Strain-Tunable Mechanical, Electronic and Optical Properties of La_2AlGaO_6 Hybrid Perovskite: A First-Principles Investigation

Chaithanya Purushottam Bhat, Jyoti Dagar, Ashwin K. Godbole, Debashis Bandyopadhyay*

Department of Physics, Birla Institute of Technology and Science Pilani, Rajasthan – 333031,

** bandy@pilani.bits-pilani.ac.in; Debashis.bandy@gmail.com*

Details of POSCAR Cubic, Ortho-rhombic and Trigonal optimized LAGO unit cell structures along with the energies

La8Al4Ga4O24 Cubic $E_{optimized}$=-302.108 eV

1.00000000000000

7.9178757667999999 0.0000000000000000 0.0000000000000000

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0.0000000000000000 0.0000000000000000 7.9178757667999999

La Al Ga O

8 4 4 24

Direct

0.0000000000000000 0.0000000000000000 0.0037200161845803

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0.0000000000000000 0.0000000000000000 0.4962799846489787

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0.4999999999494804 0.2500000000378861 0.2500000000378861

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0.7499999999873737 0.0000000000000000 0.7499999999873737
0.7499999999873737 0.4999999999494804 0.7499999999873737
0.2500000000378861 0.2500000000378861 0.0083899274194934
0.2500000000378861 0.7499999999873737 0.0083899274194934
0.7499999999873737 0.2500000000378861 0.0083899274194934
0.7499999999873737 0.7499999999873737 0.0083899274194934
0.2500000000378861 0.2500000000378861 0.4916100799814842
0.2500000000378861 0.7499999999873737 0.4916100799814842
0.7499999999873737 0.2500000000378861 0.4916100799814842
0.7499999999873737 0.7499999999873737 0.4916100799814842

La4Al2Ga2O12 Pnma Orthorhombic $E_{optimized}$=-152.096 eV

1.00000000000000
5.5463110000000002 0.0000000000000000 0.0000000000000003
0.00000000000000000 5.5942129999999999 0.0000000000000003
0.0000000000000000 0.0000000000000000 7.8505229999999999
La Al Ga O
4 2 2 12
Direct
0.4946618466683148 0.5066187079830797 0.2547251796761287
0.9946618466683148 0.9933812920169203 0.2547251796761287
0.0053381533316852 0.0066187079830797 0.7452748203238713
0.5053381533316852 0.4933812920169203 0.7452748203238713
0.0000000000000000 0.5000000000000000 0.5000000000000000
0.5000000000000000 0.0000000000000000 0.5000000000000000
0.5000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.5000000000000000 0.0000000000000000
0.7456146671770654 0.7458492101271545 0.4633593961882312
0.4972048357758467 0.9273807352086934 0.7413704811529485

0.0027951642241533 0.4273807352086934 0.2586295188470515
0.2543853328229346 0.2541507898728455 0.5366406038117688
0.5027951642241533 0.0726192647912995 0.2586295188470515
0.2440936608083319 0.7558726655219488 0.0441466993786577
0.2456146671770583 0.7541507898728455 0.4633593961882312
0.7543853328229346 0.2458492101271545 0.5366406038117688
0.9972048357758467 0.5726192647913066 0.7413704811529485
0.7440936608083391 0.7441273344780512 0.0441466993786577
0.2559063391916609 0.2558726655219488 0.9558533006213423
0.7559063391916609 0.2441273344780512 0.9558533006213423

$La_6Al_3Ga_3O_{18}$ Trigonal R3c $E_{optimized}$=-228.221 eV

1.00000000000000

2.7976921723095711 -4.8457449863779196 0.0000000000000000

2.7976921723095711 4.8457449863779196 0.0000000000000000

0.0000000000000000 0.0000000000000000 13.4644792708326442

La Al Ga O

6 3 3 18

Direct

0.3333333333333357 0.6666666666666643 0.4100600471495994
0.3333333333333357 0.6666666666666643 0.9143468669608268
0.0000000000000000 0.0000000000000000 0.7467074912233613
0.0000000000000000 0.0000000000000000 0.2452868506023904
0.6666666666666643 0.3333333333333357 0.0803485437814260
0.6666666666666643 0.3333333333333357 0.5789243986930686
0.3333333333333357 0.6666666666666643 0.1605597445175277
0.0000000000000000 0.0000000000000000 0.4946351769952315
0.0000000000000000 0.0000000000000000 0.9983969850753169
0.3333333333333357 0.6666666666666643 0.6597140309371099
0.6666666666666643 0.3333333333333357 0.8321364653841883
0.6666666666666643 0.3333333333333357 0.3283997884451608
0.5554307488477335 0.5631018010914417 0.2428014816451736
0.4368981989085583 0.9923289477562918 0.2428014816451736
0.0076710522437082 0.4445692511522665 0.2428014816451736
0.2230733719246416 0.3335339531193924 0.0795451932667604
0.6664660468806076 0.8895394188052492 0.0795451932667604
0.1104605811947508 0.7769266280753584 0.0795451932667604

0.2262893529527119 0.9010151150918091 0.5759541548206499
0.0989848849081909 0.3252742378609028 0.5759541548206499
0.6747257621390972 0.7737106470472881 0.5759541548206499
0.8993766628731947 0.6750362203272289 0.4122865750213336
0.3249637796727711 0.2243404425459659 0.4122865750213336
0.7756595574540341 0.1006233371268053 0.4122865750213336
0.8986721042105614 0.2242954805617359 0.9164415888092421
0.7757045194382570 0.6743766236488256 0.9164415888092421
0.3256233763511744 0.1013278957894386 0.9164415888092421
0.5667971046423617 0.0002241122896720 0.7459968765151004
0.9997758877103280 0.5665729923526968 0.7459968765151004
0.4334270076473032 0.4332028953576383 0.7459968765151004

Selection of K-points during structure optimization in case of Cubic system: k-point Convergence Test

The only robust way to decide k-points for structural optimization is by convergence testing: Step-by-Step Procedure

1. Choose ENCUT as 130% of Oxygen ENCUT value (400 eV).
2. Start with a coarse grid to fine grid by choosing k-points mesh as: 2×2×2 → 4×4×4 → 6×6×6 → 8×8×8
3. Calculate : Total energy, force
4. Plot these vs. k-point density; accept the mesh where changes in energy or forces are below your desired threshold (often ~1–10 meV/atom)
5. A simple rule of thumb for choosing a k-point mesh is to ensure that the product of the number of k-points and the corresponding real-space lattice dimension is sufficiently large. If this product is greater than about 20 Å in each direction, the mesh will generally provide a reasonable sampling. In many cases, using a value higher than this leads to more reliable and well-converged results