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Electronic Supplementary Information

Computational Investigation of a NASICON-type Solid Electrolyte Material $LiGe_2(PO_4)_3$

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Table S1. Two body Buckingham potentials used for dopant oxides in $LiGe_2(PO_4)_3$.

Interaction	*A* (eV)	*ρ* (Å)	*C* (eV·Å^6)	Y (e)	K (eV·Å^{-2})
Na^+–O^{2-}	1497.830598	0.287483	0.00	1.000	99,999
K^+–O^{2-}	1000.300	0.36198	10.56900	1.000	99,999
Rb^+–O^{2-}	1010.80	0.3793	0.000	1.000	99,999
Al^{3+}–O^{2-}	1114.9	0.3118	0.000	3.000	99,999
Ga^{3+}–O^{2-}	2901.12	0.2742	0.000	1.000	99,999
Sc^{3+}–O^{2-}	1575.85	0.3211	0.000	3.000	99,999
In^{3+}–O^{2-}	1495.65	0.3327	4.33	3.000	99,999
Y^{3+}–O^{2-}	1345.10	0.3491	0.000	3.000	99,999
Gd^{3+}–O^{2-}	1885.75	0.3399	20.34	3.000	99,999
La^{3+}–O^{2-}	1545.21	0.3590	0.000	−0.250	145.0
Si^{4+}–O^{2-}	1283.910	0.32052	10.66	4.000	99,999
Sn^{4+}–O^{2-}	1414.32	0.3479	13.66	4.000	99,999
Ti^{4+}–O^{2-}	5111.7	0.2625	0.00	−0.10	314.0
Zr^{4+}–O^{2-}	985.869	0.3760	0.00	1.35	169.617
Ce^{4+}–O^{2-}	1986.83	0.3511	20.40	7.70	291.75