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Supplementary Information

Defect Chemistry and Na-Ion Diffusion in $Na_3Fe_2(PO_4)_3$ Cathode Material

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Table S1. Interatomic potential parameters used in the atomistic simulations of $Na_3Fe_2(PO_4)_3$.

Two-Body [$\Phi_{ij}(r_{ij}) = A_{ij}\exp(-r_{ij}/\rho_{ij}) - C_{ij}/r_{ij}^6$]					
Interaction	***A*/eV**	**ρ/Å**	***C*/eV·Å^6**	**Y/e**	**K/eV·Å^{-2}**
Na^+–O^{2-} [1]	1497.830598	0.287483	0.00	1.000	99999
Fe^{3+}–O^{2-} [2]	1156.36	0.3299	0.00	4.970	304.7
O^{2-}–O^{2-} [3]	22764.30	0.149	27.89	–2.860	74.92
Al^{3+}–O^{2-} [4]	1114.9	0.2742	0.000	3.000	99999
Ga^{3+}–O^{2-} [5]	2901.12	0.2742	0.000	3.000	99999
Sc^{3+}–O^{2-} [4]	1299.4	0.3312	0.000	3.000	99999
Y^{3+}–O^{2-} [4]	1345.10	0.3491	0.000	3.000	99999
Gd^{3+}–O^{2-} [6]	1885.75	0.3399	20.34	3.000	99999
La^{3+}–O^{2-} [7]	1545.21	0.3590	0.000	-0.250	99999
Si^{4+}–O^{2-} [3]	1283.91	0.32052	10.66	4.000	99999
Ge^{4+}–O^{2-} [8]	1497.3996	0.325646	16.00	4.000	99999
Ti^{4+}–O^{2-} [9]	5111.7	0.2625	0.000	–0.100	314.0
Sn^{4+}–O^{2-} [10]	1414.32	0.3479	13.66	4.000	99999
Zr^{4+}–O2^{-} [11]	985.869	0.3760	0.00	1.350	169.617
Ce^{4+}–O^{2-} [8]	1986.83	0.3511	20.40	7.700	291.75

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