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Electronic Supplementary Data

Computational Study of Crystallography, Defects, Ion Migration and Dopants in Almandine Garnet

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Table S1. Two body Buckingham potentials used for dopant oxides in $Fe_2Al_2Si_3O_{12}$.

Interaction	*A* (eV)	*ρ* (Å)	*C* (eV·Å^6)	Y (e)	K (eV·Å^{-2})
Ni^{2+} - O^{2-}	683.5	0.3332	0.000	2.000	8.77
Co^{2+} - O^{2-}	696.3	0.3362	0.000	2.000	10.74
Zn^{2+} - O^{2-}	499.6	0.3595	0.000	2.050	10.28
Mn^{2+} - O^{2-}	715.80	0.3464	0.000	3.000	81.20
Mg^{2+} - O^{2-}	946.627	0.31813	0.000	2.000	99999
Ca^{2+} - O^{2-}	1090.40	0.3372	0.000	1.260	34.00
Sr^{2+} - O^{2-}	776.84	0.35867	0.000	1.526	11.406
Ba^{2+} - O^{2-}	931.79	0.3949	0.000	1.460	14.78
Ga^{3+} - O^{2-}	2901.12	0.2742	0.000	1.000	99999
Sc^{3+} - O^{2-}	1575.85	0.3211	0.000	3.000	99999
In^{3+} - O^{2-}	1495.65	0.3327	4.33	3.000	99999
Y^{3+} - O^{2-}	1345.10	0.3491	0.00	3.000	99999
Gd^{3+} - O^{2-}	1885.75	0.3399	20.34	3.000	99999
La^{3+} - O^{2-}	1545.21	0.3590	0.00	–0.250	145.0
Ge^{4+} - O^{2-}	1497.3996	0.325646	16.00	4.000	99999
Sn^{4+} - O^{2-}	1414.32	0.3479	13.66	4.000	99999
Ti^{4+} - O^{2-}	877.20	0.38096	9.00	–35.8630	65974.00
Zr^{4+} - O^{2-}	1502.11	0.3477	0.00	1.35	169.617
Ce^{4+} - O^{2-}	1986.83	0.3511	20.40	7.70	291.75