



# Application of molecular dynamics techniques and luminescent probes to the study of glass structure: the SiO<sub>2</sub>-GeO<sub>2</sub> case

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Auteur	Bernard, Christophe [1], Chaussedent, Stéphane [2], Monteil, André [3], Balu, Nathalie [4], Obriot, Jacques [5], Duverger, Claire [6], Ferrari, Maurizio [7], Bouazaoui, M [8], Kinowski, C [9], Turrell, S [10]
Editeur	Elsevier
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Résumé en anglais	<p>In this paper, we report on the results obtained from molecular dynamic simulation of a Eu<sup>3+</sup>-doped germanosilicate glass. This simulation provides further information on the structure. In particular it reveals a homogeneous distribution of SiO<sub>4</sub> and GeO<sub>4</sub> units, a decrease of defects compared to SiO<sub>2</sub> and GeO<sub>2</sub> glasses, and a trend to clustering of the doping ions. Using the modified crystal-field theory, the luminescence spectroscopic properties have been computed and comparison with experimental data has allowed a correlation of the spectral features with two main types of local environment depending on the coordination number and on the medium-range arrangement around the doping ions.</p>
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## Liens

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