Supplementary Material: Atomistic simulations of the defect chemistry and self-diffusion of Li-ion in LiAlO2

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Table S1. Interatomic potential parameters used in the atomistic simulations of LiAlO2

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Two-body [Φ*ij* (*rij*) = *Aij* exp (− *rij*/*ρij*) − *Cij / rij*6] | | | | | |
| Interaction | *A* / eV | *ρ* / Å | *C* / eV·Å6 | Y / e | K / eV·Å–2 |
| Li+‒ O2−[1] | 632.1018 | 0.2906 | 0.00 | 1.000 | 99999 |
| Al3+‒ O2−[2] | 1109.92381 | 0.31540 | 0.00 | 3.00 | 99999 |
| O2−‒ O2−[3] | 12420.5 | 0.2215 | 29.07 | ‒2.80 | 31.0 |
| Na+ - O2−[4] | 1677.83 | 0.2934 | 0.00 | 1.00 | 99999 |
| K+ - O2−[4] | 958.21 | 0.3606 | 0.00 | 1.00 | 99999 |
| Rb+ - O2−[4] | 3400.57 | 0.3167 | 0.00 | 1.00 | 99999 |
| Mg2+ - O2−[5] | 821.6 | 0.3242 | 0.000 | 2.000 | 99999 |
| Ca2+ - O2−[5] | 1228.9 | 0.3372 | 0.0000 | 1.26 | 34.00 |
| Sr2+ - O2−[5] | 1400.0 | 0.3500 | 0.0000 | 1.33 | 21.53 |
| Ba2+ - O2−[5] | 931.7 | 0.3949 | 0.000 | 1.46 | 14.78 |
| Sc3+ - O2−[6] | 1299.4 | 0.3312 | 0.000 | 3.000 | 99999 |
| Ga3+ - O2−[5] | 2901.12 | 0.2742 | 0.000 | 3.000 | 99999 |
| Fe3+ - O2−[7] | 1156.36 | 0.3299 | 0.000 | 4.970 | 304.7 |
| Mn3+ - O2−[7] | 1267.50 | 0.3214 | 0.000 | 3.00 | 95.0 |
| Co3+ - O2−[7] | 1329.82 | 0.3087 | 0.000 | 2.04 | 196.3 |
| Ni3+ - O2−[8] | 1279.23 | 0.2932 | 0.00 | 3.000 | 93.7 |
| Y3+ - O2−[6] | 1345.10 | 0.3491 | 0.00 | 3.000 | 99999 |
| La3+ - O2−[5] | 1545.21 | 0.3590 | 0.00 | ‒0.250 | 99999 |
| Zr4+ ‒ O2−[9] | 986.0 | 0.3760 | 0.00 | 1.350 | 169.617 |
| Ce4+ ‒ O2−[10] | 1986.83 | 0.3511 | 20.40 | 7.700 | 291.75 |
| Ti4+ ‒ O2−[7] | 877.20 | 0.2625 | 0.000 | ‒0.10 | 314.0 |
| Ge4+ ‒ O2−[11] | 1497.3996 | 0.325646 | 16.00 | 4.000 | 99999 |

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