

INTERNSHIP PROPOSAL

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Internship location: Sorbonne Université

Thesis possibility after internship: YES

Funding: YES/NO

If YES, which type of funding:

Probing the mesoscale dynamics of polyelectrolytes solutions by NMR relaxation: From fundamentals to applications

Polymers exhibit a wide range of behaviors for their dynamics depending on the scale of observation. Lot of efforts has been devoted to this study of several time- and length scales. A particularly suited technique to address this question is NMR relaxation dispersion since probing the dependence of NMR relaxation with Larmor frequency gives access to the molecular dynamics on the corresponding time scale. With specific instruments and methods at least three orders of magnitude can be probed and with the interplay of temperature all the polymer dynamical behaviors can be captured [1,2].

However so far little has been done with this method to study the behavior of charged polymers, polyelectrolytes, yet they are ubiquitous systems in biological, food or environmental applications, to say the least. Protein and DNA are polyelectrolytes, whose change of conformation can lead from health to illness. Naturally, food is made of a huge variety of biological macromolecules either in the raw state or transformed and raises similar fundamental questions about the multiscale dynamics of these compounds and their interaction with water. Similarly, the products of the degradation of organic matter in soils, humic substances, have a great impact on the storage and the transport of pollutants or nutrients. These three examples demonstrate the important to address the question of the dynamics of both the polyelectrolyte and the solvent at different scales.

We propose here to apply a panel of NMR relaxation methods to investigate changes in polyelectrolyte solutions. We have recently used this approach successfully to understand multiscale water dynamics in the vicinity of proteins [3] or the change of ion transport mechanisms in ionic liquids [4], and how the introduction of a supplementary species, ions in those cases, greatly modify either the approach of solvent molecules to macromolecules or the structure of the liquids.

For polyelectrolyte solutions, preliminary results obtained in the framework of an international collaboration are promising and show a significant change of the relaxation with the modification of the charge with pH or its screening with salt.

The first aim of this project is to assess this phenomenon on a simple system in order to identify the governing parameters for a relevant modeling. The influence of possible proton exchange between water and polyelectrolyte on the dynamics of water at the local (< nm), intermediate (nm- μ m) and larger scale (> μ m).

Later, the behavior of polyelectrolyte will be examined in a context closer to the applications for example gel formation of food or bio-based polyelectrolytes or the adsorption of polyelectrolyte on mineral particles.

Beyond the relaxation properties, the versatility of NMR techniques to study the solvent, guest species such as ions or the polyelectrolyte chain thanks to its isotopic and spectroscopic resolutions make it possible to acquire a complete understanding of the system.

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: YES Soft Matter and Biological Physics: YES

Quantum Physics: NO

Theoretical Physics: NO