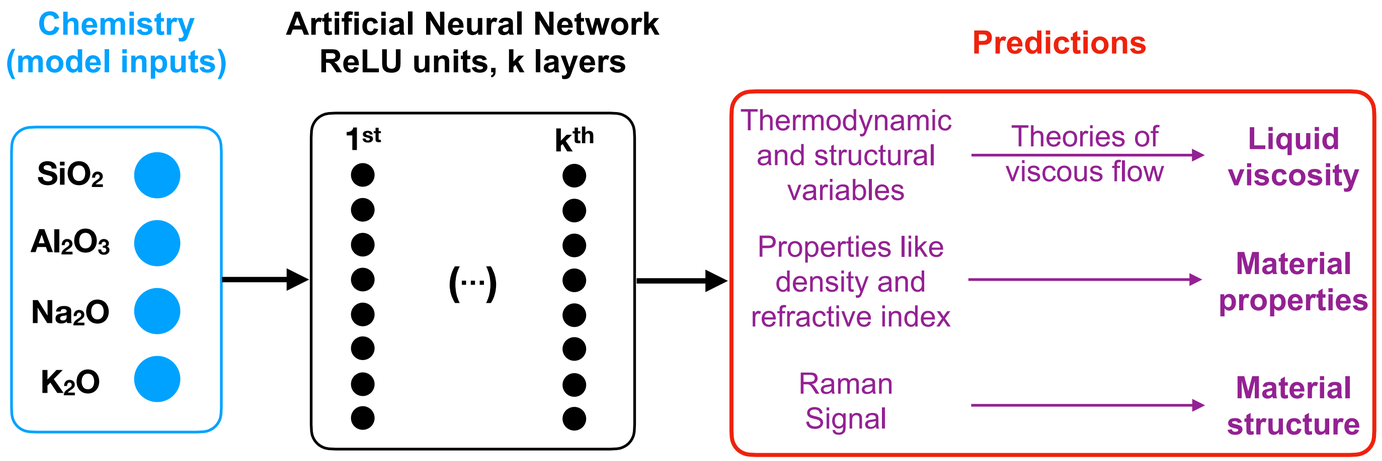
Figure and sketch for paper about neural network model

- Figure 1: a schematic drawing of the forward model
- 4 inputs (melt oxide contents) are passed to a neural network
- The neural network predicts the parameters of the VFT, AG, CG, MYEGA and AM viscosity equations (fragility, entropy, glass transition temperature, etc.).
- It also predicts glass Raman spectra, density, and optical refractive index through the Sellmeir coefficients.
- Model is trained with an existing database in the NKAS system

Figure 1



- Figure 2 : some examples > the model is actually cool and can predict accurately the viscosity of the melts with AG or CG equations.

- Even SiO2 is well predicted, which is very rare.

Figure 2

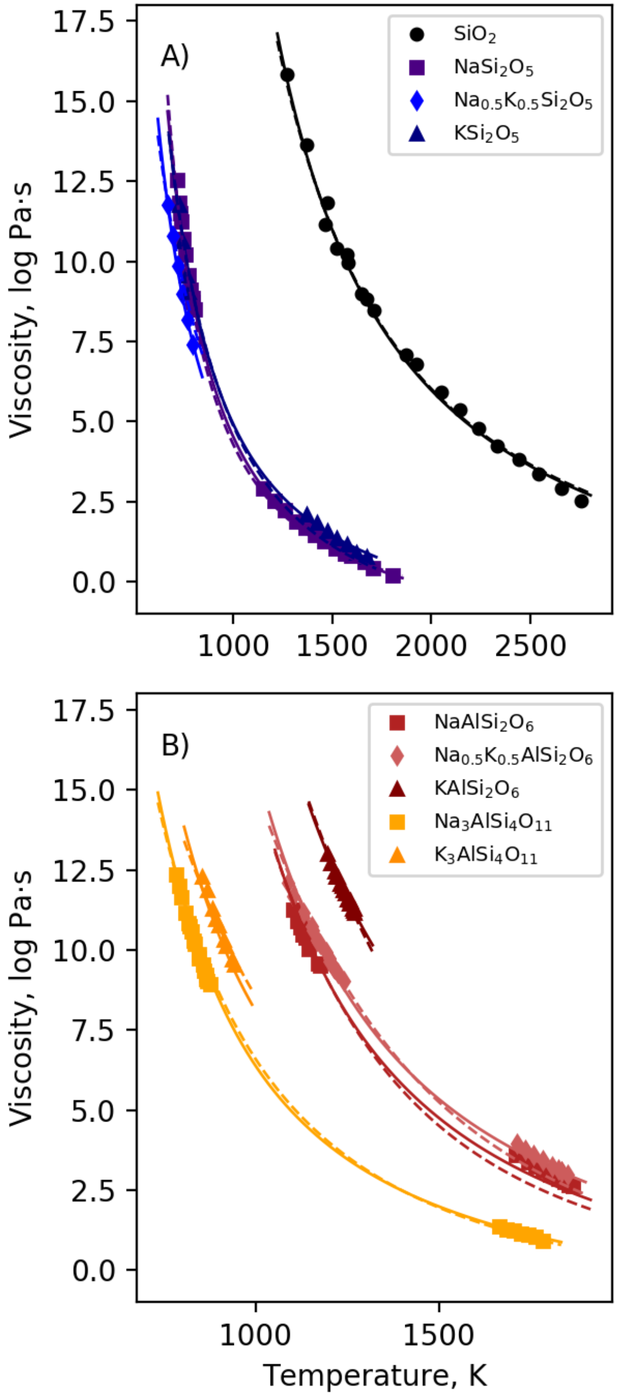
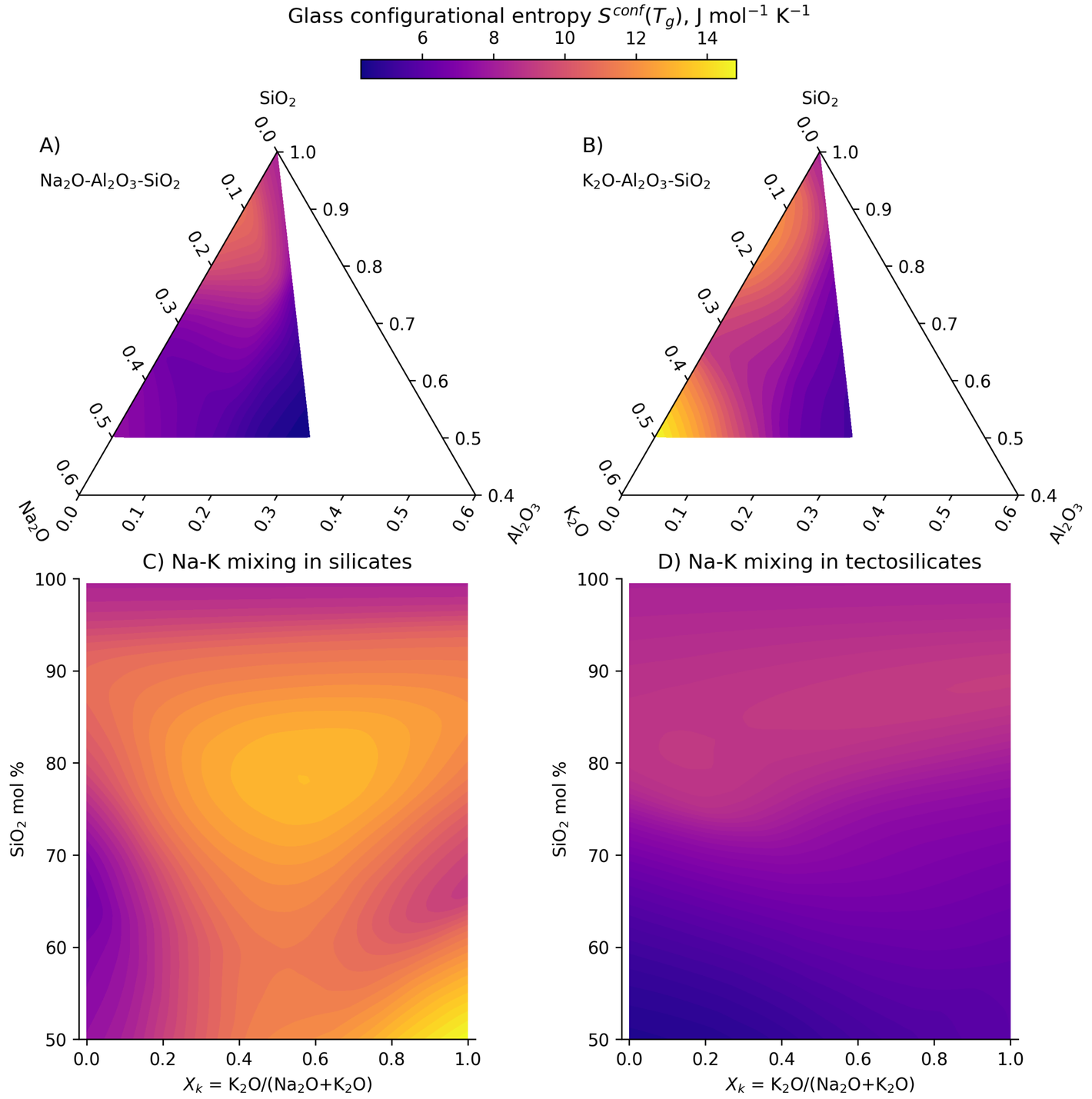


Figure 3

- Figure 3 : confident in this model, we can move on and look at latent variables like entropy.
- Glass configurational entropy is a fundamental parameter
- Variations are well predicted (supplementary figure)
- The model allows observing the variations in all the glass forming domain (A and B) as well as during alkali mixing (C and D).
- We note that the model predicts mixing effects at mostly high silica content in silicate glasses
- No mixing effect in tectosilicates, in agreement with previous data



- **General trend those days in publications : melt network controls everything. Let's explore this idea in this paper.**

- Figure 4 : now we can look how material properties are correlated with glass structure as seen by Raman spectroscopy. R_Raman is the ratio of the inter-tetrahedral Raman vibrations to intra-tetrahedral ones. It was used recently to make viscosity models…

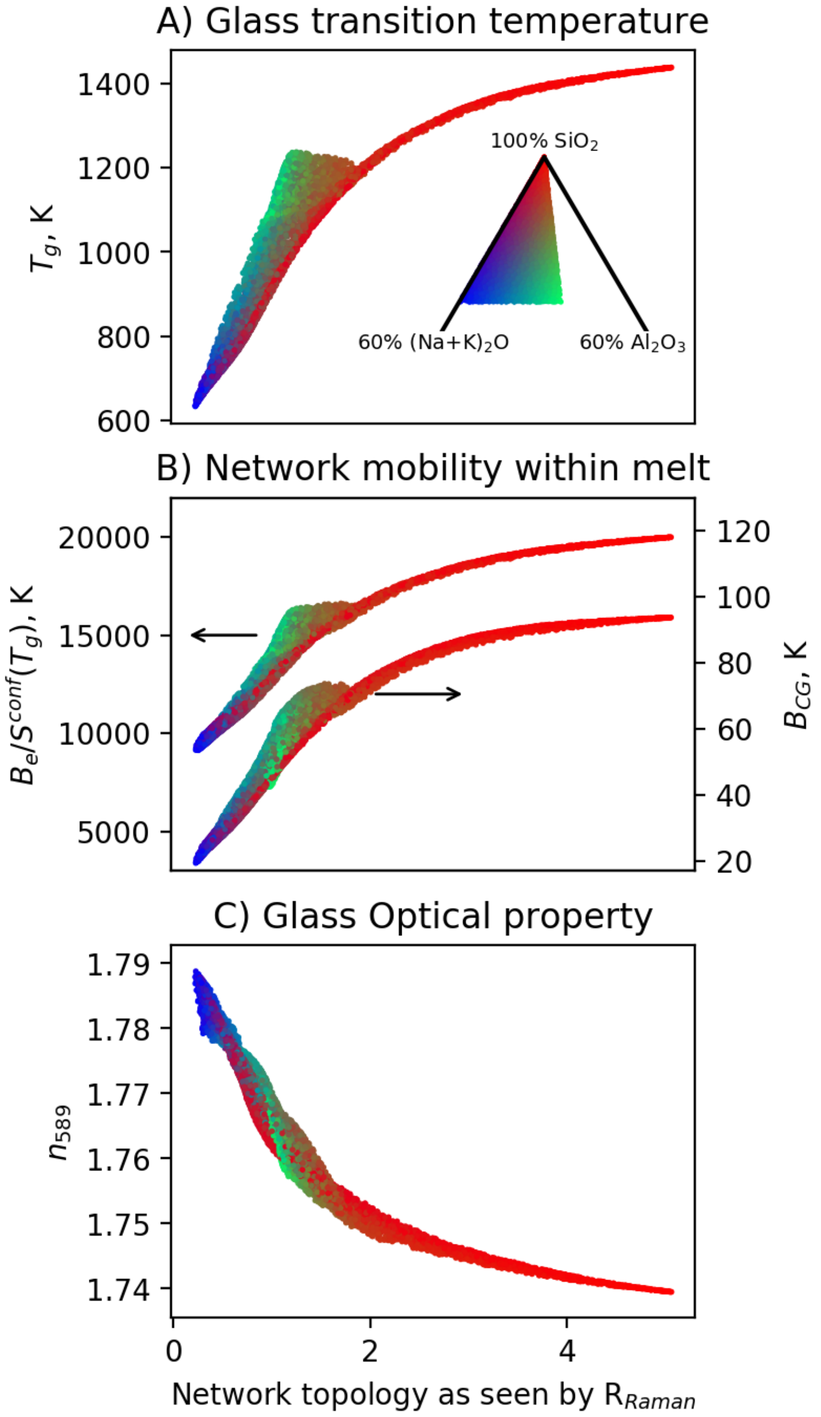
- A) The glass transition temperature correlates generally with the network topology as seen by Raman, but the correlation shows a chemical mapping and is non-linear

- B) Network mobility parameters (basically the energy barriers opposed to molecular jumps required for viscous flow) also correlate strongly with network topology, and, by extension, with the glass transition temperature

- C) interestingly, network topology correlates with the glass optical properties

- Conclusion : we directly confirm through a multi-parameter search that molecular network topology in glasses and melts determines largely some of their thermodynamic, dynamic and static properties.

Figure 4



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- Figure 5 : hum, not all properties are correlated to network topology

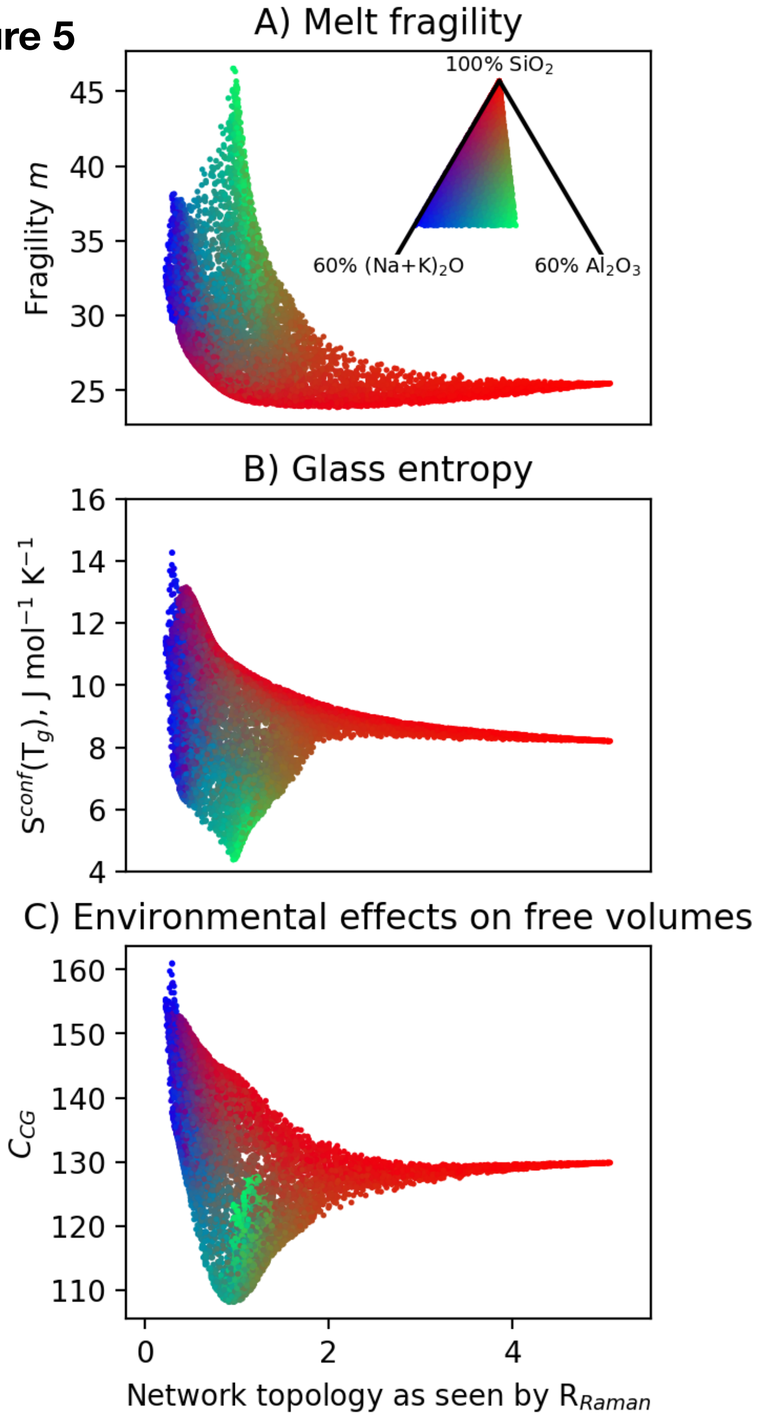
- A) the fragility (how fast melt mobility changes with temperature close to the glass transition) shows a complex mapping with the network topology parameter R_Raman

- B) same thing for the glass configurational entropy. It was proposed that it has two origins: a topological one and a chemical one. The second is due to the mixing of different ions in the glass structure. We see there that it clearly is non-negligible and varies in a complex way with composition

- C) the C_CG term of the free volume equation relates to the volumic and pressure effects on the molecular free volumes allowing viscous flow. As for entropy, we find a complex chemical mapping, indicating that the topology of the SiO2-Al2O3 network is not the main driver, but complex chemical interactions affect this parameter.

- Conclusion : the dynamic of melts is not only dependent of the SiO2-Al2O3 network mobility, but depends in a complex way of chemical effects. From previous studies, we know they are related to Si-Al mixing effects (should we add a figure about this? We can calculate this effect with the model… Maybe replace one subplot in figure 3?) and Na-K mixing (Figures 3C,D).

Figure 5



Conclusion

- The model allows observing the connections between measurable parameters from glasses (density, optical properties) and melts (viscosity) and latent variables (configurational entropy, viscosity at infinite temperature, etc.). With this, we clearly see that the static and dynamic properties of silicate melts and glasses depend on both the polyhedral network topology and complex cationic effects at play within this network.

- In particular, the model allows observing general links between different theories, like strong correlations between the C parameter of the free volume theory and the glass entropy, or between the T1 parameter of the VFT equation and the To parameter in the free volume theory. The first correlation indicates an underlying ground-truth entropic effect that controls the viscosity of silicate melts, and the second probably relates to the Kauzmann temperature.

- The informations brought by this work are thus unique in the sense that, in addition to linking static, dynamic and thermodynamic observables and latent variables, the model allows to envision the reality that controls the melt properties through its trans-theoretical nature.