

Contribution of Molecular Dynamics simulations and *ab initio* calculations to the interpretation of Mg *K*-edge experimental XANES in silicate glasses

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In spite of its influence on the glass properties [1], the structural environment of magnesium in silicate glasses have been slightly investigated due to the difficulties to obtain relevant results. The Mg role is thus still poorly understood leading to controversial conclusions [2]. In this study, we have investigated the structural environment of Mg in a *K*-bearing silicate glass of composition $K_2MgSi_3O_8$ using X-ray absorption near edge structure (XANES) spectroscopy. The study of the Mg *K*-edge XANES spectrum has been performed with the help of first principle *ab initio* calculations based on the reciprocal-space non muffin-tin plane-wave method [3]. The XANES calculations have been performed starting from structural models that have been obtained by classical molecular dynamics [4] relaxed by *ab initio* force calculation using the PARATEC code. The plausibility of the models has been checked by Bond Valence calculations [5]. The comparison between the experimental and the calculated spectra enables us to conclude that Mg atoms are located in distorted tetrahedral sites. The site distortions are found to be correlated to the theoretical shift of the XANES edge position. Using the results obtained on the $K_2MgSi_3O_8$ glass combined to results obtained previously on crystalline materials [6], the Mg coordination number in magnesio-silicate glasses in X_2O -MgO- α SiO₂ systems (where X stands for Li, Na, K, Rb and Cs and where α is the number atom of silicon) can be estimated.

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