Institut de Minéralogie et de Physique des Milieux Condensés
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SÉMINAIRE
Vendredi 27 janvier, 11h

Salle de Conférence, 4ème étage, Tour 22-23, Salle 1
IMPMC, Université P. et M. Curie, 4, Place Jussieu, 75005 Paris

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Molecular dynamics modelling of non-network oxygens in MgO-SiO_2 glasses

Although Mg is not a major component of commercial silicate glasses, the role of Mg in silicate melts is important in mineralogy, and studies of magnesium silicate glasses are a key source of information. Experimental studies in the literature give differing views on Mg coordination, and on the presence of oxygen not bonded to Si, which we refer to as "non-network" oxygen. Results from our recent molecular dynamics modelling of MgO-SiO_2 glasses with two different sets of rigid ion potentials in meta- and ortho-silicate compositions will be presented [1]. This stimulates reflection on several issues such as the interpretation of previous NMR studies in the literature, the wider applicability of the bridging and non-bridging oxygen scheme for silicate structures, and the relationship between heterogeneity and phase separation.

[1] G. Mountjoy, B. M. Al-Hasni, and C. Storey (2011) J. Non-Cryst. Solids 357 2522 - "Structural organisation in oxide glasses from molecular dynamics modelling".

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