Supporting Information

Atomic and Electronic Structure in $MgO–SiO_2$

Yuta Shuseki[a,b], *Shinji Kohara*[b*], *Tomoaki Kaneko*[c], *Keitaro Sodeyama*[b], *Yohei Onodera*[b], *Chihiro Koyama*[d], *Atsunobu Masuno*[a,b], *Shunta Sasaki*[e], *Shohei Hatano*[e], *Motoki Shiga*[f,g,h], *Ippei Obayashi*[i], *Yasuaki Hiraoka*[j], *Junpei T. Okada*[k], *Akitoshi Mizuno*[l], *Yuki Watanabe*[m], *Yui Nakata*[m], *Koji Ohara*[n], *Motohiko Murakami*[o], *Matthew G. Tucker*[p], *Marshall T. McDonnell*[q], *Hirohisa Oda*[d] *and Takehiko Ishikawa*[r]

[a] *Graduate School of Engineering, Kyoto University, Kyoto 615-8520, Japan*

[b] *Center for Basic Research on Materials, National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0047, Japan*

[c] *Department of Computational Science and Technology, Research Organization for Information Science and Technology (RIST), Tokyo 105-0013, Japan*

[d] *Human Spaceflight Technology Directorate, Japan Aerospace Exploration Agency (JAXA), Tsukuba, Ibaraki 305-8505, Japan*

[e] *Graduate School of Science and Technology, Hirosaki University, Hirosaki, Aomori 036-8561, Japan*

[f] *Unprecedented-Scale Data Analytics Center, Tohoku University, Sendai, Miyagi 980-8578, Japan*

[g] *Graduate School of Information Science, Tohoku University, Sendai, Miyagi 980-8579, Japan*

[h] *RIKEN Center for Advanced Intelligence Project, Tokyo 103-0027, Japan*

[i] *Center for Artificial Intelligence and Mathematical Data Science, Okayama University, Okayama 700-8530, Japan*

[j] *Institute for the Advanced Study of Human Biology (WPI-ASHBi), Kyoto University, Kyoto* 606-8303*, Japan*

[k] *Institute for Materials Research, Tohoku University, Sendai, Miyagi 980-8577, Japan*

[l] *National Institute of Technology, Hakodate College, Hakodate, Hokkaido 042-8501, Japan*

[m] *Advanced Engineering Services Co., Ltd., Tsukuba, Ibaraki* 305-0032*, Japan*

[n] *Faculty of Materials for Energy, Shimane University, Matsue, Shimane 690-8504, Japan*

[o] *Department of Earth Sciences, ETH Zürich, Zürich 8092, Switzerland*

[p] *Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States*

[q] *Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, United States*

[r] *Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency (JAXA), Tsukuba, Ibaraki 305-8505, Japan*

[*]Corresponding author: Shinji Kohara, email:KOHARA.Shinji@nims.go.jp

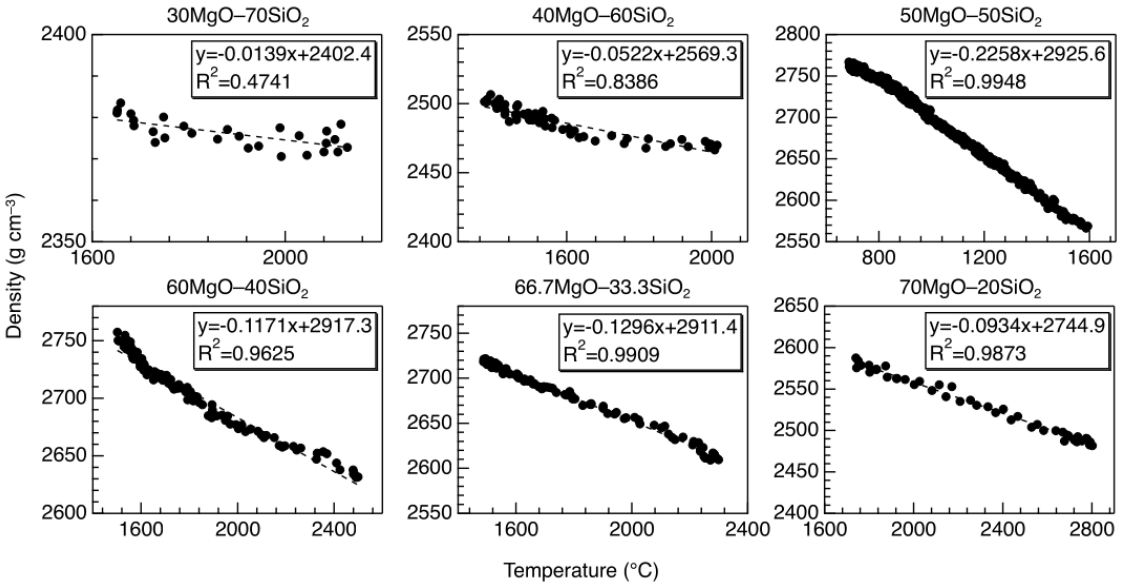

Fig. S1 Measured density of *l*-*x*MgO–(100-*x*)SiO_2 as a function of temperature.

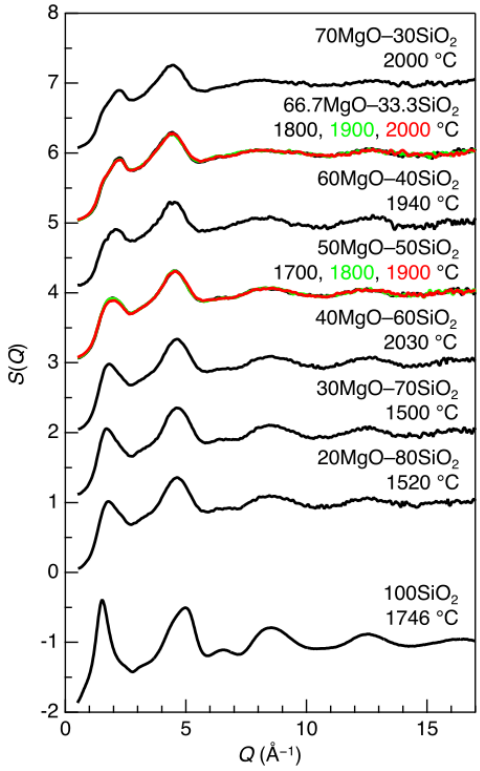

Fig. S2 X-ray total structure factors, $S(Q)$, for *l*-xMgO–(100-x)SiO_2 and *l*-SiO_2[1].

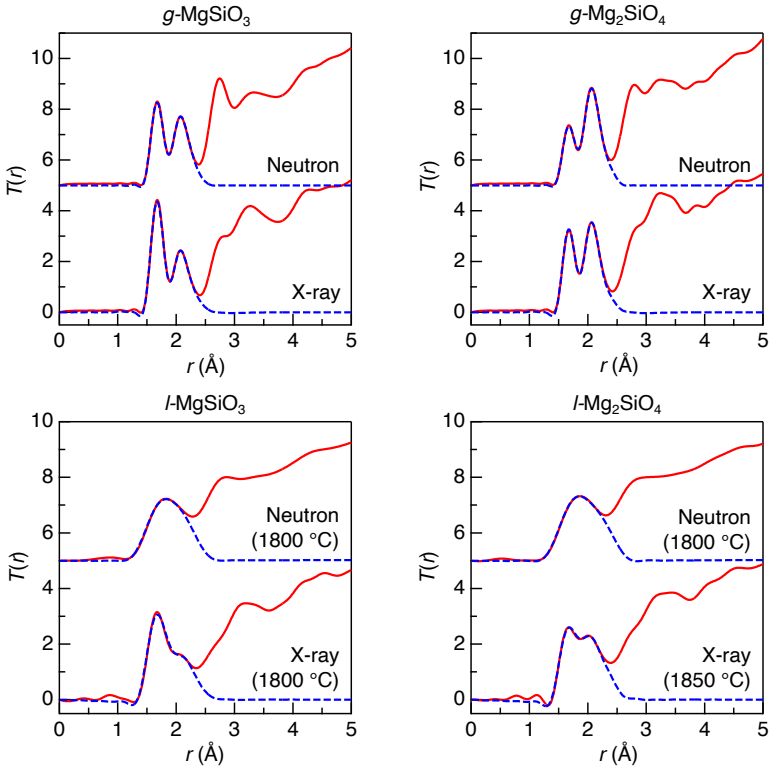

Fig. S3 Pair function analysis of total correlation functions $T(r)$. Red; experimental data, bule; pair function.

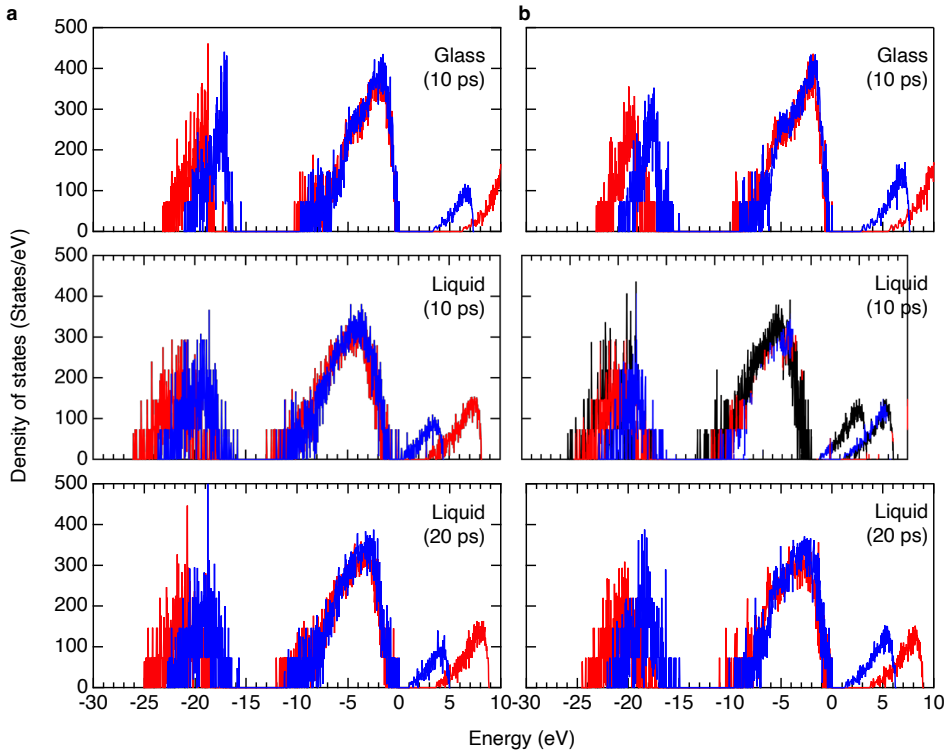

Fig. S4 Electron density of states for **a** *g*- and *l*-$MgSiO_3$ and **b** *g*- and *l*-Mg_2SiO_4 calculated by DF–MD simulations. Red; PBE0 (0.3), blue; GGA–PBE.

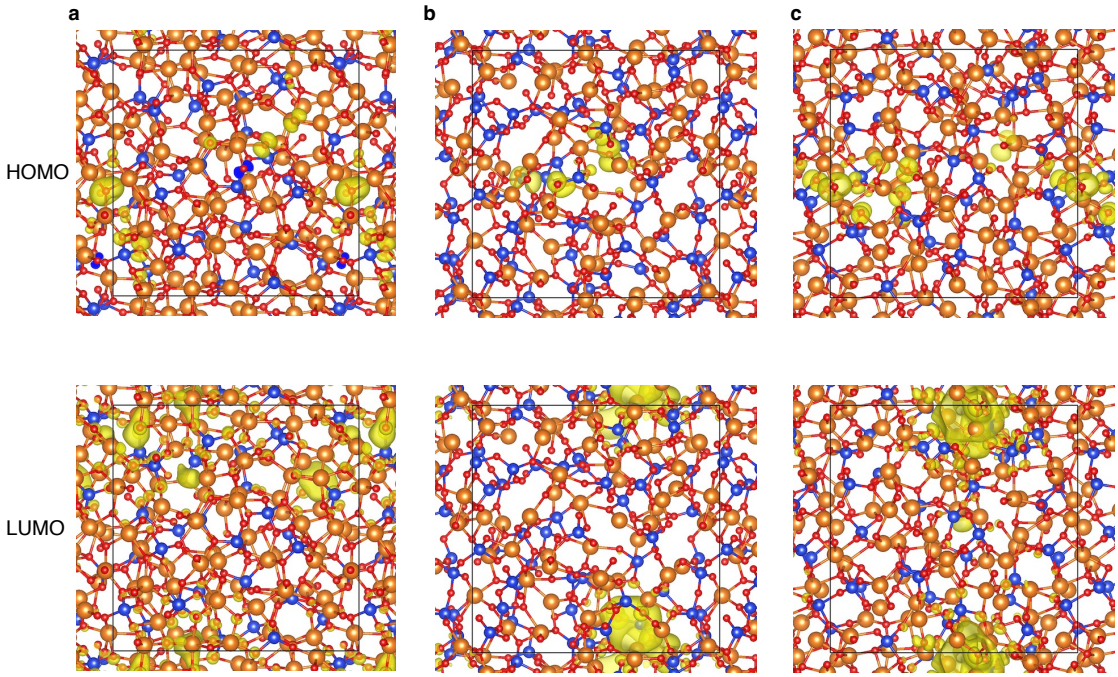

Fig. S5 Isosurface plots of the partial charge density around the HOMO and the LUMO levels for **a** *g*-Mg_2SiO_4 density of states, **b** *l*-$MgSiO_3$ (10 ps) and **c** *l*-Mg_2SiO_4 (10 ps).

Table S1 Coordination numbers obtained by pair function analysis of X-ray and neutron total correlation functions $T(r)$.

		$N_{Si–O}$	$N_{Mg–O}$
l-$MgSiO_3$	neutron	3.85	4.8 (3.7+1.1)
	X-ray	3.85	4.8 (4.0+0.8)
g-$MgSiO_3$	neutron	3.95	5.0 (4.5+0.5)
	X-ray	3.95	5.0 (4.5+0.5)
l-Mg_2SiO_4	neutron	3.85	4.8 (3.55+1.25)
	X-ray	3.85	4.8 (3.9+0.9)
g-Mg_2SiO_4	neutron	4.00	5.0 (4.4+0.6)
	X-ray	3.95	5.0 (4.5+0.5)

Table S2 Coordination numbers obtained by DF–MD models.

DF–MD model	$N_{Si–O}$ (cut off 1.9 Å)	$N_{O–O}$ (cut off 4.0 Å)	$N_{Mg–O}$ (cut off 2.8 Å)
l-$MgSiO_3$	3.84	11.24	4.82
l-Mg_2SiO_4	3.88	11.82	4.93
g-$MgSiO_3$	4.00	12.17	5.19
g-Mg_2SiO_4	4.03	12.70	5.15

Table S3 Electron band gaps (eV) for several crystals calculated by GGA–PBE and PBE0.

Method	MgO	α-quartz	$MgSiO_3$	Mg_2SiO_4
Exp.	7.7[2]/7.8[3]	9.34-9.55[4]	8.9[5]	8.4[6]/8.8[5]
GGA–PBE	4.82779	5.53158	4.88708	5.27906
PBE0 (0.25)	7.33461	8.06809	7.44759	7.85018
PBE0 (0.30)	7.84888	8.58155	7.96749	8.37234
PBE0 (0.35)	8.36677	9.09690	8.48946	8.89693

Values in brackets show fractions of the exact exchange term for the exchange correlation functional.

References

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