Laboratoire CIMAP
Centre de recherche sur les Ions, les Matériaux et la Photonique
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✓ Proposition de sujet de stage M2

Titre : ***Theoretical study of isolated and solvated peptides***	
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Missions

In the last 20 years, there has been a growing interest for mass spectrometry as a powerful tool to unravel the structure of isolated molecular systems. This way, one may further perform experiment on molecular systems by storing and irradiating them in an ion trap by means of synchrotron radiation in the VUV and soft X-ray ranges. VUV and soft X-ray action spectroscopy techniques are powerful methods to investigate the electronic and some aspects of the geometric structure of biomolecules.

In her thesis,Juliette LEROUX (PhD from CIMAP), combines both action spectroscopy and structural approaches to study radiation-induced processes in biomolecular systems (peptides and proteins). In particular, she demonstrated that the NEXAMS (near-edge X-ray absorption mass spectrometry) technique is sensitive to backbone protonation by studying protonated triglycine at the nitrogen and oxygen K-edge [1]. She will later study the influence of a controlled number of water molecules on radiation-induced processes in peptides and proteins.

Project:

The master student will study theoretically small model peptides like triglycine in the (de)protonated form. First, the student will have to generate different isomers for the isolated and hydrated peptide (1 to 5 and 10 water molecules). This exploration of potential energy surface (PES) will be done using a program based on the Molecular Dynamics where the energy will be described with the AMBER force field [2]. In a second step, the student will have to reoptimize these geometries with DFT-B3LYP calculations. For the lowest-energy isomers the student will calculate infrared and X-ray spectra to analyze the role of the water environment. These calculations will be done with the ORCA program [3].

[1] J. Leroux et al., Physical Chemistry Chemical Physics, 25, 37, 25 603–25 618, (2023)
[2] J. Wang et al., J Comput Chem 21, 1049 (2000).
[3] F. Neese et al., J Chem.Phys., (2020), 152, 224108.