Supplementary Materials

Theoretical Modelling of Defects, Dopants and Diffusion in the Mineral Ilmenite

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Table S1. Interatomic potential parameters used in the atomistic simulations of $FeTiO_3$

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}**
$Fe^{2+} – O^{2-}$	694.10	0.3399	0.00	2.00	10.92
$Ti^{4+} – O^{2-}$	5111.7	0.2625	0.000	–0.10	314.0
$O^{2-} – O^{2-}$	22764.3	0.1490	27.879	−2.86902	74.92
$Ni^{2+} – O^{2-}$	683.5	0.3332	0.000	2.00	8.77
$Zn^{2+} – O^{2-}$	499.6	0.3595	0.000	2.05	10.28
$Co^{2+} – O^{2-}$	696.3	0.3362	0.000	2.00	10.74
$Mn^{2+} – O^{2-}$	715.80	0.3464	0.000	3.00	81.20
$Ca^{2+} – O^{2-}$	1090.4	0.3372	0.000	1.26	34.00
$Sr^{2+} – O^{2-}$	1400.0	0.3500	0.000	1.33	21.53
$Ba^{2+} – O^{2-}$	931.79	0.3949	0.000	3.000	99999
$Al^{3+} – O^{2-}$	1725.20	0.28971	0.000	3.00	99999
$Mn^{3+} – O^{2-}$	1267.50	0.3214	0.000	4.97	304.7
$Ga^{3+} – O^{2-}$	1625.72	0.3019	0.000	3.000	99999
$Sc^{3+} – O^{2-}$	1299.40	0.3312	0.000	3.000	99999
$In^{3+} – O^{2-}$	1495.65	0.3327	4.330	3.000	99999
$Yb^{3+} – O^{2-}$	1309.60	0.3462	0.000	3.000	99999
$Y^{3+} – O^{2-}$	1766.40	0.33849	0.000	3.000	99999
$Gd^{3+} – O^{2-}$	1885.75	0.3399	20.34	3.000	99999
$La^{3+} – O^{2-}$	2088.79	0.3460	23.25	3.000	99999
$Si^{4+} – O^{2-}$	1283.91	0.32052	10.66	4.000	99999
$Ge^{4+} – O^{2-}$	1497.3996	0.325646	16.00	4.000	99999
$Sn^{4+} – O^{2-}$	1414.32	0.3479	13.66	4.000	99999
$Zr^{4+} – O^{2-}$	985.869	0.3760	0.000	1.350	169.617
$Ce^{4+} – O^{2-}$	1986.83	0.3511	20.40	7.700	291.75