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Structural Study of Mg-containing Silicate Glasses by Raman Spectroscopy, ^{29}Si MAS NMR and Molecular Dynamics

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Magnesium is a common transition element in silicate glasses (a few wt % in industrial and natural glasses) and its introduction in melts largely influences glass and melt properties. In crystalline systems, Mg^{2+} and Fe^{2+} often share the same sites leading to a broad range of solid solutions. For this reason, Mg^{2+} in glasses and melts is often considered as having a behaviour similar to Fe^{2+}.

In order to investigate the structural role of Mg^{2+} in glasses, we present in this study preliminary results on the structure of Mg-containing silicate glasses by Raman spectroscopy and ^{29}Si MAS NMR. In particular, effect of polymerisation and network modifier nature (Na^{+}, K^{+} and Ca^{2+}) are separately studied.

Experimental results are interpreted and compared to classical Molecular Dynamics simulations. A first approach of Mg^{2+} speciation in glasses is obtained by analysing the numerical models.