# Supporting Information

**CIF file for the structural information**

```
data_LiAl5O8
_symmetry_space_group_name_H-M    'P 1'
_cell_length_a    7.98736707
_cell_length_b    7.98736707
_cell_length_c    7.98736707
_cell_angle_alpha    90.00000000
_cell_angle_beta    90.00000000
_cell_angle_gamma    90.00000000
_symmetry_Int_Tables_number    1
_chemical_formula_structural    LiAl5O8
_chemical_formula_sum    'Li4 Al20 O32'
_cell_volume    509.57830561
_cell_formula_units_Z    4
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
```

| | | | | | | |
|---|---|---|---|---|---|---|
| Li | Li1 | 1 | 0.125000 | 0.875000 | 0.375000 | 1.0 |
| Li | Li2 | 1 | 0.875000 | 0.375000 | 0.125000 | 1.0 |
| Li | Li3 | 1 | 0.375000 | 0.125000 | 0.875000 | 1.0 |
| Li | Li4 | 1 | 0.625000 | 0.625000 | 0.625000 | 1.0 |
| Al | Al5 | 1 | 0.118726 | 0.625000 | 0.131274 | 1.0 |
| Al | Al6 | 1 | 0.125000 | 0.368726 | 0.881274 | 1.0 |
| Al | Al7 | 1 | 0.381274 | 0.375000 | 0.631274 | 1.0 |
| Al | Al8 | 1 | 0.375000 | 0.631274 | 0.381274 | 1.0 |
| Al | Al9 | 1 | 0.618726 | 0.875000 | 0.868726 | 1.0 |
| Al | Al10 | 1 | 0.625000 | 0.131274 | 0.118726 | 1.0 |
| Al | Al11 | 1 | 0.881274 | 0.125000 | 0.368726 | 1.0 |
| Al | Al12 | 1 | 0.875000 | 0.868726 | 0.618726 | 1.0 |
| Al | Al13 | 1 | 0.131274 | 0.118726 | 0.625000 | 1.0 |
| Al | Al14 | 1 | 0.631274 | 0.381274 | 0.375000 | 1.0 |
| Al | Al15 | 1 | 0.868726 | 0.618726 | 0.875000 | 1.0 |
| Al | Al16 | 1 | 0.368726 | 0.881274 | 0.125000 | 1.0 |
| Al | Al17 | 1 | 0.002378 | 0.497622 | 0.502378 | 1.0 |
| Al | Al18 | 1 | 0.252378 | 0.252378 | 0.252378 | 1.0 |
| Al | Al19 | 1 | 0.497622 | 0.502378 | 0.002378 | 1.0 |
| Al | Al20 | 1 | 0.247622 | 0.747622 | 0.752378 | 1.0 |
| Al | Al21 | 1 | 0.502378 | 0.002378 | 0.497622 | 1.0 |
| Al | Al22 | 1 | 0.752378 | 0.247622 | 0.747622 | 1.0 |
| Al | Al23 | 1 | 0.997622 | 0.997622 | 0.997622 | 1.0 |
| Al | Al24 | 1 | 0.747622 | 0.752378 | 0.247622 | 1.0 |
| O | O25 | 1 | 0.114717 | 0.133106 | 0.384526 | 1.0 |
| O | O26 | 1 | 0.616894 | 0.364717 | 0.134526 | 1.0 |
| O | O27 | 1 | 0.385283 | 0.866894 | 0.884526 | 1.0 |
| O | O28 | 1 | 0.883106 | 0.635283 | 0.634526 | 1.0 |
| O | O29 | 1 | 0.614717 | 0.3668 | | |

**The atomic configuration of different defects**

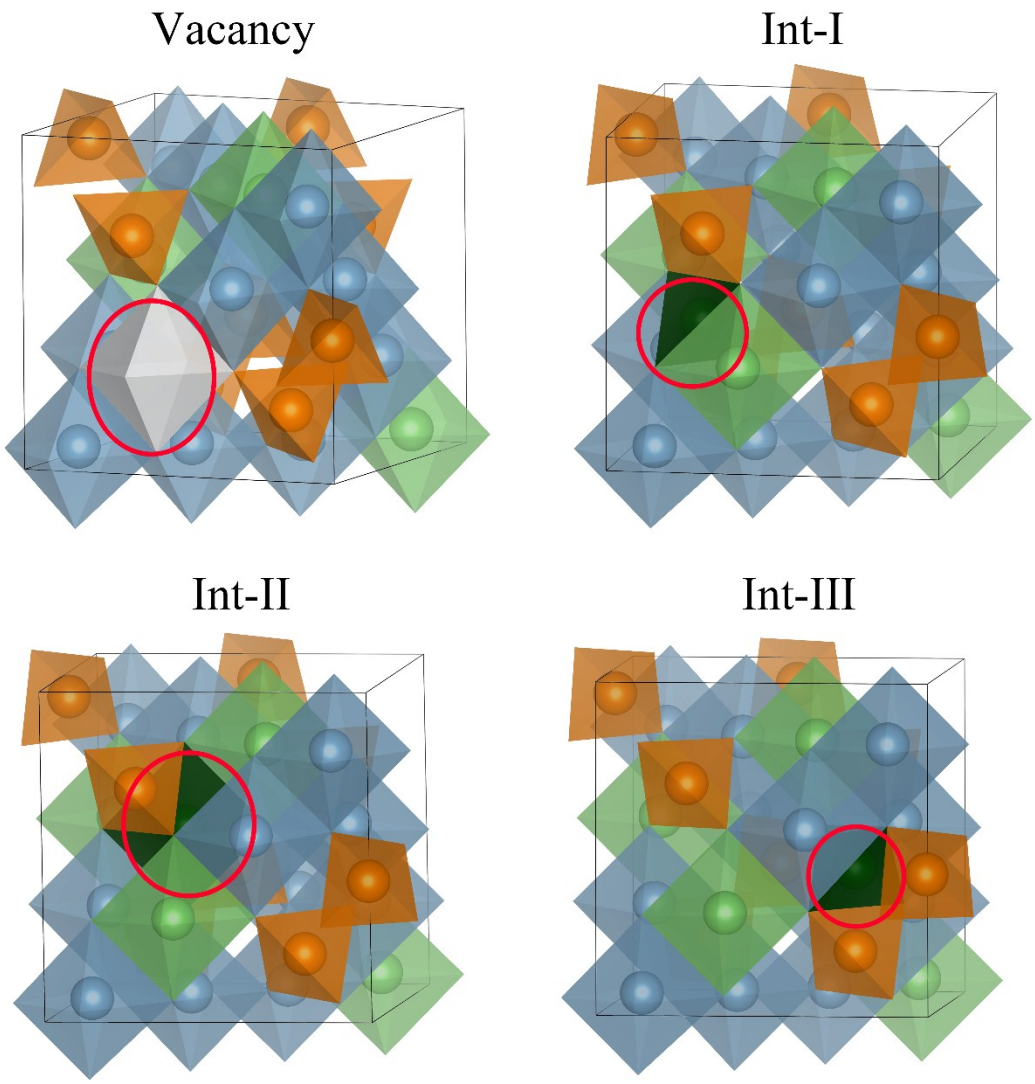


**Figure S1.** The atomic configuration of different defects