Supporting Information

Transferability of Interatomic Potentials with insights on the Structure-Property Relationship of SiO_2-CaO-MgO-Al_2O_3 Melts

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Tables

Table S 1 Effective charge of oxygen for the 4 potentials

	Matsui	Kawamura	Miyake	Guillot
Effective charge	-0.945	-2	-0.96	-0.945

Table S 2 Selected compositions (wt.%) and estimated melting points (MP) and density

Samples	SiO_2	CaO	MgO	Al_2O_3	SUM	CaO/SiO_2	MgO/Al_2O_3	MP (°C)	Density (g/cc)
S35-1	35	35	15	15	100.00	1.00	1.00	1341.15	2.85
S35-2	35	35	10	20	100.00	1.00	0.50	1353.97	2.82
S35-3	35	35	5	25	100.00	1.00	0.20	1401.56	2.78
S35-4	35	40	15	10	100.00	1.14	1.50	1451.53	2.87
S35-5	35	40	10	15	100.00	1.14	0.67	1368.35	2.84
S35-6	35	40	5	20	100.00	1.14	0.25	1386.31	2.81
S40-1	40	35	20	5	100.00	0.88	4.00	1412.56	2.85
S40-2	40	35	15	10	100.00	0.88	1.50	1341.59	2.82
S40-3	40	35	10	15	100.00	0.88	0.67	1252.18	2.79
S40-4	40	40	15	5	100.00	1.00	3.00	1345.02	2.85
S40-5	40	40	10	10	100.00	1.00	1.00	1254.94	2.82
S40-6	40	40	5	15	100.00	1.00	0.33	1364.12	2.79
S45-1	45	30	20	5	100.00	0.67	4.00	1281.69	2.80
S45-2	45	30	15	10	100.00	0.67	1.50	1233.22	2.77
S45-3	45	30	10	15	100.00	0.67	0.67	1299.13	2.74
S45-4	45	35	15	5	100.00	0.78	3.00	1232.16	2.80
S45-5	45	35	10	10	100.00	0.78	1.00	1361.3	2.77
S45-6	45	35	5	15	100.00	0.78	0.33	1270.82	2.73
S50-1	50	25	20	5	100.00	0.50	4.00	1266.28	2.76
S50-2	50	25	15	10	100.00	0.50	1.50	1250.52	2.72
S50-3	50	25	10	15	100.00	0.50	0.67	1270.67	2.69
S50-4	50	30	15	5	100.00	0.60	3.00	1341.15	2.75
S50-5	50	30	10	10	100.00	0.60	1.00	1353.97	2.72
S50-6	50	30	5	15	100.00	0.60	0.33	1401.56	2.68

Table S 3 Bond lengths (Å) of Si-O, Ca-O, Mg-O and Al-O for sample S35-1 obtained with 4 potentials and comparison with neutron diffraction experiment obtained in literature[1, 2].

	Matsui	Kawamura	Miyake	Guillot	Experiment
Si-O	1.62	1.67	1.61	1.62	1.61-1.65
Ca-O	2.37	2.41	2.32	2.39	2.32-2.36
Mg-O	1.99	2.08	2.03	2.02	1.98-2.05
Al-O	1.74	1.84	1.73	1.71	1.74-1.78

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Figures

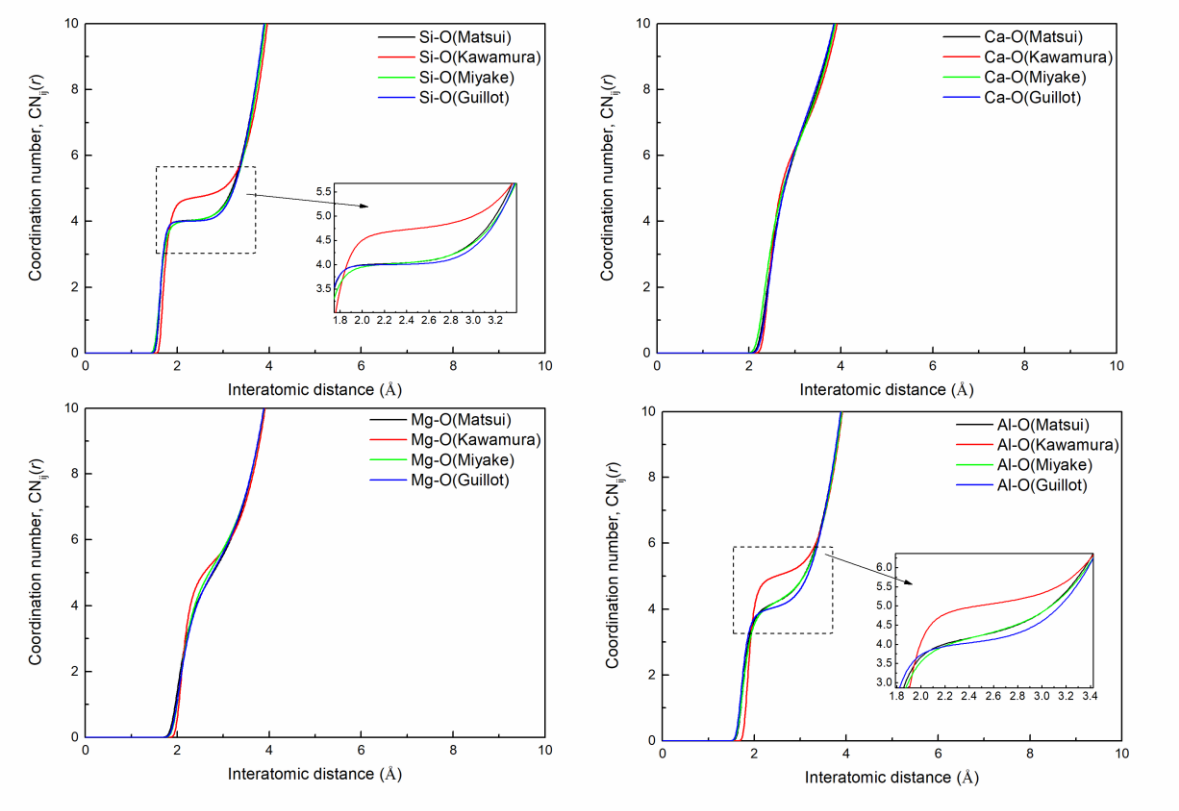

Fig.S 1 Comparison of coordination number curved obtained with 4 potentials (take s35-1 as an example)

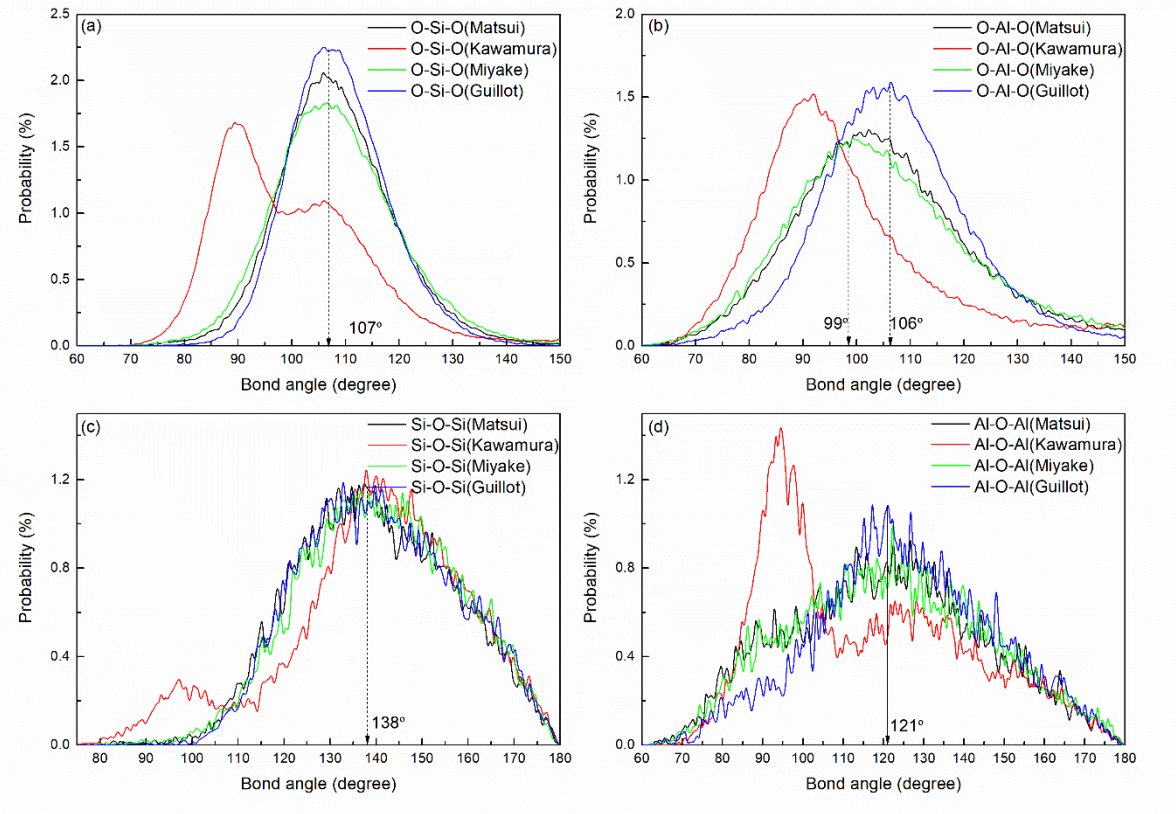

Fig.S 2 Bond angle distribution for O-Si-O, O-Al-O, Si-O-Si and Al-O-Al with 4 potentials. (Take sample S35-1 as an example)

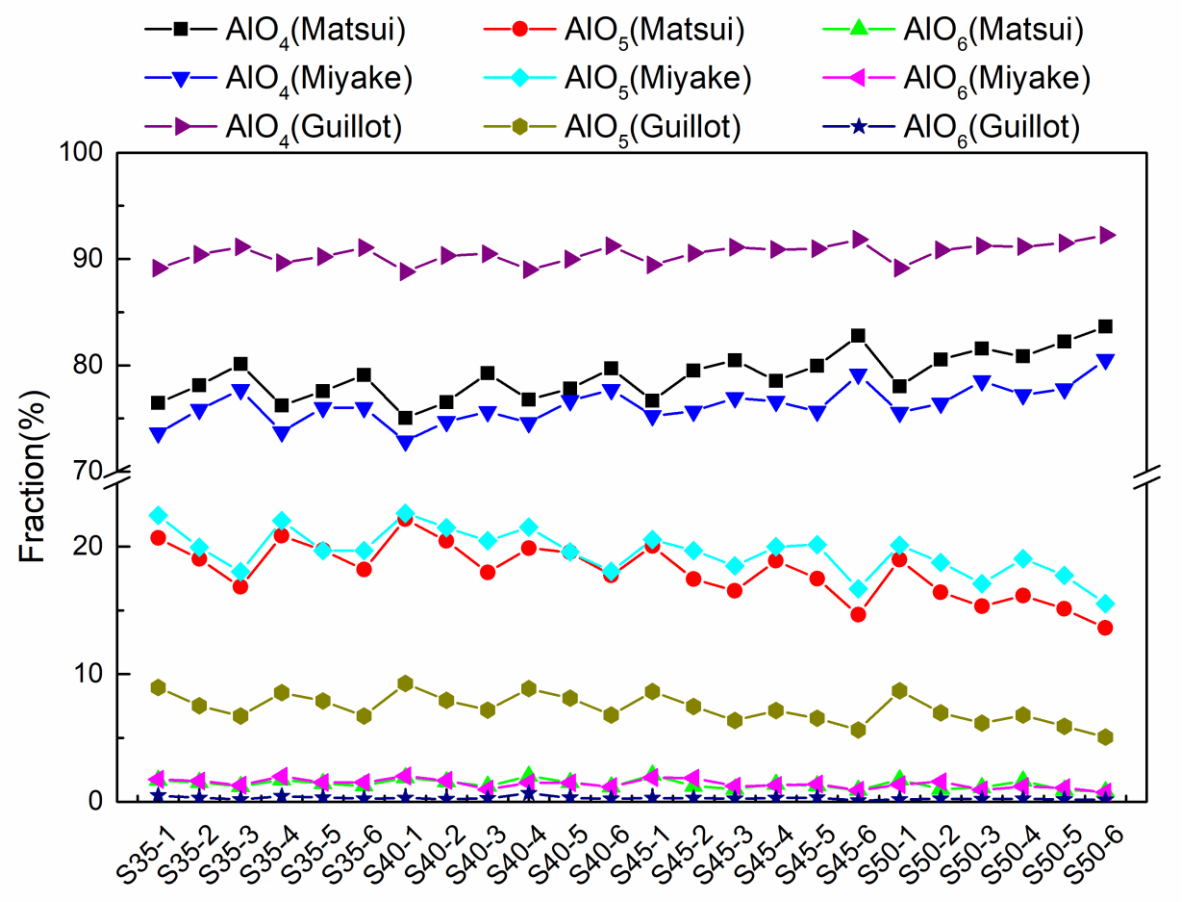

Fig.S 3 Aluminum coordination number for all the samples obtained with Matsui, Miyake and Guillot potentials

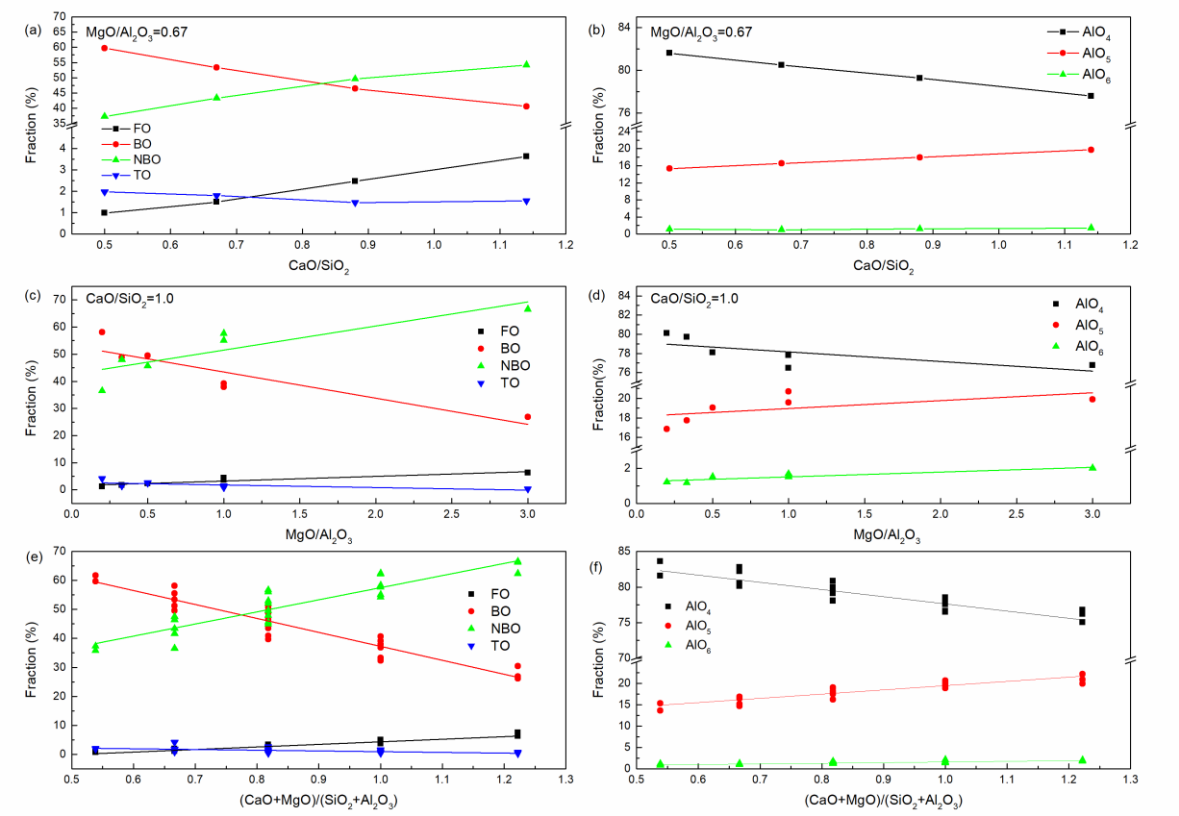

Fig.S 4 Fraction evolution of oxygen bond types and three type's aluminum with the change of MgO/Al_2O_3 ratio (a-b), CaO/SiO_2 ratio (c-d) and $(CaO+MgO)/(SiO_2+Al_2O_3)$ ratio (e-f). Take the results using Matsui potential as example.

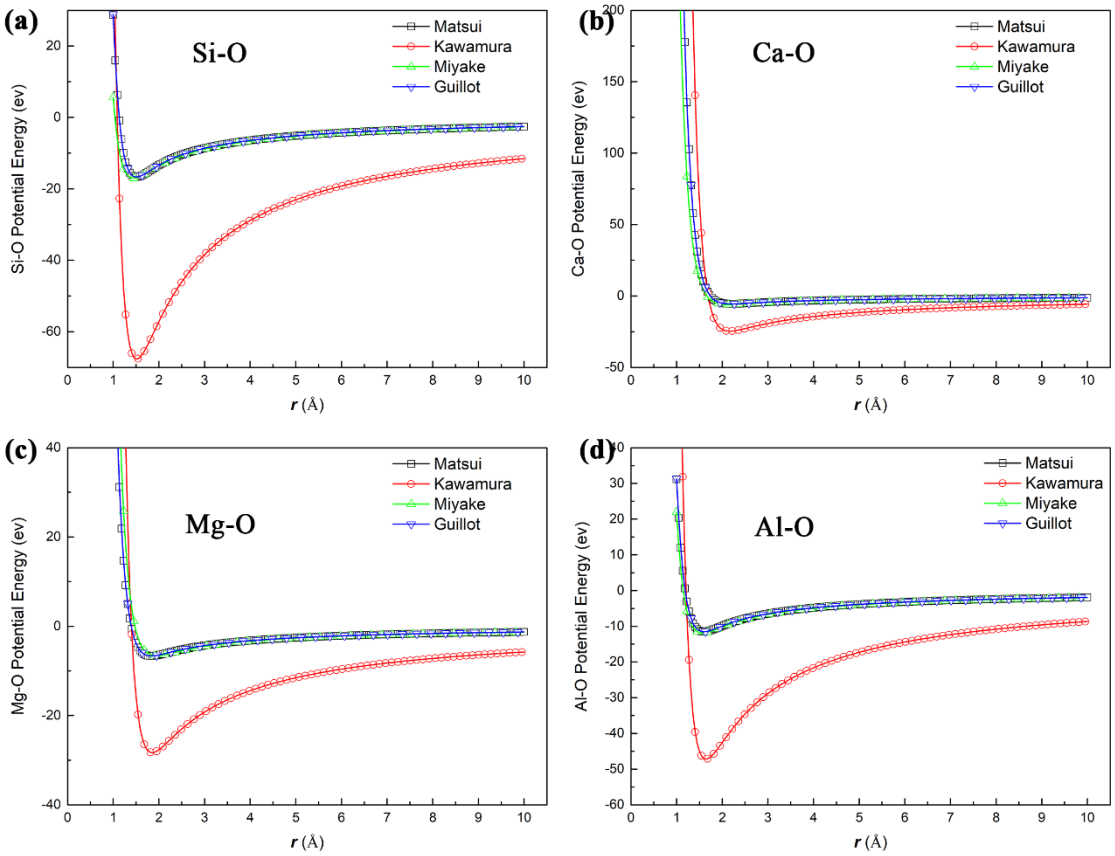

Fig.S 5 Interatomic potential energy for different atomic pairs using the selected four potentials: (a) Si-O; (b) Ca-O; (c) Mg-O; (d) Al-O

Regerences

[1] M. Guignard, L. Cormierl, Environments of Mg and Al in MgO–Al2O3–SiO2 glasses: A study coupling neutron and X-ray diffraction and Reverse Monte Carlo modeling, Chemical Geology 256 (2008) 111-118.

[2] L. Hennet, J.W. Drewitt, D.R. Neuville, V. Cristiglio, J. Kozaily, S. Brassamin, D. Zanghi, H.E. Fischerl, Neutron diffraction of calcium aluminosilicate glasses and melts, Journal of Non-Crystalline Solids 451 (2016) 89-93.