

# Modeling of Rare Earth-doped Silicate Glasses: Codoping Effects on the Luminescent Sites Structures and Formation of Dielectrics Nanoparticles

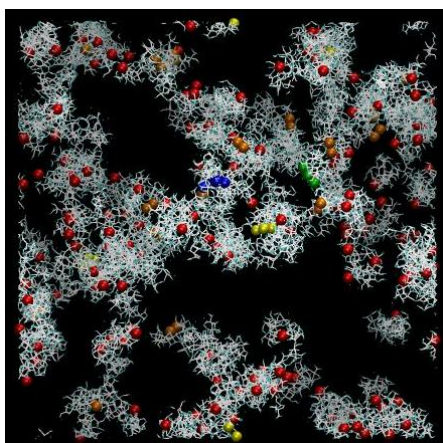
S. Chaussedent<sup>1\*</sup>, J. Turlier<sup>1</sup>, X. Bidault<sup>1</sup>, F. Ben Slimen<sup>1</sup>, N. Gaumer<sup>1</sup>, P. Raso<sup>1</sup>,  
D. Guichaoua<sup>1</sup>, W. Blanc<sup>2</sup>

<sup>1</sup> Université d'Angers, Laboratoire de Photonique d'Angers (LPhA – EA 4464), Angers, France

<sup>2</sup> Université Nice Sophia Antipolis, Laboratoire de Physique de la Matière Condensée (LPMC – UMR 7336), Nice, France

\*stephane.chaussedent@univ-angers.fr

Rare-earth (RE) containing glasses are known to be good candidate materials for devices such as optical fiber amplifiers, upconversion lasers and glass lasers. In such materials, strong changes in the luminescent properties can be induced by changes in the distribution and local environment of the RE ions. The investigation of the local structure around the RE ions in glasses is therefore a key issue to interpret their luminescent properties in terms of local structure.



Snapshot of a modeled structure: Er<sup>3+</sup>-doped nanoparticles of Mg-rich phase in a silica matrix.

ions but strongly modify the local structure of the luminescent ions. Another unexpected result is the striking difference between Al<sup>3+</sup> and P<sup>5+</sup> in the way they modify the first and the second coordination shell of RE<sup>3+</sup> [2][3].

Mg-codoping of a RE-doped silica glass is another route to tailor the spectroscopic features of optical fibers. Since it was experimentally evidenced that the RE ions can be embedded in nanoparticles (NP) formed *in situ* in silica through phase separation, we have developed an adaptive and transferable MD potential to model and track the formation of Mg-rich amorphous NP in a Si-rich matrix [4]. We present here our results on the dependence between the RE environment and the size of the containing NP.

Our group is for a long time involved in the study of these properties by means of an original approach which combines photoluminescence measurements and Molecular Dynamics (MD) modeling [1]. We use the Fluorescence Line Narrowing (FLN) as a site-selective technique to determine the different types of site occupied by the Eu<sup>3+</sup> ions. Structural information on these sites is deduced from FLN spectra and from the structures modeled by MD simulations. Using this methodology, we especially study the effective role of a codoping in the enhancement of the fluorescence of RE ions, which is commonly attributed to the ability of certain cations to avoid the RE clustering.

The presented work focuses on the comparison between Al<sup>3+</sup> and P<sup>5+</sup> codoping of a RE-doped silica glass. Surprisingly, both cations do not act to disperse significantly the clustered RE

- [1] S. Chaussedent, V. Teboul, A. Monteil, *Curr. Opin. Solid State Mater. Sci.* **7**, 111 (2003)
- [2] A. Monteil, S. Chaussedent, G. Alombert-Goget, N. Gaumer, J. Obriot, S.J.L. Ribeiro, Y. Messaddeq, A. Chiasera, M. Ferrari, *J. Non-Cryst. Solids* **348**, 44 (2004)
- [3] F. Ben Slimen, M. Haouari, H. Ben Ouada, D. Guichaoua, P. Raso, X. Bidault, J. Turlier, N. Gaumer, S. Chaussedent, *Opt. Mat.* (in press)
- [4] X. Bidault, S. Chaussedent, W. Blanc, *J. Chem. Phys.* **143**, 154501 (2015)