A Computational Study of Defects, Li-ion Migration and Dopants in Li2ZnSiO4 Polymorphs

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**Table S1**. Interatomic potential parameters used in the atomistic simulations of Li2ZnSiO4.

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] | 479.837 | 0.3000 | 0.00 | 1.000 | 99999 |
| Zn2+–O2−[2] | 499.60 | 0.3595 | 0.00 | 2.050 | 10.28 |
| Si4+–O2–[3] | 1315.2478 | 0.317759 | 10.141118 | 4.000 | 99999 |
| O2−–O2−[4] | 22764.30 | 0.1490 | 27.89 | -2.86902 | 74.92 |
| Ni2+ - O2−[5] | 1760.0 | 0.2800 | 0.000 | 0.000 | 93.7 |
| Mg2+ - O2−[6] | 946.627 | 0.31813 | 0.000 | 0.000 | 99999 |
| Co2+ - O2−[5] | 1670.2416 | 0.2859 | 0.0000 | -1.5030 | 110.5 |
| Fe2+ - O2−[5] | 694.10 | 0.3399 | 0.0000 | 2.000 | 10.92 |
| Ca2+ - O2−[5] | 1090.4 | 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 |
| Al3+ - O2−[5] | 1114.90 | 0.2742 | 0.000 | 3.000 | 99999 |
| Sc3+ - O2−[5] | 1299.40 | 0.3312 | 0.000 | 3.000 | 99999 |
| Ga3+ - O2−[5] | 2901.12 | 0.2742 | 0.000 | 3.000 | 99999 |
| Fe3+ - O2−[5] | 1156.36 | 0.3299 | 0.000 | 4.970 | 304.7 |
| In3+ - O2−[5] | 1495.65 | 0.3327 | 4.33 | 3.000 | 99999 |
| Y3+ - O2−[5] | 1345.10 | 0.3491 | 0.00 | 3.000 | 99999 |
| Gd3+ - O2−[5] | 1885.75 | 0.3399 | 20.34 | 3.000 | 99999 |
| La3+ - O2−[5] | 1545.21 | 0.3590 | 0.00 | ‒0.250 | 145.0 |
| Ce4+ - O2−[5] | 1986.83 | 0.3511 | 20.40 | 7.700 | 291.75 |
| Sn4+ - O2−[7] | 1414.32 | 0.3479 | 13.66 | 4.00 | 99999 |
| Ge4+ - O2−[8] | 1497.3996 | 0.325646 | 16.00 | 4.000 | 99999 |
| Ti4+ - O2−[9] | 5111.7 | 0.2625 | 0.00 | ‒0.10 | 314.0 |
| Zr4+ - O2−[5] | 985.869 | 0.3760 | 0.0000 | 1.35 | 169.617 |

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