Post Doctoral Position:

Nano-structural investigation of Silica glasses combining MD simulations and hyper-Rayleigh and hyper-Raman scattering spectroscopies

**Envisaged Job Starting Date:** April 2012  *(duration: ≥12 months)*

**Application Deadline:** 15 September 2012

**Skills:** Quantum Chemistry, physical-chemistry in condensed phases, classical and quantum MD simulations.

**Scientific responsible:**
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**Country:** FRANCE

Subject

Non linear optical spectroscopies are powerful investigational techniques in the research field of new materials having specific optical properties. In this context, hyper-Rayleigh and hyper-Raman scattering are particularly well-adapted tools to investigate both structural and dynamical properties of macroscopically isotropic materials such as silica glasses at room temperature\(^1\,^2\).

We propose here a study aimed at assessing a further understanding of the harmonic light scattering processes taking place in silica glasses. Our methodology will be mainly based on theoretical approaches (at the nanometric spatial scale) combining both quantum chemistry calculations as well as numerical simulations well-adapted to investigate condensed media. Firstly, the elaboration of a sophisticated modelling associated with a distribution of elementary (short-ranged) structural scattering units (ESU) could be helping to interpret quantitatively the main observed harmonic scattered light signatures (quasi elastic and inelastic responses). For that, the development of theoretical procedures adapted for these kinds of systems for determining both structure and the non linear response (hyper-polarizability components) of the ESU will constitute likely a preliminary step of this work. Moreover, the results of these quantum chemistry calculations will be useful in the elaboration of interaction potentials including (hyper-) polarization effects for simulations (classical and quantum MD simulations) aimed at investigating in a second step the influence on the spectral features due to long-ranged interaction processes (beyond a first shell of neighbours) between a distribution of different environments. These models could be straightforwardly confronted with hyper-Rayleigh and hyper-Raman measurements.

This work is included in a network of collaborations involving both University of Bordeaux I the Aquitaine regional Council (project «*Laser Interaction and New Optical Functionality*» (LasInof) in the network « Advanced Materials in Aquitaine »). The subject is also strongly coupled to an international research program gathering chemists and physicists in France, Europe and USA.

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