

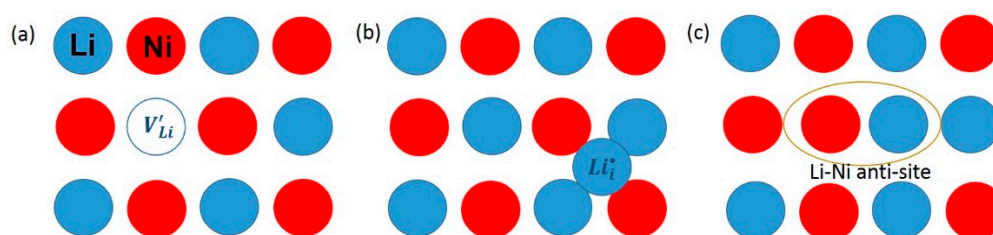
# Defect Properties of $\text{Li}_2\text{NiGe}_3\text{O}_8$

Navaratnarajah Kuganathan <sup>1,\*</sup>, Raveena Sukumar <sup>2</sup> and Poobalasuntharam Iyngaran <sup>2</sup>

<sup>1</sup> Department of Materials, Faculty of Engineering, Imperial College London, London SW7 2AZ, UK

<sup>2</sup> Department of Chemistry, University of Jaffna, Sir. Pon Ramanathan Road, Thirunelvely, Jaffna 40000, Sri Lanka

\* Correspondence: n.kuganathan@imperial.ac.uk



**Figure S1.** Schematic diagrams showing vacancy, interstitial, and anti-site defects.

**Table S1.** Two body Buckingham potentials used for dopant oxides in  $\text{Li}_2\text{NiGe}_3\text{O}_8$ .

Interaction	$A$ (eV)	$\rho$ (Å)	$C$ (eV·Å <sup>6</sup> )	$\gamma$ (e)	$K$ (eV·Å <sup>-2</sup> )
$\text{Na}^+ - \text{O}^{2-}$	1497.830598	0.287483	0.00	1.00	99999
$\text{K}^+ - \text{O}^{2-}$	1000.30	0.36198	10.56900	1.00	99999
$\text{Rb}^+ - \text{O}^{2-}$	1010.80	0.3793	0.000	1.00	99999
$\text{Fe}^{2+} - \text{O}^{2-}$	1207.6	0.3084	0.000	2.000	99999
$\text{Co}^{2+} - \text{O}^{2-}$	696.3	0.3362	0.000	2.000	10.74
$\text{Zn}^{2+} - \text{O}^{2-}$	499.6	0.3595	0.000	2.050	10.28
$\text{Mn}^{2+} - \text{O}^{2-}$	715.80	0.3464	0.000	3.000	81.20
$\text{Cu}^{2+} - \text{O}^{2-}$	3799.3	0.24273	0.000	2.000	99999
$\text{Ca}^{2+} - \text{O}^{2-}$	1090.40	0.3372	0.000	1.260	34.00
$\text{Sr}^{2+} - \text{O}^{2-}$	776.84	0.35867	0.000	1.526	11.406
$\text{Ba}^{2+} - \text{O}^{2-}$	931.79	0.3949	0.000	1.460	14.78
$\text{Al}^{3+} - \text{O}^{2-}$	1114.9	0.3118	0.000	1.000	99999
$\text{Ga}^{3+} - \text{O}^{2-}$	2901.12	0.2742	0.000	1.000	99999
$\text{Sc}^{3+} - \text{O}^{2-}$	1575.85	0.3211	0.000	3.000	99999
$\text{In}^{3+} - \text{O}^{2-}$	1495.65	0.3327	4.33	3.000	99999
$\text{Y}^{3+} - \text{O}^{2-}$	1345.10	0.3491	0.00	3.000	99999
$\text{Gd}^{3+} - \text{O}^{2-}$	1885.75	0.3399	20.34	3.000	99999
$\text{La}^{3+} - \text{O}^{2-}$	1545.21	0.3590	0.00	−0.250	145.0
$\text{Si}^{4+} - \text{O}^{2-}$	1283.91	0.320520	10.66	4.000	99999
$\text{Sn}^{4+} - \text{O}^{2-}$	1414.32	0.3479	13.66	4.000	99999
$\text{Ti}^{4+} - \text{O}^{2-}$	5111.7	0.2625	0.00	−0.10	314.0
$\text{Zr}^{4+} - \text{O}^{2-}$	985.869	0.3760	0.00	1.35	169.617
$\text{Ce}^{4+} - \text{O}^{2-}$	1986.83	0.3511	20.40	7.70	291.75