



# Simulation-Based Defect Engineering in “ $\alpha$ -Spodumene”

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**Table S1.** Interatomic potential parameters used for dopant in the atomistic simulations of  $\text{LiAlSi}_2\text{O}_6$ .

Two-body [ $\Phi_{ij}(r_{ij}) = A_{ij} \exp(-r_{ij}/\rho_{ij}) - C_{ij}/r_{ij}^6$ ]

Interaction	$A / \text{eV}$	$\rho / \text{\AA}$	$C / \text{eV}\cdot\text{\AA}^6$	$Y / \text{e}$	$K / \text{eV}\cdot\text{\AA}^{-2}$
$\text{Na}^+ - \text{O}^{2-}$	1497.830598	0.287483	0.00	1.000	99999
$\text{K}^+ - \text{O}^{2-}$	1000.300	0.36198	10.56900	1.000	99999
$\text{Rb}^+ - \text{O}^{2-}$	1010.80	0.3793	0.00	1.000	99999
$\text{Ga}^{3+} - \text{O}^{2-}$	1625.72	0.3019	0.0000	3.000	99999
$\text{Sc}^{3+} - \text{O}^{2-}$	1575.85	0.3211	0.0000	3.000	99999
$\text{In}^{3+} - \text{O}^{2-}$	1495.65	0.3327	0.0000	3.000	99999
$\text{Y}^{3+} - \text{O}^{2-}$	1766.40	0.33849	19.43	3.000	99999
$\text{Gd}^{3+} - \text{O}^{2-}$	1885.75	0.3399	20.34	3.000	99999
$\text{La}^{3+} - \text{O}^{2-}$	2088.79	0.3460	23.25	3.000	99999
$\text{Ge}^{4+} - \text{O}^{2-}$	1497.3996	0.325646	16.00	4.000	99999
$\text{Sn}^{4+} - \text{O}^{2-}$	1414.32	0.3479	13.660	4.000	99999
$\text{Ti}^{4+} - \text{O}^{2-}$	5111.7	0.2625	0.0000	−0.10	314.0
$\text{Zr}^{4+} - \text{O}^{2-}$	985.869	0.3760	0.0000	1.35	169.617
$\text{Ce}^{4+} - \text{O}^{2-}$	1986.83	0.3511	20.40	7.700	291.75