

## Contrat doctoral – ED Galilée

## Titre du sujet : Laser induced liquid bead desorption for biomolecular structure analysis

- > Unité de recherche : Laboratoire de Physique des Lasers
- > Discipline : Physique
- > Direction de thèse : Nicolas Nieuwjaer
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- > Domaine de recherche : physique moléculaire pour la biologie
- Mots clés : laser desorption, microdroplets, gas phase, mass spectrometry, IR spectroscopy, quadrupolar ion trap, molecular structure, biomolecules.

**Context :** The Biomolecules and Spectroscopy team performs structural studies of biomolecules, molecular complexes (biocaptors, vectorisation) and small nanoagregates (imaging, therapy) using gas phase physical chemistry technics. In addition to collaborative experiments performed on state-of-the-art devices<sup>1</sup> (infrared multi photon dissociation with free eleectron lasers, ion mobility spectrometry), the team is currently developping an innovative gas phase ion source. This source, unique in France, is based on laser desorption of liquid microdroplets directly under vacuum<sup>2</sup>. It allows to benefit from the numerous advantages of the gas phase (stoechiometric control, trapping and manipulation of ions, interrogation with different spectroscopic structural probes) while preserving biomolecules native structure<sup>3,4</sup>.

**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  $\mu$ m diameter) under vacuum. Underlying mechanisms are poorly undestood (supercritical phase transition, supersonic shock wave...) and the way energy is deposited into the microdroplet strongly influences the nature and quantity of desorbed species (biomolecules into the droplet). Pulse energy and wavelength effects will be studied using an optical parametric oscillator with a short bandwidth and allowing to get pulse energies higher than 10 mJ. The desorbed species are analysed by time-of-flight mass spectrometry. Once the desorption process characterized, the candidate will implement the coupling of the gas phase source with a quadrupole ion trap to perform structural studies of biomolecules by means of infrared spectroscopy. The structures of polypeptides and of water-amino acids complexes will be determined and compared with those obtained with an electrospray ionization source. Eventually, the quadrupole ion trap 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.



- <sup>1</sup> Nieuwjaer et al. J. Mol. Spec. 383 (2022) 111562.
- <sup>2</sup> Morgner et al. Aust. J. Chem 59 (2006) 109.
- <sup>3</sup> Peetz et al. J. Am. Soc. Mass Spectrom. 30 (2019) 181.
- <sup>4</sup> Hellwig et al. *Biochem. Soc. Trans.* 50 (2022) 1057.

