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Supporting Information

Intrinsic defects, diffusion and dopants in $AVSi_2O_6$ (A= Li and Na) electrode materials

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Table S1. Two body Buckingham potentials used for dopant oxides in $LiVSi_2O_6$ and $NaVSi_2O_6$.

Interaction	*A* (eV)	*ρ* (Å)	*C* (eV·Å^6)	Y (e)	K (eV·Å^{-2})
K^+–O^{2-}	1000.300	0.36198	10.56900	1.000	99999
Rb^+–O^{2-}	1010.80	0.3793	0.00	1.000	99999
Al^{3+} - O^{2-}	1725.20	0.28971	0.000	3.000	99999
Ga^{3+} - O^{2-}	1625.72	0.3019	0.000	1.000	99999
Sc^{3+} - O^{2-}	1575.85	0.3211	0.000	3.000	99999
In^{3+} - O^{2-}	1495.65	0.3327	4.33	3.000	99999
Y^{3+} - O^{2-}	1766.40	0.33849	19.43	3.000	99999
Gd^{3+} - O^{2-}	1885.75	0.3399	20.34	3.000	99999
La^{3+} - O^{2-}	2088.79	0.3460	23.25	3.000	99999
Ge^{4+} - O^{2-}	1497.3996	0.325646	16.00	4.000	99999
Sn^{4+} - O^{2-}	1414.32	0.3479	13.66	4.000	99999
Ti^{4+} - O^{2-}	5111.7	0.2625	0.00	–0.10	314.0
Zr^{4+} - O^{2-}	1502.11	0.3477	0.00	1.35	169.617
Ce^{4+} - O^{2-}	1986.83	0.3511	20.40	7.70	291.75

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