

COMPOSITION AND TEMPERATURE EFFECTS ON SHORT AND MEDIUM-RANGE ORDER IN LITHIUM SILICATE GLASSES: A MOLECULAR DYNAMICS STUDY

Pham Thi Lien^{1,*}, Nguyen Thi Thao² and Tran Duc Hiep²

¹*University of Economics - Technology for Industries, Hanoi, Vietnam*

²*Hanoi National University of Education, Hanoi, Vietnam*

*Corresponding author: Pham Thi Lien, e-mail: ptlien@uneti.edu.vn

Received August 14, 2026. Revised September 3, 2026. Accepted September 30, 2026.

Abstract. Molecular dynamics (MD) simulations were employed to examine the composition- and temperature-dependent structure of $\text{Li}_2\text{O}_m\text{SiO}_2$ glasses with $m = 1, 2$, and 4, denoted LS1, LS2, and LS4, over 300–973 K. The simulated models reproduce the principal peak positions and overall features of available neutron structure-factor and pair-distribution data, providing a basis for comparative structural analysis. The internal geometry of the SiO_4 tetrahedra is comparatively stable, with Si–O distances of approximately 1.55–1.60 Å and Si–O coordination close to four. Network connectivity changes strongly with composition through the balance between bridging oxygens (BOs) and non-bridging oxygens (NBOs): increasing SiO_2 raises the average O–Si coordination from about 1.33 in LS1 to 1.78 in LS4 and decreases NBO/T from approximately 2.0 to 0.5, while Li retains a broad oxygen-coordination environment dominated by four- and fivefold states. Temperature produces only minor changes in characteristic bond distances and NBO/T. Quantitative first sharp diffraction peak (FSDP) parameters show a weak and composition-dependent thermal response, whereas increasing SiO_2 content produces a more pronounced and narrower neutron-weighted FSDP. These results identify composition as the dominant control on network connectivity and the neutron-weighted medium-range structural signature, while temperature causes comparatively modest changes without substantially reconstructing the local SiO_4 framework or the average BO/NBO topology. The principal contribution is the direct, internally consistent separation of composition- and temperature-induced responses using the same interaction potential, preparation protocol, and structural descriptors.

Keywords: lithium silicate glass, MD, short-range order, medium-range order, NBO

1. Introduction

Lithium silicate glasses are model network formers composed of SiO_4 tetrahedra linked by bridging oxygens (BOs). Li_2O breaks Si–O–Si linkages, creates non-bridging oxygens (NBOs), and thereby modifies network connectivity and transport.

Diffraction and reverse Monte Carlo (RMC) studies show nearly tetrahedral Si coordination and heterogeneous Li–O environments [1], [2]. Nuclear magnetic resonance and Raman measurements describe depolymerization through Q^n distributions [3], [4], while simulations and diffusion experiments relate composition to Li hopping, pathways, and mobility [5]–[8]. Recent work addresses conduction channels, interfaces, medium-range topology, and structure–transport relations [9]–[12].

These descriptors are established; the remaining question is their relative sensitivity to composition and temperature when evaluated with one potential, preparation protocol, and set of definitions.

Here, LS1, LS2, and LS4 are studied at 300, 573, 773, and 973 K. The analysis separates local SiO_4 geometry, network connectivity, and the neutron-weighted FSDP. It shows that composition strongly changes O–Si connectivity and NBO/T, whereas local geometry and the thermal FSDP response vary less. Table 1 summarizes the distinction from representative MD studies.

Table 1. Comparison of representative MD studies of lithium silicate glasses with the present work

Study	Main focus	Difference from this work
Banhatti and Heuer [5]	Structure and Li dynamics at high T	Melt dynamics and ion motion
Habasaki and Hiwatari [6]; Lammert and Heuer [9]	Li sites, jumps, and conduction channels	Microscopic transport mechanisms
Prasada Rao et al. [7]	BO/NBO, Q^n , composition, and Li pathways	Broad composition range; transport focus
Firooz et al. [11]	Topology, rings, and the FSDP	Composition and medium-range topology
Present work	LS1, LS2, and LS4 at 300–973 K	Unified separation of composition and temperature effects

2. Computational method

2.1. Model construction and simulation protocol

The three compositions LS1, LS2, and LS4 were simulated using the MXDORTO MD code. They were deliberately selected as representative states spanning a broad range of silicate-network polymerization rather than as a uniformly spaced compositional series. For LS_m , the nominal stoichiometric relation $\text{NBO}/\text{T} = 2/m$ gives values of 2.0, 1.0, and 0.5 for LS1, LS2, and LS4, respectively, corresponding to strongly depolymerized, intermediate, and more polymerized networks. LS2 was additionally retained as an experimental benchmark because lithium disilicate is well characterized by neutron-scattering and density measurements [13], [14]. LS3 and other intermediate compositions were not excluded because of anomalous behavior; they were outside the representative composition set selected for this study. The LS1, LS2, and LS4 cells contained 10,008, 9,999, and 10,005 atoms, respectively, with the atomic populations listed in Table 2. Periodic boundary conditions were applied in all three spatial directions. The relatively large cells improve the statistics of pair and coordination distributions and

reduce, although they do not by themselves eliminate, possible finite-size effects. Initial configurations were generated by random placement according to the required stoichiometry. Each system was first equilibrated at 1573 K in the constant-number, constant-pressure, constant-temperature (NPT) ensemble and then cooled to the target temperatures of 300, 573, 773, and 973 K at an approximate rate of 10^{12} K s⁻¹. At each target temperature, an additional NPT equilibration was performed until the cell volume reached a stable average value. This volume was subsequently fixed for a 150-ps constant-number, constant-volume, constant-energy (NVE) production run with a time step of 1 fs. For each state point, one production trajectory was generated, and 144 configurations recorded at 1-ps intervals were retained for structural averaging. Long-range Coulomb interactions were evaluated using Ewald summation.

The cooling rate used here ($\sim 10^{12}$ K s⁻¹) is many orders of magnitude higher than typical experimental glass-processing rates, as is common in classical MD simulations because of their limited accessible timescale. Rapid cooling may retain excess frozen-in disorder and can affect the simulated density, structural relaxation, and medium-range organization. Absolute comparison with slowly cooled experimental glasses should therefore be made cautiously. Nevertheless, the same cooling protocol was applied to all compositions and temperatures, so the relative trends discussed below remain internally comparable within the present model set. The 144 configurations constitute a correlated time series from a single production trajectory at each state point and were not treated as independent replicas. Additional trajectories generated from independently prepared initial configurations could not be included within the available computational resources and project timeframe. Consequently, the reported quantities are temporal averages from one trajectory and do not include model-to-model uncertainty across independent glass realizations; small differences should therefore be interpreted cautiously.

Table 2. Model compositions and simulated densities, ρ (g cm⁻³), at 300, 573, 773, and 973 K

	Sample				ρ (g cm ⁻³)			
	N _{Li}	N _{Si}	N _O	N	300 K	573 K	773 K	973 K
LS1	3336	1668	5004	10008	2.3654	2.3169	2.2759	2.2269
LS2	2222	2222	5555	9999	2.4528	2.4173	2.3862	2.3594
LS4	1334	2668	6003	10005	2.5037	2.4816	2.4658	2.4432

2.2. Interatomic potential

Interatomic interactions were described using the rigid-ion potential developed by Pedone and co-workers for oxides and silicate glasses [15].

Table 3. Interaction-potential parameters adopted without modification from Pedone et al. [15] and used in Eq. (1)

Pair	D _{ij} (eV)	a _{ij} (Å ⁻¹)	r _{0,ij} (Å)	C _{ij} (eV Å ¹²)
Li–O	0.001114	3.429506	2.681360	1.0
Si–O	0.340554	2.006700	2.100000	1.0
O–O	0.042395	1.379316	3.618701	22.0

The potential consists of long-range Coulomb, short-range Morse, and steep repulsive contributions:

$$U_{ij}(r) = Z_i Z_j e^2 / r + D_{ij} \{ [1 - \exp(-a_{ij}(r - r_{0,ij}))]^2 - 1 \} + C_{ij} / r^{12} \quad (1)$$

Here, Z_i and Z_j are effective charges. All charges and Li–O, Si–O, and O–O parameters were taken unchanged from Pedone et al. [15]. Their General Utility Lattice Program (GULP) parameterization used relaxed fitting and Gibbs free-energy minimization at 300 K and 1 atm: Si–O and O–O were constrained by α -quartz structure and elasticity, whereas Li–O was fitted to crystalline $\text{Li}_2\text{Si}_2\text{O}_5$. The adopted charges are +0.6e (Li), +2.4e (Si), and –1.2e (O). Because Coulomb and Morse terms act together, D_{ij} , a_{ij} , and $r_{0,ij}$ are effective force-field parameters.

2.3. Structural analysis

Partial radial distribution functions (RDFs) were calculated for all atomic pairs. Characteristic distances were determined from the first-peak positions, while coordination numbers were obtained by direct neighbor counting. Cutoff distances of 2.40 Å for Si–O and 2.85 Å for Li–O were selected from the first-minimum regions following the corresponding first RDF peaks and were applied consistently to all systems and temperatures. The Si–O first shell is sharply defined, whereas the Li–O minimum is broader; consequently, the absolute LiO_x fractions are more sensitive to the exact Li–O cutoff. The discussion therefore emphasizes comparative trends obtained with the same cutoff rather than treating individual LiO_x fractions as cutoff-independent quantities. For comparison with neutron-scattering data, the partial functions were combined using Faber–Ziman weighting to obtain the neutron-weighted RDF and total structure factor $S_N(q)$. O–Si coordination was determined using the 2.40 Å cutoff. Oxygen atoms with one and two Si neighbors were classified as NBOs and BOs, respectively. Network polymerization was characterized by NBO/T, where T denotes tetrahedrally coordinated Si. Medium-range order was analyzed from the FSDP in $S_N(q)$. FSDP peak positions, peak values, and full-width-at-half-maximum (FWHM) values were extracted using the same peak-profile procedure for all reported state points.

3. Results and discussion

3.1. Validation of the simulated models

The experimental $S_N(q)$ dataset of Kitamura et al. [13] corresponds to an undensified $\text{Li}_2\text{O} \cdot 0.2\text{SiO}_2$ glass prepared by liquid quenching: reagent-grade Li_2CO_3 and SiO_2 were melted at approximately 1475 °C for 4 h in a platinum crucible, cast in a carbon mold, and annealed at the glass-transition temperature, $T_g = 470$ °C. The undensified glass had a density of $2.34 \pm 0.01 \text{ g cm}^{-3}$.

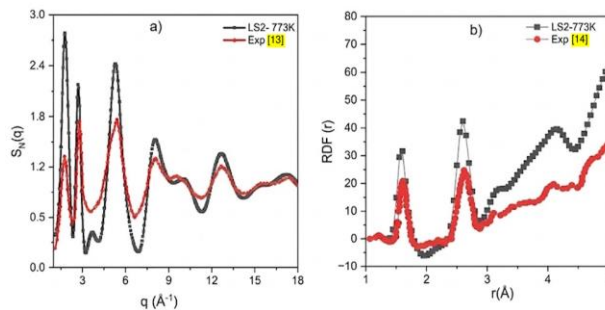


Figure 1. Comparison of the simulated LS2 neutron-weighted structure factor at 773 K and RDF with room-temperature experimental data [13], [14]

Misawa et al. [14] reported room-temperature time-of-flight pulsed-neutron total-scattering data for LS2 glass; a detailed melt-quench and annealing history was not specified in that cited report. Thus, neither experimental dataset corresponds to an in-situ 773 K state or to the present MD cooling history. The comparison is therefore restricted to characteristic peak positions and overall structural features; differences in absolute intensities and widths are not interpreted as direct quantitative validation. Figure 1 compares the LS2 model at 773 K with available neutron-scattering data.

The simulated density decreases monotonically with temperature for each composition (Figure 2), consistent with the larger volumes assigned to the higher-temperature states. Within the present models, the density order is $LS4 > LS2 > LS1$ at every temperature; this ordering is specific to the present potential and preparation protocol. For LS2 at 300 K, the calculated density is 2.4528 g cm^{-3} , whereas Kitamura et al. reported $2.34 \pm 0.01 \text{ g cm}^{-3}$ for their undensified, melt-quenched and annealed glass measured by the Archimedes method [13]. The simulation therefore overestimates this reference value by approximately 4.8%.

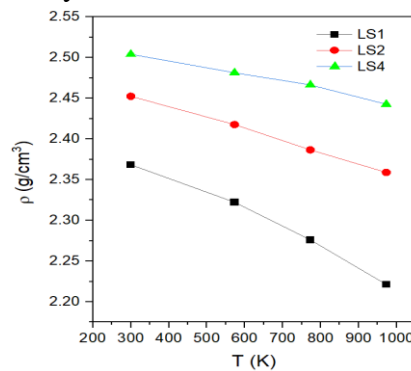


Figure 2. Simulated density of LS1, LS2, and LS4 as a function of temperature
Lines connect the calculated state points

This discrepancy may affect atomic packing and, consequently, RDF and $SN(q)$ amplitudes and widths. Plausible contributors include the empirical potential, the rapid MD cooling rate, the simulation-volume procedure, and the different thermal histories. Accordingly, density and scattering comparisons are used to validate characteristic structural scales and comparative trends rather than exact experimental values.

The comparison can also be expressed quantitatively. For LS2, the calculated FSDP position at 773 K is 1.772 Å^{-1} , whereas Kitamura et al. reported the room-temperature experimental FSDP at approximately 1.70 Å^{-1} , a difference of about 4.2% [13]. The representative simulated Si–O and O–O distances, 1.60 and 2.60 Å, differ from the corresponding experimental values of 1.62 and 2.65 Å by approximately 1.2% and 1.9%, respectively [13]. Together with the 4.8% density overestimation discussed above, these values show that the model reproduces the principal structural length scales but not all absolute experimental observables. Because the simulation and experiments correspond to different temperatures and preparation histories, this validation supports comparative analysis among the simulated systems and should not be interpreted as an exact, condition-matched reproduction of the experimental glasses.

3.2. Short-range atomic structure

The partial pair-distribution functions show a clear separation between the network-forming and modifier-related environments (Figure 3a). The Si–O first peak is narrow and intense, reflecting the well-defined first coordination shell of the SiO_4 tetrahedron. The O–O first peak represents the tetrahedral edge length, while the first Si–Si maximum reflects the separation between neighboring tetrahedral centers. In contrast, Li-containing correlations are broader and overlap over a wider r range, indicating a more heterogeneous local environment around the modifier cation.

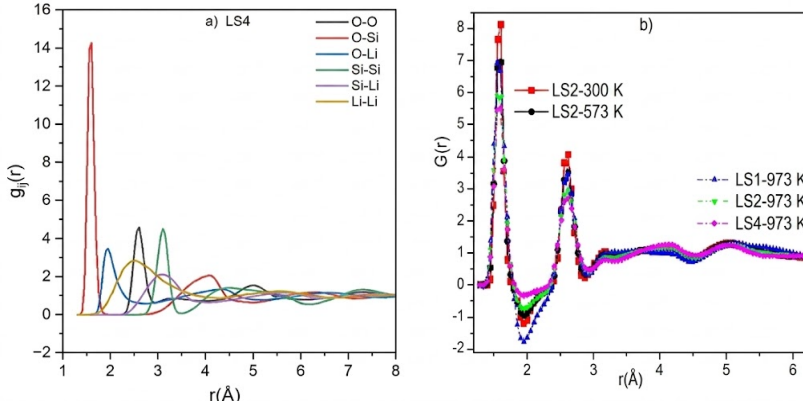


Figure 3. (a) Partial pair-distribution functions for LS4 at 773 K. (b) Neutron-weighted total pair-distribution functions for selected temperatures and compositions

The simulated characteristic distances at 573 K are summarized in Table 4 after conversion to $\text{\AA}$. The Si–O distance lies between 1.55 and 1.60 $\text{\AA}$, the nearest O–O distance is approximately 2.60 $\text{\AA}$, and the Si–Si distance is approximately 3.10 $\text{\AA}$. These values are close to the ranges obtained from neutron diffraction, RMC, and previous MD analyses, which typically place Si–O near 1.60–1.62 $\text{\AA}$, O–O near 2.62–2.65 $\text{\AA}$, and Li–O near 1.9–2.0 $\text{\AA}$ [1], [2], [5]. The simulated Li–O first-neighbor distance remains approximately 1.95 $\text{\AA}$. The peak positions vary only slightly with temperature in the total $G(r)$, supporting the relative stability of the local bond-length scale over 300–973 K.

Table 4. Simulated atomic-pair distances and partial coordination numbers at 573 K. All distances are reported in $\text{\AA}$

Sys.	r_{SiO}	r_{OO}	r_{SiSi}	r_{LiO}	r_{LiSi}	r_{LiLi}	Z_{SiO}	Z_{OSi}	Z_{LiO}
LS1	1.55	2.60	3.10	1.95	3.10	2.50	4.000	1.333	4.508
LS2	1.60	2.60	3.10	1.95	3.10	2.45	4.001	1.600	4.482
LS4	1.60	2.60	3.10	1.95	3.10	2.40	4.005	1.778	4.422

The Si–O coordination number remains essentially four in all three compositions, confirming that the internal tetrahedral coordination is preserved. This statement is restricted to the internal geometry and fourfold coordination of SiO_4 ; it does not imply that the entire short-range structure is composition independent. The O–Si coordination changes substantially because the fraction of BOs changes, and the Li coordination distribution also varies with composition. Because the Li–O first minimum is broad, the absolute Li coordination numbers and LiO_x fractions depend on the selected cutoff; the

same 2.85 Å criterion is therefore used throughout so that the relative composition and temperature trends are directly comparable.

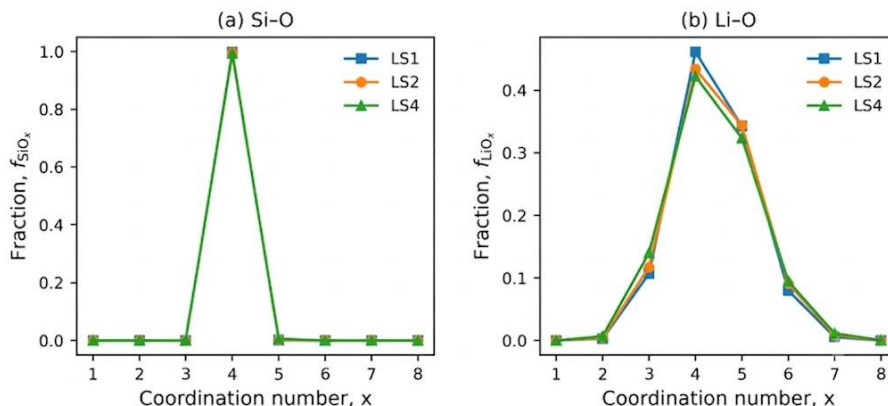


Figure 4. Coordination-number distributions at 973 K: (a) Si–O and (b) Li–O for LS1, LS2, and LS4

Table 5. Fractions (%) of fourfold Si coordination and the dominant Li–O coordination states at 573, 773, and 973 K

T(K)	Sample	SiO ₄ (%)	LiO ₄ (%)	LiO ₅ (%)	LiO ₄ + LiO ₅ (%)
573	LS1	99.962	47.039	36.914	83.953
	LS2	99.903	44.909	36.061	80.969
	LS4	99.537	43.071	34.918	77.989
773	LS1	99.960	46.336	35.896	82.232
	LS2	99.880	46.335	35.896	82.231
	LS4	99.450	42.811	33.668	76.479
973	LS1	99.900	46.175	34.264	80.439
	LS2	99.732	43.429	34.406	77.835
	LS4	99.413	42.261	32.366	74.628

The Li–O coordination analysis was extended to 573 and 773 K in addition to 973 K (Table 5). LiO₄ and LiO₅ remain the dominant environments in all three compositions over 573–973 K. Their combined fractions are 83.95%, 80.97%, and 77.99% for LS1, LS2, and LS4 at 573 K; 82.23%, 82.231%, and 76.48% at 773 K; and 80.44%, 77.84%, and 74.63% at 973 K. Heating and increasing SiO₂ content therefore produce a modest redistribution toward lower-coordination Li environments, particularly LiO₃, without changing the dominance of LiO₄ and LiO₅. In contrast, more than 99.4% of Si atoms remain fourfold coordinated in every analyzed state. Figure 4 illustrates the full distributions at 973 K.

3.3. Network connectivity and oxygen speciation

Oxygen speciation shows the strongest composition effect: NBO fractions are approximately 0.664, 0.399, and 0.220 in LS1, LS2, and LS4, with little temperature variation. Corresponding NBO/T values are approximately 2.0, 1.0, and 0.5 (Table 6), close to stoichiometric expectations for Li₂O.mSiO₂.

Table 6. NBO/T as a function of composition and temperature

Sample	300 K	573 K	773 K	973 K
LS1	1.993	1.991	1.991	1.991
LS2	1.000	0.998	0.999	0.996
LS4	0.496	0.497	0.495	0.494

NBO/T is used here as an average measure of network depolymerization. A value near 2.0 in LS1 is compatible with an average degree of depolymerization often associated with Q²-rich environments, whereas the lower values in LS2 and LS4 indicate progressively greater network connectivity. However, NBO/T does not uniquely determine the complete Qⁿ distribution, and no unique Qⁿ population is inferred from NBO/T alone; coexisting Qⁿ species may produce the same average value [3], [4], [7], [11]. A full Qⁿ distribution was not calculated in the present analysis, so the discussion is deliberately limited to average connectivity. Consistently, the average O–Si coordination increases from approximately 1.34 in LS1 to 1.60 in LS2 and 1.78 in LS4, reflecting the increasing number of intertetrahedral Si–O–Si connections with increasing SiO₂ content. NBO/T varies by less than approximately 0.01 from 300 to 973 K for each composition, indicating little temperature-induced change in average BO/NBO topology. This is consistent with high-temperature Raman observations [4] and suggests that thermal effects mainly involve rearrangement of existing structural units rather than substantial changes in oxygen speciation.

3.4. Medium-range order

The neutron-weighted structure factors show an FSDP at 1.71 - 1.78 Å⁻¹ and a principal peak at 2.57 - 2.78 Å⁻¹ (Figure 6). Because both partial correlations S_{ij}(q) and Faber–Ziman weights vary with composition, total S_n(q) cannot uniquely separate structural and neutron-weighting contributions. The FSDP is therefore interpreted together with BO/NBO, NBO/T, and O–Si coordination.

At 573 K, the FSDP peak value increases from 2.594 in LS1 to 2.921 in LS4, while FWHM decreases from 0.731 to 0.532 Å⁻¹; similar contrasts occur at 773 and 973 K (Table 7). The higher, narrower FSDP in SiO₂-rich models is consistent with greater connectivity, but is not assigned solely to structure because scattering weights also change.

Table 7. Quantitative FSDP parameters at 573 - 973 K

Sample	T(K)	q _{FSDP} (Å ⁻¹)	S _N (q _{FSDP})	FWHM (Å ⁻¹)
LS1	573	1.7351	2.5939	0.7313
	773	1.7274	2.6195	0.7173
	973	1.7108	2.6475	0.7054
LS2	573	1.7788	2.7154	0.6019
	773	1.7715	2.7474	0.6020
	973	1.7693	2.7154	0.5943
LS4	573	1.7681	2.9207	0.5322
	773	1.7648	2.9385	0.5321
	973	1.7625	2.9174	0.5213

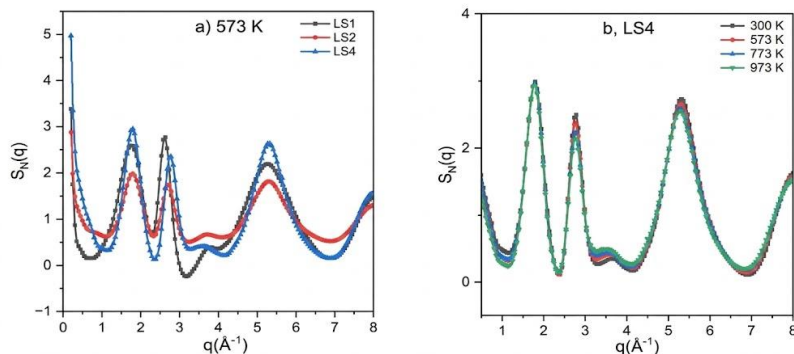


Figure 6. Neutron-weighted total structure factors showing (a) the composition dependence for LS1, LS2, and LS4 at 573 K and (b) the temperature dependence of LS4 from 300 to 973 K

Thermal changes are weaker: from 573 to 973 K, q_{FSDP} decreases by only $0.024 \text{ \AA}^{-1}$ in LS1, $0.010 \text{ \AA}^{-1}$ in LS2, and $0.006 \text{ \AA}^{-1}$ in LS4, while peak values and FWHM vary weakly or non-monotonically. Thus, composition produces the clearer FSDP contrast.

3.5. Unified structural interpretation and implications

Together, the results establish a hierarchy: composition strongly controls O–Si connectivity, NBO/T, and the neutron-weighted FSDP, whereas temperature causes small changes in local SiO_4 coordination, BO/NBO speciation, and the FSDP. The data therefore do not support universal thermal weakening of medium-range order.

These static trends are consistent with reports of modifier-rich Li pathways, reduced Li mobility with increasing silica, cooperative motion, and structure–transport relations [6]–[8], [12]. Direct pathway and dynamical analyses are outside the present scope.

4. Conclusions

MD simulations were used to investigate the effects of composition and temperature on the structure of LS1, LS2, and LS4 lithium silicate glasses from 300 to 973 K. The models reproduce the principal structural features observed experimentally. The local SiO_4 tetrahedral geometry remains comparatively stable, whereas Li exhibits a broader and more heterogeneous oxygen-coordination environment. Composition has the dominant effect on network topology: increasing SiO_2 increases O–Si connectivity and decreases NBO/T, indicating progressive network polymerization. Quantitative FSDP analysis shows a weak and composition-dependent thermal response, while the compositional dependence is more pronounced, with a higher and narrower neutron-weighted FSDP in SiO_2 -rich systems. Taken together, the results identify composition as the dominant control parameter for network connectivity and the neutron-weighted medium-range structural signature, whereas temperature produces comparatively modest changes without substantially reconstructing the local SiO_4 framework or the average BO/NBO topology. The contribution of the present work lies in establishing this hierarchy of structural sensitivities within an internally consistent composition–temperature MD dataset, rather than in identifying the individual structural descriptors themselves.

Note for contributor:

- Short bio: Pham Thi Lien is a researcher at the University of Economics - Technology for Industries, Vietnam. Nguyen Thi Thao and Tran Duc Hiep are researchers at Hanoi National University of Education, Vietnam.

- Author contributions: Pham Thi Lien, Nguyen Thi Thao: conceptualization, simulation, data analysis, and writing; Nguyen Thi Thao: validation and review; Tran Duc Hiep: methodology, supervision, and review.

Conflict of interest. The authors declare no conflict of interest.

Acknowledgments. This research was funded by the Vietnam National Foundation for Science and Technology Development (NAFOSTED), grant number 103.01-2025.107.

REFERENCES

- [1] H. Uhlig, M. J. Hoffmann, H.-P. Lamparter, F. Aldinger, R. Bellissent & S. Steeb, "Short-range and medium-range order in lithium silicate glasses, Part I: diffraction experiments and results", *Journal of the American Ceramic Society*, vol. 79, no. 11, pp. 2833-2838, 1996. DOI: 10.1111/j.1151-2916.1996.tb08716.x
- [2] H. Uhlig, M. J. Hoffmann, H. P. Lamparter, F. Aldinger, R. Bellissent & S. Steeb, "Short-range and medium-range order in lithium silicate glasses, Part II: simulation of the structure by the reverse Monte Carlo method", *Journal of the American Ceramic Society*, vol. 79, no. 11, pp. 2839-2846, 1996. DOI: 10.1111/j.1151-2916.1996.tb08717.x
- [3] B. H. W. S. De Jong, C. M. Schramm & V. E. Parziale, "Silicon-29 magic angle spinning NMR study on local silicon environments in amorphous and crystalline lithium silicates", *Journal of the American Chemical Society*, vol. 106, no. 16, pp. 4396-4402, 1984. DOI: 10.1021/ja00328a018
- [4] O. N. Koroleva, "The structure of lithium silicate melts revealed by high-temperature Raman spectroscopy", *Spectroscopy Letters*, vol. 50, no. 5, pp. 257-264, 2017. DOI: 10.1080/00387010.2017.1316743
- [5] R. D. Banhatti & A. Heuer, "Structure and dynamics of lithium silicate melts: molecular dynamics simulations", *Physical Chemistry Chemical Physics*, vol. 3, pp. 5104-5108, 2001. DOI: 10.1039/B106013A
- [6] J. Habasaki & Y. Hiwatari, "Molecular dynamics study of the mechanism of ion transport in lithium silicate glasses: characteristics of the potential energy surface and structures", *Physical Review B*, vol. 69, no. 14, pp. 144207, 2004. DOI: 10.1103/PhysRevB.69.144207
- [7] R. Prasada Rao, T. D. Tho & S. Adams, "Ion transport pathways in molecular dynamics simulated lithium silicate glasses," *Solid State Ionics*, vol. 181, no. 1-2, pp. 1-6, 2010. DOI: 10.1016/j.ssi.2009.12.003
- [8] U. Bauer, A.-M. Welsch, H. Behrens, J. Rahn, H. Schmidt & I. Horn, "Li diffusion and the effect of local structure on Li mobility in Li₂O–SiO₂ glasses," *The Journal of Physical Chemistry B*, vol. 117, no. 48, pp. 15184-15195, 2013. DOI: 10.1021/jp408805e

- [9] H. Lammert & A. Heuer, “Emergence of conduction channels in lithium silicate”, *Physical Review B*, vol. 70, no. 2, pp. 024204, 2004. DOI: 10.1103/PhysRevB.70.024204
- [10] J. Du & C. H. Chen, “Structure and lithium ion diffusion in lithium silicate glasses and at their interfaces with lithium lanthanum titanate crystals”, *Journal of Non-Crystalline Solids*, vol. 358, pp. 3531–3538, 2012. DOI: 10.1016/j.jnoncrysol.2012.05.015
- [11] A. F. Firooz, R. Christensen, C. A. N. Biscio & M. M. Smedskjaer, “Characterizing medium-range order structure of binary silicate glasses using ring analysis and persistent homology”, *Journal of the American Ceramic Society*, vol. 107, no. 12, pp. 7739–7750, 2024. DOI: 10.1111/jace.19924
- [12] P. T. Lien, N. T. Thao & P. K. Hung, “Structure and ion transport in lithium silicates: insights from molecular dynamics simulations”, *The European Physical Journal B*, vol. 99, article 10, 2026. DOI: 10.1140/epjb/s10051-026-01120-7
- [13] N. Kitamura, K. Fukumi, H. Mizoguchi, M. Makihara, A. Higuchi, N. Ohno & T. Fukunaga, “High pressure densification of lithium silicate glasses”, *Journal of Non-Crystalline Solids*, vol. 274, no. 1-3, pp. 244–248, 2000. DOI: 10.1016/S0022-3093(00)00190-3
- [14] M. Misawa, D. L. Price & K. Suzuki, “The short-range structure of alkali disilicate glasses by pulsed neutron total scattering”, *Journal of Non-Crystalline Solids*, vol. 37, pp. 85–97, 1980. DOI: 10.1016/0022-3093(80)90481-0
- [15] A. Pedone, G. Malavasi, M. C. Menziani, A. N. Cormack & U. Segre, “A new self-consistent empirical interatomic potential model for oxides, silicates, and silica-based glasses”, *The Journal of Physical Chemistry B*, vol. 110, no. 24, pp. 11780–11795, 2006. DOI: 10.1021/jp0611018