

Contrat doctoral – ED Galilée

Titre du sujet : Gas phase structural analysis of microsolvated biomolecules

- Unité de recherche : Laboratoire de Physique des Lasers
- Discipline : Physique
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- Domaine de recherche : Physique moléculaire pour la biologie
- Mots clés : Action spectroscopy, mass spectrometry, laser desorption, molecular structure, microsolvation.

Context : The Biomolecules and Spectroscopy team performs structural studies of biomolecules, molecular complexes (biocaptors, vectorization) and small nanoaggregates (imaging, therapy) using gas phase physical chemistry technics. In addition to collaborative experiments performed on state-of-the-art devices (infrared multi photon dissociation with free electron lasers, ion mobility spectrometry), the team is currently developing an innovative gas phase ion source. This source, unique in France, is based on laser desorption of liquid microdroplets directly under vacuum. It allows to benefit from the numerous advantages of the gas phase (stoichiometric control, trapping and manipulation of ions, interrogation with different spectroscopic structural probes) while preserving biomolecules native structure.

Objectives : The candidate will perform the experimental investigation of the desorption phenomena induced by the interaction of an infrared laser pulse (tuned to water absorption band) with a liquid water microdroplet (50 μm diameter) under vacuum. Pulse energy and wavelength will be optimized to preserve hydrated biomolecules during their gas phase transfer. The desorbed species will be analyzed by infrared multiphoton dissociation spectroscopy coupled with time-of-flight mass spectrometry. Their structure will be determined by comparison with quantum chemistry calculations: exploration of the potential energy landscape at the force-field level, followed by geometry optimization and infrared spectrum calculation at the density functional theory level. The influence of solvation on the helicity of polypeptides and on the structure of small glycopeptides such as Tn antigens. Eventually, the quadrupole ion trap used for infrared action spectroscopy will be cryogenically cooled to obtain an improved spectral resolution which will open the way to structural studies of larger biomolecules.

Applicant skills : experimental liking and skills, strong background in general physics, basic knowledge in laser physics and in spectroscopy.

Group webpage : <https://bms.lpl.univ-paris13.fr/>