INTERNSHIP PROPOSAL

(One page maximum)

Laboratory name: Physicochimie des Électrolytes et Nanosystèmes interfaciaux (PHENIX)
CNRS identification code: UMR 8234
Internship director'surname: MÉRIGUET
e-mail: guillaume.meriguet@sorbonne-universite.fr Phone number: +33 1 44 27 31 09
Web page: https://phenix.cnrs.fr/annuaire-user/?uid=guillaume-meriguet
Internship location: Lab. PHENIX – Sorbonne University – 75005 PARIS
Thesis possibility after internship: YES
Funding: YES

Colloidal suspensions: study of solvent dynamics using a combination of NMR and molecular dynamics

Interactions between dispersed colloidal objects, for example between nanoparticles, polymers, and/or ions, modify the dynamic properties of all species in the mixture. In particular, it has been established that the dynamics of the solvent, most often water, are altered when one species adsorbs onto another. Thus, the dynamics of the solvent can indirectly provide information about this adsorption. The study of NMR relaxation of water has even been successfully proposed as a method for studying this phenomenon [1,2].

This method has recently seen a resurgence of interest because rapid, easy-to-implement measurements allow for non-invasive evaluation of drug stability for example [3-5]. Nevertheless, the mechanism behind the modification of water dynamics remains poorly understood and is the subject of this research project, which combines two complementary methods, experimental, nuclear magnetic resonance (NMR), and theoretical, molecular dynamics (MD).

To control the interactions and behavior of the colloidal suspension, the chosen study system is developed and characterized in parallel within the research team. These are mixtures based on polyhedral oligomeric siloxanes (POSS) and polyelectrolytes. POSS are small molecular colloids (~1 nm) whose pendant groups can be easily modified to adjust interactions. The relatively small size of POSS allows them to be studied using molecular dynamics.

This internship will involve conducting a simultaneous analysis of the dynamic properties of water using experimental NMR methods (diffusion and relaxation) and modeling them using molecular dynamics (MD). The properties measurable by these NMR methods are related to correlation functions that can be calculated by molecular dynamics [6]. While the focus is on the properties of the solvent, both NMR and MD provide information on the behavior of other species, which will help to understand the microscopic mechanisms
involved.

First, the approach and methods will be adjusted for suspensions of POSS alone, with varying types of functionalization and concentrations, before being deployed on more complex systems also involving polyelectrolytes.

References

[1] Van der Beek et al.*Langmuir* 7, 327-334 (1991) 10.1021/la00050a022
[2] Cooper et al. *Soft Matter* 9, 7211-7228 (2013) 10.1039/C3SM51067K
[3] Feng, et al. *Chem. Commun.* 51, 6804-6807 (2015) 10.1039/C5CC00741K
[4] Taraban et al. *Pharm. Res.* 42, 987–1001 (2025). 10.1007/s11095-025-03880-w
[5] Janc et al. *Phys. Chem. Chem. Phys.* 20, 30340-30350 (2018) 10.1039/C8CP06061D
[6] Hostnik et al. *Macromolecules* 53, 1119-1128 (2020) 10.1021/acs.macromol.9b02161

Specific techniques or methods

- Dynamic nuclear magnetic resonance methods (diffusion, relaxation)
- Molecular dynamics (LAMMPS code)

Internship period: February – July 2026

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