chemistry

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Supplementary Information

Defects and Calcium Diffusion in Wollastonite

Sumudu Nimasha [1], Sashikesh Ganeshalingam [1], Navaratnarajah Kuganathan[2,3*] and Alexander Chroneos[2,3]

[1] Department of Chemistry, University of Jaffna, Sir. Pon Ramanathan Road, Thirunelvely, Jaffna, 40000, Srilanka

[2] Department of Materials, Imperial College London, London, SW7 2AZ, United Kingdom

[3] Faculty of Engineering, Environment and Computing, Coventry University, Priory Street, Coventry CV1 5FB, United Kingdom

*Correspondence: n.kuganathan@imperial.ac.uk; ad0636@coventry.ac.uk (N.K)

Table S1. Interatomic potential parameters used in the atomistic simulations of $CaSiO_3$

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}**
$Co^{2+} - O^{2-}$	696.3	0.3362	0.00	2.00	10.74
$Mn^{2+} - O^{2-}$	715.80	0.3464	0.00	3.42	81.20
$Ni^{2+} - O^{2-}$	683.5	0.3332	0.00	2.00	8.77
$Mg^{2+} - O^{2-}$	946.627	0.31813	0.00	2.00	99999
$Zn^{2+} - O^{2-}$	499.6	0.3595	0.00	2.05	10.28
$Sr^{2+} - O^{2-}$	776.84	0.35867	0.00	1.526	11.406
$Ba^{2+} - O^{2-}$	931.79	0.3949	0.00	1.46	14.78
$Al^{3+} - O^{2-}$	1114.9	0.3118	0.00	3.00	99999
$Ga^{3+} - O^{2-}$	2901.12	0.2742	0.00	3.00	99999
$Fe^{3+} - O^{2-}$	1156.36	0.3299	0.00	4.97	304.7
$In^{3+} - O^{2-}$	1495.65	0.3327	4.33	3.00	99999
$Sc^{3+} - O^{2-}$	1575.85	0.3211	0.000	3.00	99999
$Y^{3+} - O^{2-}$	1345.10	0.3491	0.000	3.00	99999
$Gd^{3+} - O^{2-}$	1885.75	0.3399	20.34	3.00	99999
$La^{3+} - O^{2-}$	1545.21	0.3590	0.000	-0.25	145.0
$Ge^{4+} - O^{2-}$	1497.3996	0.325646	16.00	4.00	99999
$Ti^{4+} - O^{2-}$	877.200	0.380960	9.00	-35.863	65974.0
$Sn^{4+} - O^{2-}$	1414.32	0.3479	13.66	4.00	99999
$Zr^{4+} - O^{2-}$	1502.11	0.3477	5.10	1.65	189.70
$Ce^{4+} - O^{2-}$	1986.83	0.3511	20.40	7.70	291.75