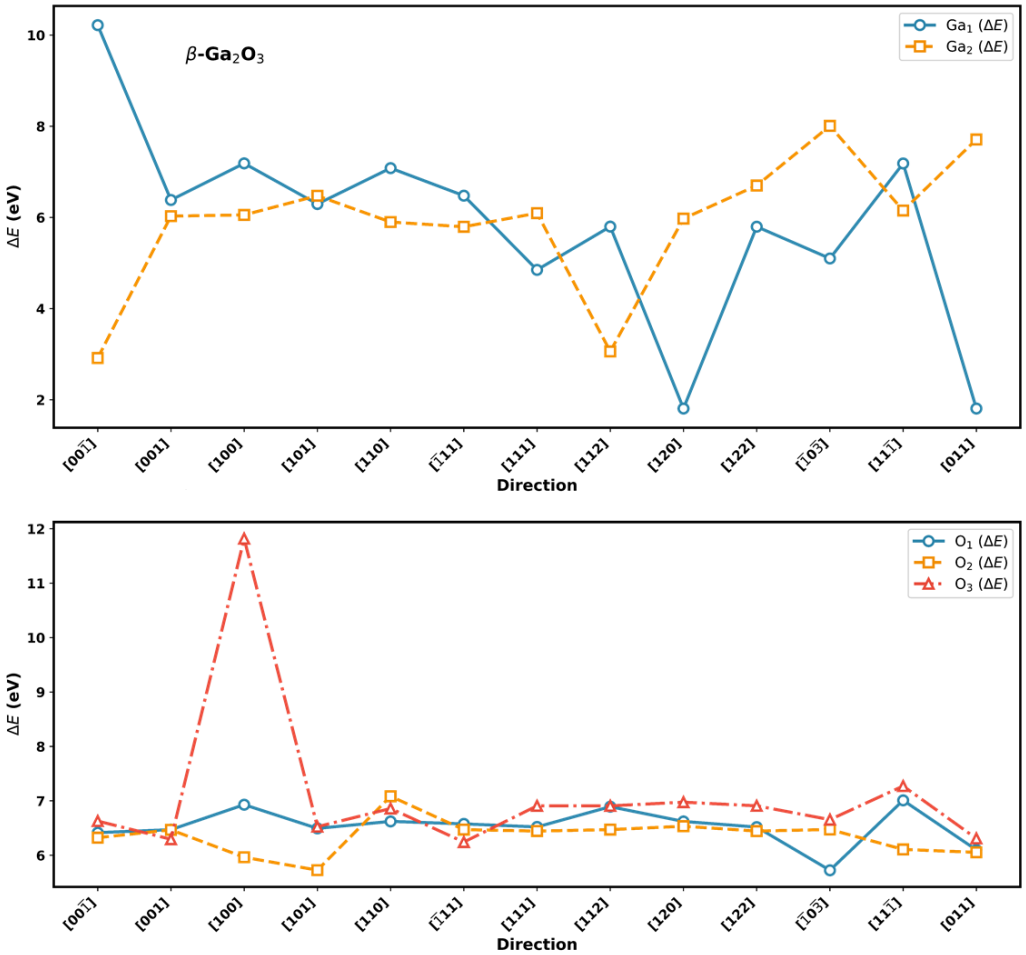

FIG. 6: Formation energy difference (ΔE) for Ga1, Ga2, and O PKAs in β-Ga_2O_3.

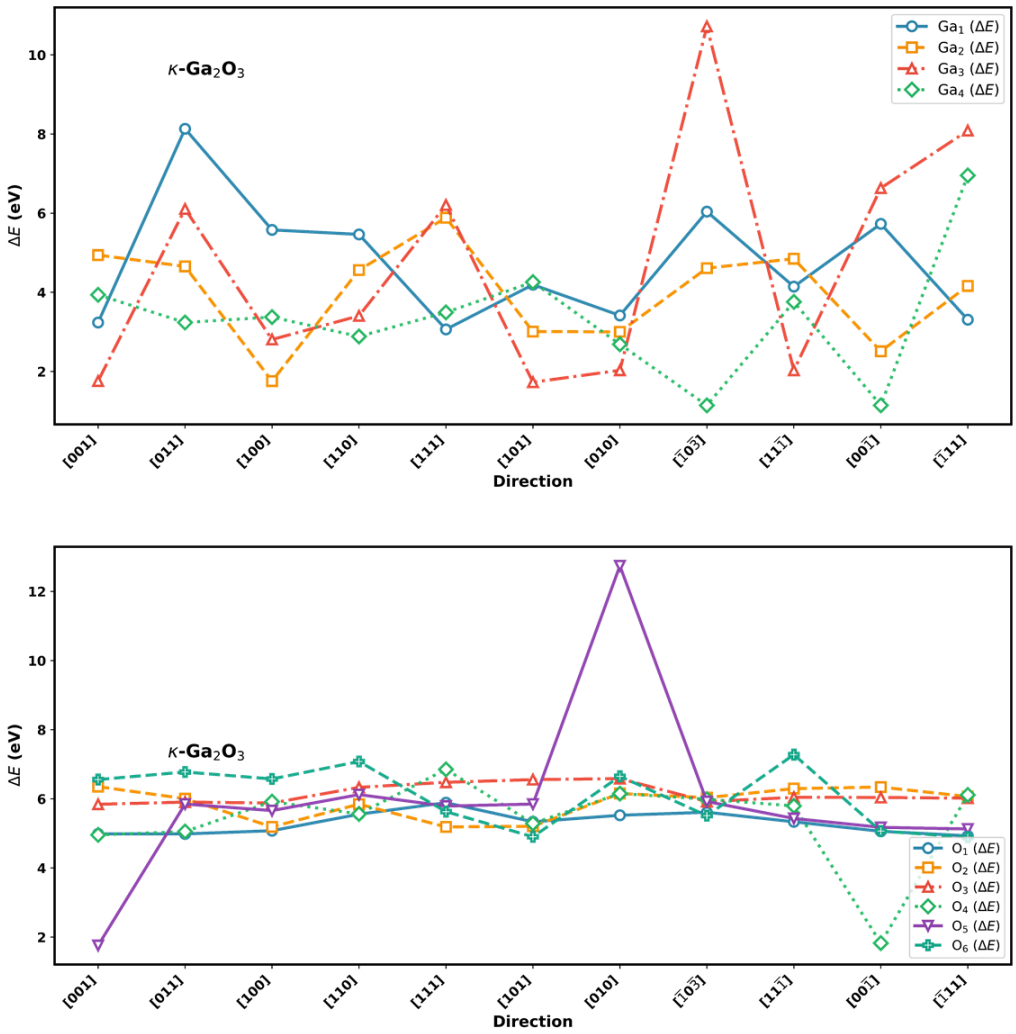

FIG. 7: Formation energy difference (ΔE) for Ga and O PKAs in κ-Ga_2O_3.

TABLE I: Calculated and experimental band gap values for different Ga_2O_3 phases.

System	**PBE**	**HSE06**				**EXP Value**
		0.25	0.30	0.35	0.37	
α-Ga_2O_3	2.91 eV	4.63 eV	4.99 eV	5.36 eV	5.51 eV	5.3 eV
β-Ga_2O_3	2.29 eV	4.04 eV	4.40 eV	4.78 eV	4.93 eV	4.9 eV
κ-Ga_2O_3	2.34 eV	4.09 eV	4.45 eV	4.83 eV	4.98 eV	4.8 eV

TABLE II: Average distances of Ga–O and O–O bonds in α-, β-, and κ-Ga_2O_3 phases, respectively.

Compound	Ga–O Octahedral	Ga–O Tetrahedral	O–O Octahedral	O–O Tetrahedral
α-Ga_2O_3	1.994	—	2.81	—
β-Ga_2O_3	1.994	1.860	2.88	3.050
κ-Ga_2O_3	1.994	1.861	2.89	3.018

TABLE III: Area under the plot (vacancies ions^{-1}) obtained from TRIM calculations in Default -,α-, β-, and κ-Ga_2O_3 phases, respectively.

Compound	Ga	O	Total
$Default$-Ga_2O_3	5.3538	5.2103	10.5641
α-Ga_2O_3	2.2490	5.2983	7.5473
β-Ga_2O_3	2.2000	5.7085	7.9085
κ-Ga_2O_3	3.0290	5.2130	8.2420

TABLE IV: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by Ga PKA along different directions for α-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[**001**]	107	No defect	6.514
[**-120**]	48	$V_{Ga} + I_{Ga}$	2.684
[**2-10**]	77	$V_{Ga} + I_{Ga} + V_O + I_O$	4.916
[**110**]	22	$V_{Ga} + I_{Ga}$	2.711
[**113**]	56	$V_{Ga} + I_{Ga}$	4.887
[**100**]	52	$V_{Ga} + I_{Ga}$	0.006
[**116**]	70	$V_{Ga} + I_{Ga}$	2.708
[**012**]	43	$V_{Ga} + I_{Ga} + V_O + I_O$+D	4.155
[**-243**]	55	$V_{Ga} + I_{Ga}$	0.095
[**2-13**]	40	$V_{Ga} + I_{Ga}$	3.591
[**0-11**]	48	$V_{Ga} + I_{Ga}$	3.514
[**221**]	31	$V_O + I_O$	0.350
[**021**]	44	$V_{Ga} + I_{Ga}$	0.096
[**112**]	42	$V_{Ga} + I_{Ga}$	1.899
[**416**]	47	$V_O + I_O$+D	3.656
[**443**]	33	$V_O + I_O$	0.295
[**-111**]	52	$V_{Ga} + I_{Ga}$	2.681

TABLE V: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by O PKA along different directions for α-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[**001**]	28	V_O + I_O+D	3.993
[**-120**]	29	V_O + I_O+D	2.608
[**2-10**]	29	V_O + I_O+D	2.614
[**110**]	31	V_O + I_O+D	4.890
[**113**]	24	V_O + I_O+D	2.690
[**100**]	21	V_O + I_O+D	2.085
[**116**]	33	V_O + I_O+D	3.989
[**012**]	47	V_O + I_O+D	0.026
[**-243**]	24	V_O + I_O+D	4.066
[**2-13**]	20	V_O + I_O+D	0.004
[**0-11**]	18	V_O + I_O+D	3.462
[**221**]	44	V_O + I_O+D	2.577
[**021**]	23	V_O + I_O	4.391
[**112**]	35	V_O + I_O+D	3.462
[**416**]	22	V_O + I_O+D	3.462
[**443**]	38	V_O + I_O+D	2.953
[**-111**]	30	V_O + I_O+D	4.061

TABLE VI: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by Ga1 PKA along different directions for β-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[00-1]	70	3 V_{Ga} + 3 V_O + 3 I_{Ga} + 3 I_O	5.404
[001]	54	V_O + I_O	1.219
[010]	42	V_O + I_O	3.463
[100]	74	2 V_{Ga} + 2 I_{Ga}	3.042
[101]	34	V_O + I_O	0.036
[110]	59	2 V_{Ga} + 2 I_{Ga}	4.504
[-111]	29	V_O + I_O+D	0.070
[111]	42	3 V_{Ga} + 3 I_{Ga}	3.949
[112]	47	6 V_{Ga} + 6 I_{Ga}	3.322
[120]	68	2 V_{Ga} + 2 I_{Ga}	3.575
[122]	50	6 V_{Ga} + 6 I_{Ga}	1.461
[-10-3]	89	4 V_{Ga} + 4 I_{Ga}	4.448
[11-1]	52	2 V_{Ga} + 2 I_{Ga}	3.280
[011]	30	4 V_{Ga} + 4 I_{Ga}	3.578

TABLE VII: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by Ga2 PKA along different directions for β-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[00-1]	80	3 V_{Ga} + 3 I_{Ga}	5.380
[001]	35	3 V_{Ga} + 3 I_{Ga}	2.750
[010]	118	No Defect	10.150
[100]	31	V_O + I_O+D	0.140
[101]	28	V_O + I_O+D	0.030
[110]	43	3 V_{Ga} + 3 I_{Ga}	2.750
[-111]	36	3 V_{Ga} + 3 I_{Ga}	2.990
[111]	48	6 V_{Ga} + 6 I_{Ga}	5.530
[112]	64	2 V_{Ga} + 2 I_{Ga}	0.020
[120]	59	V_O + I_O+D	3.200
[122]	52	V_O + I_O+D	0.070
[-10-3]	35	2 V_{Ga} + 2 I_{Ga}	4.440
[11-1]	20	3 V_{Ga} + 3 I_{Ga}	2.52
[011]	38	V_{Ga} + I_{Ga} + V_O + I_O+D	0.210

TABLE VIII: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by O1 PKA along different directions for β-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[00-1]	20	$V_{Ga} + I_{Ga} + 2\ V_O + 2\ I_O$	3.980
[001]	22	$V_O + I_O$ + D	2.400
[010]	22	$V_O + I_O$ + D	2.780
[100]	15	$V_O + I_O$ + D	4.260
[101]	18	$V_{Ga} + I_{Ga} + 2\ V_O + 2\ I_O$	3.610
[110]	19	$V_O + I_O$ + D	4.730
[-111]	47	$V_O + I_O$ + D	4.280
[111]	22	$V_O + I_O$ + D	3.380
[112]	57	$V_O + I_O$ + D	2.880
[120]	18	$V_O + I_O$ + D	5.228
[122]	30	$V_O + I_O$ + D	2.100
[-10-3]	30	$V_{Ga} + I_{Ga} + 2\ V_O + 2\ I_O$	4.800
[11-1]	17	$V_O + I_O$ + D	2.820
[011]	70	$V_{Ga} + I_{Ga} + 2\ V_O + 2\ I_O$	2.746

TABLE IX: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by O2 PKA along different directions for β-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[00-1]	28	$V_O + I_O$ + D	2.670
[001]	10	$V_O + I_O$ + D	2.840
[010]	26	$V_O + I_O$ + D	2.730
[100]	17	$V_O + I_O$ + D	3.430
[101]	47	3 V_{Ga} + 3 I_{Ga}	0.070
[110]	44	$V_{Ga} + I_{Ga} + V_O + I_O$	9.360
[-111]	33	$V_O + I_O$ + D	2.620
[111]	18	$V_O + I_O$ + D	2.840
[112]	29	$V_O + I_O$ + D	4.390
[120]	38	$V_O + I_O$ + D	2.830
[122]	14	$V_O + I_O$ + D	2.840
[-10-3]	27	$V_O + I_O$ + D	2.710
[11-1]	27	$V_O + I_O$ + D	5.520
[011]	19	$V_O + I_O$	2.890

TABLE X: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by O3 PKA along different directions for β-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[00-1]	17	$V_O + I_O$ + D	2.090
[001]	31	$V_{Ga} + I_{Ga} + V_O + I_O$	9.110
[010]	25	$V_O + I_O$ + D	3.600
[100]	67	$3\ V_{Ga} + 3\ I_{Ga} + V_O + I_O$ + D	3.410
[101]	16	$V_O + I_O$ + D	2.480
[110]	24	$V_O + I_O$ + D	2.150
[-111]	31	$V_{Ga} + I_{Ga} + 3\ V_O + 3\ I_O$	3.020
[111]	15	$V_O + I_O$ + D	4.390
[112]	23	$V_O + I_O$ + D	4.380
[120]	25	$V_O + I_O$ + D	4.720
[122]	14	$V_O + I_O$ + D	4.390
[-10-3]	25	$V_O + I_O$ + D	2.290
[11-1]	25	$V_O + I_O$	4.520
[011]	16	$V_{Ga} + I_{Ga} + 2\ V_O + 2\ I_O$	4.220

TABLE XI: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by Ga1 PKA along different directions for κ-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[001]	42	3 V_{Ga} + 3 I_{Ga}	1.827
[011]	77	4 V_{Ga} + 4 I_{Ga}	5.036
[100]	24	V_{Ga} + I_{Ga} + V_O + I_O	0.416
[110]	55	V_{Ga} + I_{Ga} + 3 V_O + 3 I_O	0.211
[111]	49	3 V_{Ga} + 3 I_{Ga}	3.573
[101]	53	3 V_{Ga} + 3 I_{Ga}	4.919
[010]	37	2 V_{Ga} + 2 I_{Ga}	4.392
[-10-3]	28	V_O + I_O + D	0.439
[11-1]	58	2 V_{Ga} + 2 I_{Ga}	5.189
[00-1]	36	V_O + I_O + D	0.428
[-111]	30	2 V_{Ga} + 2 I_{Ga}	3.266

TABLE XII: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by Ga2 PKA along different directions for κ-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[001]	33	4 V_{Ga} + 4 I_{Ga}	4.360
[011]	49	4 V_{Ga} + 4 I_{Ga}	3.338
[100]	18	3 V_{Ga} + 3 I_{Ga}	1.342
[110]	56	3 V_{Ga} + 3 I_{Ga}	4.410
[111]	28	V_O + I_O + D	0.000
[101]	49	4 V_{Ga} + 4 I_{Ga}	4.781
[010]	41	4 V_{Ga} + 4 I_{Ga}	5.382
[-10-3]	36	4 V_{Ga} + 4 I_{Ga}	2.668
[11-1]	52	4 V_{Ga} + 4 I_{Ga}	4.685
[00-1]	35	3 V_{Ga} + 3 I_{Ga}	2.942
[-111]	48	3 V_{Ga} + 3 I_{Ga}	0.138

TABLE XIII: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by Ga3 PKA along different directions for κ-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[001]	26	3 V_{Ga} + 3 I_{Ga}	2.0068
[011]	30	V_O + I_O + D	0.0596
[100]	68	2 V_{Ga} + 2 I_{Ga}	3.5625
[110]	49	2 V_{Ga} + 2 I_{Ga}	2.5990
[111]	22	V_O + I_O + D	0.1567
[101]	20	2 V_{Ga} + 2 I_{Ga}	1.4661
[010]	13	2 V_{Ga} + 2 I_{Ga}	2.8981
[-10-3]	52	2 V_{Ga} + 2 I_{Ga} + V_O + I_O + D	5.0824
[11-1]	32	2 V_{Ga} + 2 I_{Ga}	2.7469
[00-1]	30	V_O + I_O + D	0.1092
[-111]	36	2 V_{Ga} + 2 I_{Ga} + 2V_O + 2I_O	3.6934

TABLE XIV: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by Ga4 PKA along different directions for κ-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[001]	56	5 V_{Ga} + 5 I_{Ga}	4.7553
[011]	59	3 V_{Ga} + 3 I_{Ga}	2.8365
[100]	44	3 V_{Ga} + 3 I_{Ga}	4.9530
[110]	62	3 V_{Ga} + 3 I_{Ga}	2.6457
[111]	73	3 V_{Ga} + 3 I_{Ga}	5.1136
[101]	55	3 V_{Ga} + 3 I_{Ga}	3.8915
[010]	21	3 V_{Ga} + 3 I_{Ga}	3.0880
[-10-3]	12	2 V_{Ga} + 2 I_{Ga}	1.6458
[11-1]	42	3 V_{Ga} + 3 I_{Ga}	3.5924
[00-1]	21	2 V_{Ga} + 2 I_{Ga}	1.6466
[-111]	36	V_O + I_O + D	0.1090

TABLE XV: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by O1 PKA along different directions for κ-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[001]	14	$V_O + I_O$ + D	2.6402
[011]	10	$V_O + I_O$ + D	2.6392
[100]	40	$V_O + I_O$ + D	4.2800
[110]	20	$V_O + I_O$ + D	2.9968
[111]	17	$V_O + I_O$ + D	2.6985
[101]	19	$V_O + I_O$ + D	2.9511
[010]	61	$V_O + I_O$ + D	5.3144
[-10-3]	53	$V_O + I_O$ + D	3.4051
[11-1]	17	$V_O + I_O$ + D	3.3539
[00-1]	22	$V_O + I_O$ + D	13.5800
[-111]	15	$V_O + I_O$ + D	2.0848

TABLE XVI: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by O2 PKA along different directions for κ-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[001]	21	$V_O + I_O$ + D	2.8330
[011]	27	$V_O + I_O$ + D	4.8186
[100]	17	$V_O + I_O$ + D	2.0550
[110]	26	$V_O + I_O$ + D	2.3489
[111]	41	$V_O + I_O$ + D	2.8869
[101]	44	2 V_O + 2 I_O	2.2637
[010]	25	$V_O + I_O$ + D	5.5384
[-10-3]	40	$V_O + I_O$ + D	12.7270
[11-1]	17	$V_O + I_O$ + D	4.0030
[00-1]	17	$V_O + I_O$ + D	2.5183
[-111]	19	$V_O + I_O$ + D	3.3096

TABLE XVII: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by O3 PKA along different directions for κ-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[001]	56	$V_O + I_O$ + D	3.0289
[011]	37	$V_O + I_O$ + D	4.3028
[100]	42	$V_O + I_O$ + D	4.7739
[110]	16	$V_O + I_O$ + D	2.2667
[111]	43	$V_O + I_O$ + D	4.9124
[101]	16	$V_O + I_O$ + D	3.6639
[010]	18	$V_O + I_O$ + D	3.1634
[-10-3]	30	$V_O + I_O$ + D	15.6798
[11-1]	28	$V_O + I_O$ + D	16.6212
[00-1]	21	$V_O + I_O$ + D	16.1882
[-111]	19	$V_O + I_O$ + D	4.3974

TABLE XVIII: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by O4 PKA along different directions for κ-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[001]	52	V_{Ga} + I_{Ga} + V_O + I_O	2.3518
[011]	15	V_{Ga} + I_{Ga} + 2 V_O + 2 I_O	2.8224
[100]	16	V_O + I_O + D	2.3973
[110]	18	V_O + I_O	2.7165
[111]	17	V_{Ga} + I_{Ga} + V_O + I_O + D	3.5241
[101]	19	V_{Ga} + I_{Ga} + 2 V_O + 2 I_O	3.3198
[010]	24	V_O + I_O + D	2.8009
[-10-3]	33	V_O + I_O + D	2.3249
[11-1]	36	V_O + I_O + D	2.2255
[00-1]	70	2 V_{Ga} + 2 I_{Ga}	2.8337
[-111]	22	V_O + I_O + D	3.5952

TABLE XIX: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by O5 PKA along different directions for κ-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[001]	58	3 V_{Ga} + 3 I_{Ga}	0.1024
[011]	22	V_O + I_O + D	2.7726
[100]	70	V_{Ga} + I_{Ga} + 2 V_O + 2 I_O	16.2148
[110]	21	V_O + I_O + D	3.7895
[111]	47	V_O + I_O + D	4.6768
[101]	31	V_O + I_O + D	2.7751
[010]	34	2 V_O + 2 I_O + 2 D	4.7382
[-10-3]	41	V_O + I_O + D	12.1325
[11-1]	27	2 V_O + 2 I_O	14.9949
[00-1]	30	V_O + I_O + D	11.7162
[-111]	14	2 V_O + 2 I_O	3.1303

TABLE XX: Threshold displacement energies E_d (eV), types of defects, and distances d (Å) traveled by O6 PKA along different directions for κ-Ga_2O_3

Direction	E_d (eV)	Defect	d (Å)
[001]	22	V_O + I_O + D	4.2978
[011]	40	V_O + I_O + D	3.2207
[100]	18	2 V_O + 2 I_O + D	2.6037
[110]	38	V_O + I_O + D	3.4544
[111]	25	2 V_O + 2 I_O	4.7772
[101]	31	V_O + I_O	2.2687
[010]	23	V_O + I_O + D	2.9493
[-10-3]	25	V_O + I_O	2.8464
[11-1]	17	V_O + I_O + D	3.9390
[00-1]	26	V_O + I_O	4.4176
[-111]	45	V_O + I_O	3.8376