

PhD Thesis on Theoretical Physical Chemistry

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

This thesis is aimed at modelling and understanding the electrospray technique at an atomistic level. This work is part of a global laboratory project devoted to theoretically describe electrospray/mass spectrometry experiments (ESI/MS). Electrospray - daily used in experiments performed in our laboratory to produce ions in the gas phase which are subsequently analysed by mass spectrometry - is supposed to produce ions in a "soft way". This technique is thought to preserve the ion liquid phase structure, after evaporation of all the water molecules. Many experiments show that this is not true, though. The thesis proposed here will try to answer the following question: during the electrospray process, are liquid phase structures preserved in the gas phase (where they are characterised by mass spectrometry) ?

To understand the mechanism producing ions in the gas phase from a system initiated in an aqueous medium, we will set up molecular dynamics simulations using a classical description of interactions between the different particles (quantum chemistry calculations will help in the parameterisation procedure) and Newton dynamics (including dissipation). At this end, the laboratory has a home made molecular dynamics code (MDVRY). In the dynamics algorithm, electric field and pressure gradient effects will be added. Also ab initio molecular dynamics will be performed as reference for classical simulations.

During the thesis, the PhD student will gain skills in different domains of molecular modelling: quantum chemistry, ab initio and classical molecular dynamics simulations and force field development. Furthermore, he/she will be involved in developing our MDVRY molecular dynamics code, such that he/she will also gain skills in scientific programming.

The thesis will be held in France near Paris (about 40' from downtown by city train) in a laboratory with researchers from CEA (Saclay), CNRS and University (Evry). Part of the project could be done in collaboration with F.Calvo (LASIM, Lyon), P.-A.Hervieux (IPCMS, Strasbourg), R.Vuilleumier (LPTMC, Paris) and F.Martin (Universidad Autonoma De Madrid). The supervisors are specialists in atomistic modelling and theoretical physical-chemistry. A master in chemistry or physics is required.

The thesis is founded by CEA and the gross montly salary will be around 1990 euro during the first two years and 2050 euro the third year.

Applications should be done as quickly as possible and the thesis will begin in september/october 2008.

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