

Direct Molecular Modelling of Electrospray Processes in Mass Spectrometry (ESI-MS)

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Laboratory

Laboratoire Analyse et Modelisation pour la Biologie et l'Environnement

UMR8587

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Subjects / Tools-Methodologies

1 : charged nano-droplets / Molecular Dynamics simulations

2 : modeling evaporation of biomolecular edifices / Monte Carlo simulations

3 : mesoscopic models / develop mesoscopic interaction models

Summary of lab's interests

Laboratory acronym : LAMBE (Laboratoire Analyse et Modelisation pour la Biologie et l'Environnement) Our laboratory is nationally recognized as a specialist of Mass Spectrometry experiments, in particular with the development of new methods. The lab has especially developed recent investigations on proteomics. The Theoretical Modeling Group of the lab headed by Prof. MP Gageot has the aim of bringing the methods of theoretical computation in Physics and Chemistry for a precise understanding and interpretation of the experiments performed in the lab. In particular, we have recently launched a research program on the modeling of ElectroSpray Ionisation processes as they occur in Mass Spectrometry experiments of biomolecules. The PhD subject proposed here is related to this research program.

Summary of project

The goal of the proposed PhD research is to theoretically characterise the evaporation mechanisms that take place during Electrospray (ESI) processes in Mass Spectrometry. The ESI technique consists in forming charged droplets, from which solvent molecules gradually evaporate, eventually producing charged solutes in the gas phase. Evaporation mechanisms and their consequences on properties of the molecules that are formed in the gas phase are still not well understood. The PhD research will tackle this problem in a detailed and systematic way. To that end, Monte Carlo (MC) and molecular dynamics (MD) simulations of charged clusters composed of classical mesoscopic particles will be developed. Structures of charged clusters, and their thermodynamic and kinetic properties will be characterised, with a special emphasis on the interplay between thermodynamics and kinetics. Our main focus will be on the study of ESI processes on non-covalent biomolecular structures such as DNA-DNA and DNA-protein complexes, or multi-domain proteins. Mesoscopic interaction models of such systems will therefore be developed. Related codes are under development in the group in collaboration with Dr Mark Miller from the University of Cambridge, UK. The PhD student will participate in all these developments. The general project has been granted by PHC Alliance France-UK (2009-10), with a collaboration between the LAMBE in Paris (Prof. MP Gageot) and the Chemistry Department of Cambridge-UK (Dr. M. Miller).