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Defect, Diffusion and Dopant Properties of $NaNiO_2$: Atomistic Simulation Study

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Table S1. Interatomic potential parameters used in the atomistic simulations of $NaNiO_2$.

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
Ni^{3+}–O^{2-}[2]	1018.36	0.3299	0.00	4.97	304.7
O^{2-}–O^{2-}[3]	22764.30	0.149	43.0	–2.86	42.0
Mg^{2+}–O^{2-}[4]	946.627	0.31813	0.000	0.000	99999
Co^{2+}–O^{2-}[5]	1670.2416	0.2859	0.000	−1.5030	110.5
Fe^{2+}–O^{2-}[6]	1207.6	0.3084	0.000	2.000	99999
Ca^{2+}–O^{2-}[5]	1090.4	0.3372	0.0000	1.26	34.00
Sr^{2+}–O^{2-}[5]	1400.0	0.3500	0.0000	1.33	21.53
Ba^{2+}–O^{2-}[5]	931.7	0.3949	0.000	1.46	14.78
Al^{3+}–O^{2-}[7]	1725.20	0.28971	0.000	3.000	99999
Sc^{3+}–O^{2-}[5]	1299.4	0.3312	0.000	3.000	99999
Ga^{3+}–O^{2-}[5]	2901.12	0.2742	0.000	3.000	99999
Fe^{3+}–O^{2-}[5]	1156.36	0.3299	0.000	4.970	304.7
In^{3+}–O^{2-}[5]	1495.65	0.3327	4.33	3.000	99999
Gd^{3+}–O^{2-}[5]	1885.75	0.3399	20.34	3.000	99999
Y^{3+}–O^{2-}[5]	1345.10	0.3491	0.00	3.000	99999
La^{3+}–O^{2-}[5]	1545.21	0.3590	0.00	−0.250	99999
Sn^{4+}–O^{2-}[8]	1414.32	0.3479	13.66	4.000	99999
Zr^{4+}–O^{2-}[5]	985.869	0.3760	0.00	1.350	169.617
Ce^{4+}–O^{2-}[5]	1986.83	0.3511	20.40	7.700	291.75
Ti^{4+} – O^{2-}[9]	5111.7	0.2625	0.000	−0.10	314.0
Ge^{4+}–O^{2-}[10]	1497.3996	0.325646	16.00	4.0000	99999
Si^{4+}–O^{2-}[11]	1315.2478	0.317759	10.141118	0.000	99999

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