Supporting Information

Mg_6MnO_8 as a magnesium-ion battery material: defects, dopants and Mg-ion transport

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Table S1. Interatomic potential parameters used in the atomistic simulations of Mg_6MnO_8.

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}
Mg^{2+}–O^{2-}(1)	946.627	0.31813	0.0000	2.000	999999
Mn^{4+} - O^{2-}(2)	3087.826	0.2642	0.0000	4.000	99999
O^{2-}–O^{2-}(3)	22764.30	0.1490	27.879	-2.86902	74.92
Ca^{2+} - O^{2-}(4)	1090.40	0.3372	0.0000	0.7400	34.00
Sr^{2+} - O^{2-}(4)	1400.00	0.3500	0.0000	0.6700	21.53
Ba^{2+} - O^{2-}(4)	931.79	0.3949	0.0000	0.5400	14.78
Fe^{2+} - O^{2-}(4)	694.10	0.3399	0.0000	2.000	10.92
Co^{2+} - O^{2-}(4)	1670.2416	0.2859	0.0000	3.503	110.5
Ni^{2+} - O^{2-}(4)	1760.0	0.2800	0.0000	2.000	93.7
Zn^{2+} - O^{2-}(4)	499.60	0.3595	0.0000	2.050	10.28
Al^{3+} - O^{2-}(4)	1114.9	0.2742	0.0000	3.000	99999
Ga^{3+} - O^{2-}(4)	2901.12	0.2742	0.0000	3.000	99999
Fe^{3+} - O^{2-}(4)	1156.36	0.3299	0.0000	4.970	304.70
Sc^{3+} - O^{2-}(4)	1299.40	0.3312	0.0000	3.000	99999
In^{3+} - O^{2-}(4)	1495.65	0.3327	0.0000	3.000	99999
Y^{3+} - O^{2-}(4)	1345.10	0.3491	0.0000	3.000	99999
Gd^{3+} - O^{2-}(4)	1885.75	0.3399	20.34	3.000	99999
La^{3+} - O^{2-}(4)	1545.21	0.3590	0.000	3.000	99999
Si^{4+} - O^{2-}(5)	1283.91	0.32052	10.66	4.000	99999
Ge^{4+} - O^{2-}(6)	1497.3996	0.325646	16.00	4.000	99999
Sn^{4+} - O^{2-}(7)	1414.32	0.3479	13.660	4.000	99999
Ti^{4+} - O^{2-}(8)	5111.7	0.2625	0.0000	-0.10	314.0
Zr^{4+} - O^{2-}(4)	985.869	0.3760	0.0000	1.350	169.617
Ce^{4+} - O^{2-}(4)	1986.83	0.3511	20.40	7.700	291.75

Table S2. Energetics of intrinsic defect process in Mg_6MnO_8

Defect process/equation	Reaction energy/eV	Reaction energy per defect/eV
Mg Frenkel /1	5.68	2.84
Mn Frenkel /2	20.42	10.21
O Frenkel /3	12.32	6.16
Schottky /4	62.02	4.13
MgO Schottky/5	7.92	3.96
MnO_2 Schottky/6	20.76	6.92
Mg/Mn antisite (isolated) /7	6.18	3.09
Mg/Mn antisite (cluster) /8	3.46	1.73

Table S3. Calculation formulas for intrinsic and extrinsic defect processes.

Defect process	Equation number	Calculation formula
Mg Frenkel	1	$E(V''_{Mg}) + E(Mg^{\bullet\bullet}_i)$
O Frenkel	2	$E(V^{\bullet\bullet}_O) + E(O''_i)$
Mn Frenkel	3	$E(V''''_{Mn}) + E(Mn^{\bullet\bullet\bullet\bullet}_i)$
Schottky	4	$6\,E(V''_{Mg}) + E(V''''_{Mn}) + 8E(V^{\bullet\bullet}_O) + E_{lat}(Mg_6MnO_8)$
MgO Schottky	5	$E(V''_{Mg}) + E(V^{\bullet\bullet}_O) + E_{lat}(MgO)$
MnO_2 Schottky	6	$E(V''''_{Mn}) + 2\,E(V^{\bullet\bullet}_O) + E_{lat}(MnO_2)$
Mg/Mn antisite (isolated)	7	$E(Mg''_{Mn}) + E(Mn^{\bullet\bullet}_{Mg})$
Mg/Mn antisite (cluster)	8	$E\{(Mg''_{Mn} : Mn^{\bullet\bullet}_{Mg})^X\}$
M^{2+} on Mg site	9	$E(MgO) - E(MO)$

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