Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary material:

Low-energy Ga_2O_3 polymorphs with low carrier effective masses

Qingyang Fan,[1,2,*] Ruida Zhao[1], Wei Zhang[3], Yanxing Song[3], Minglei Sun[4], Udo Schwingenschlögl[4,*]

[1]College of Information and Control Engineering, Xi'an University of Architecture and Technology, Xi'an 710055, China
[2]Shaanxi Key Laboratory of Nano Materials and Technology, Xi'an, 710055, China
[3]School of Microelectronics, Xidian University, Xi'an 710071, China
[4]Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia
*fanqy@xauat.edu.cn, udo.schwingenschlogl@kaust.edu.sa

Crystallographic Information $P2_1/c$ Ga_2O_3

```
_symmetry_space_group_name_H-M    'P21/C'
_symmetry_Int_Tables_number       14
_symmetry_cell_setting            monoclinic
loop_
_symmetry_equiv_pos_as_xyz
   x,y,z
   -x,y+1/2,-z+1/2
   -x,-y,-z
   x,-y+1/2,z+1/2
_cell_length_a                    9.7704
_cell_length_b                    8.7618
_cell_length_c                    5.8104
_cell_angle_alpha                 90.0000
_cell_angle_beta                  149.5868
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
O1    O    0.67952    0.29563    0.77246    0.00000    Uiso    1.00
O2    O    0.83087    0.88921    0.73081    0.00000    Uiso    1.00
O3    O    0.74889    0.52154    0.58037    0.00000    Uiso    1.00
Ga4   Ga   0.05258    0.54083    0.82169    0.00000    Uiso    1.00
Ga5   Ga   0.46712    0.65729    0.73249    0.00000    Uiso    1.00
```

Crystallographic Information Pnma-I Ga_2O_3

```
_symmetry_space_group_name_H-M    'PNMA'
_symmetry_Int_Tables_number       62
_symmetry_cell_setting            orthorhombic
loop_
_symmetry_equiv_pos_as_xyz
   x,y,z
   -x+1/2,-y,z+1/2
   -x,y+1/2,-z
   x+1/2,-y+1/2,-z+1/2
   -x,-y,-z
   x+1/2,y,-z+1/2
   x,-y+1/2,z
   -x+1/2,y+1/2,z+1/2
_cell_length_a                    7.0734
_cell_length_b                    3.3107
_cell_length_c                    9.8351
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
O1     O     0.41147   0.75000   0.41452   0.00000   Uiso   1.00
Ga5    Ga    0.02396   0.75000   0.27556   0.00000   Uiso   1.00
O2     O     0.08469   0.25000   0.36673   0.00000   Uiso   1.00
O3     O     0.73881   0.25000   0.83710   0.00000   Uiso   1.00
Ga4    Ga    0.80285   0.25000   0.01866   0.00000   Uiso   1.00
```

Crystallographic Information Pnma-II Ga_2O_3

```
_symmetry_space_group_name_H-M    'PNMA'
_symmetry_Int_Tables_number       62
_symmetry_cell_setting            orthorhombic
loop_
_symmetry_equiv_pos_as_xyz
   x,y,z
   -x+1/2,-y,z+1/2
   -x,y+1/2,-z
   x+1/2,-y+1/2,-z+1/2
   -x,-y,-z
   x+1/2,y,-z+1/2
   x,-y+1/2,z
   -x+1/2,y+1/2,z+1/2
_cell_length_a                    5.9003
_cell_length_b                    3.0933
_cell_length_c                    12.1263
_cell_angle_alpha                 90.0000
_cell_angle_beta                  90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
O1    O    0.84749    0.25000    0.41503    0.00000    Uiso    1.00
O3    O    0.39839    0.25000    0.42279    0.00000    Uiso    1.00
Ga4   Ga   0.12405    0.25000    0.34039    0.00000    Uiso    1.00
O2    O    0.62506    0.75000    0.24579    0.00000    Uiso    1.00
Ga5   Ga   0.64094    0.75000    0.40866    0.00000    Uiso    1.00
```

Elastic constants C_{ij} (GPa) of P2$_1$/c Ga_2O_3

175. 48445	62. 04100	66. 13096	0. 00000	7. 56231	0. 00000
62. 04100	252. 58488	87. 88119	0. 00000	- 43. 59696	0. 00000
66. 13096	87. 88119	203. 85126	0. 00000	- 8. 76458	0. 00000
0. 00000	0. 00000	0. 00000	45. 05845	0. 00000	- 16. 88817
7. 56231	- 43. 59696	- 8. 76458	0. 00000	59. 21376	0. 00000
0. 00000	0. 00000	0. 00000	- 16. 88817	0. 00000	47. 04479

Elastic constants C_{ij} (GPa) of Pnma-I Ga_2O_3

210. 45319	90. 45296	180. 71827	0. 00000	0. 00000	0. 00000
90. 45296	269. 32226	121. 76815	0. 00000	0. 00000	0. 00000
108. 71827	121. 76815	256. 73331	0. 00000	0. 00000	0. 00000
0. 00000	0. 00000	0. 00000	53. 07579	0. 00000	0. 00000
0. 00000	0. 00000	0. 00000	0. 00000	72. 56831	0. 00000
0. 00000	0. 00000	0. 00000	0. 00000	0. 00000	51. 38698

Elastic constants C_{ij} (GPa) of Pnma-II Ga_2O_3

310. 78212	58. 79830	115. 83764	0. 00000	0. 00000	0. 00000
58. 79830	299. 78024	120. 04074	0. 00000	0. 00000	0. 00000
115. 83764	120. 04074	193. 35150	0. 00000	0. 00000	0. 00000
0. 00000	0. 00000	0. 00000	80. 87248	0. 00000	0. 00000
0. 00000	0. 00000	0. 00000	0. 00000	95. 87205	0. 00000
0. 00000	0. 00000	0. 00000	0. 00000	0. 00000	41. 26736

Born mechanical stability conditions for monoclinic symmetry (P2$_1$/c Ga_2O_3)

$C_{11}>0,\ C_{22}>0,\ C_{33}>0,\ C_{44}>0,\ C_{55}>0,\ C_{66}>0,$

$[C_{11}+C_{22}+C_{33}+2(C_{12}+C_{13}+C_{23})]>0,$

$(C_{33}C_{55}-C_{35}^2)>0,\ (C_{44}C_{66}-C_{46}^2)>0,\ (C_{22}+C_{33}-2C_{23})>0,$

$[C_{22}(C_{33}C_{55}-C_{35}^2)+2C_{23}C_{25}C_{35}-C_{23}^2C_{55}-C_{25}^2C_{33}]>0,$

$\{2[C_{15}C_{25}(C_{33}C_{12}-C_{13}\ C_{23})+C_{15}C_{35}(C_{22}C_{13}-C_{12}C_{23})+C_{25}C_{35}(C_{11}C_{23}-C_{12}C_{13})]-[C_{15}^2(C_{22}C_{33}-C_{23}^2)+C_{25}^2(C_{11}C_{33}-C_{13}^2)+C_{35}^2(C_{11}C_{22}-C_{12}^2)]+C_{55}D\}>0,$

$D=C_{11}C_{22}C_{33}-C_{11}C_{23}^2-C_{22}C_{13}^2-C_{33}C_{12}^2+2C_{12}C_{13}C_{23}.$

Born mechanical stability conditions for orthorhombic symmetry (Pnma-I and Pnma-II Ga_2O_3)

$C_{11}>0,\ C_{11}C_{22}>C_{12}^2,$

$C_{11}C_{22}C_{33}\ +2C_{12}C_{13}C_{23}\ -C_{11}C_{23}^2-C_{22}C_{13}^2-C_{33}C_{12}^2>0,$

$C_{44}>0,\ C_{55}>0,\ C_{66}>0.$