MASTER DE CHIMIE DE PARIS CENTRE - M2S2
Proposition de stage 2017-2018
Internship Proposal 2017-2018

Spécialité(s) / *Specialty(ies) :*

X Chimie Analytique, Physique, et Théorique / *Analytical, Physical and Theoretical Chemistry* :
□ Chimie Moléculaire / *Molecular Chemistry* :
□ Matériaux / *Materials:*
□ Ingénierie Chimique / *Chemical Engineering:*

Laboratoire d'accueil / *Host Institution*

Intitulés / *Name* : PHENIX UMR 8234
Adresse / *Address* : Campus Jussieu Couloirs 42-43 étages 2&3, 32-42 étages 2&3
Directeur / *Director (legal representative) :* Pierre Levitz
Tél / *Tel* : 01 44 27 31 66
E-mail : pierre.levitz@upmc.fr

Equipe d'accueil / *Hosting Team :*

Adresse / *Address :* Campus Jussieu, couloir 42-43 2ème étage
Responsable équipe / *Team leader* : Marie Jardat
Site Web / *Web site :* www. phenix.cnrs.fr
Responsable du stage (encadrant) / *Direct Supervisor :* Marie Jardat & Vincent Dahirel
Fonction / *Position :* Professeur (M. J.) et Maître de Conférences (V.D.)
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Période de stage / *Internship period* * : 1er février - 1er juillet

Sujet / Title Numerical Simulations of polyelectrolytes dynamics

Projet scientifique (1 page maximum) / *Scientific Project (maximum 1 page):*

1. Projet / *Project*

Polyelectrolytes (polymers whose repeating units bear a charge) have applications in many industrial fields including water treatment or oil recovery, and are essential elements of biological media. They turn out to have a very rich and complex behaviour in particular from the dynamical point of view, which is much less investigated than structural properties. In PHENIX laboratory, we seek to determine, understand and predict the behavior of colloidal and porous systems from short (picosecond) to large (hour) time scales, by using a unique combination of experimental and theoretical tools.

This internship deals with the modeling of the dynamical properties of polyelectrolytes in water. The aim of this theoretical work is to build simplified but realistic models of polyelectrolytes, namely coarse-grained models, whose dynamic properties in various conditions will be studied by numerical simulations. The first system which will be investigated is the sodium polyacrylate. Some numerical simulations of this polyelectrolyte in water have been carried out at the atomic scale. Experimental determinations of the diffusion coefficient of the center of mass of the polyelectrolyte for several chain lengths have also been conducted in the team. The goal of the internship is to derive effective coarse-

* 5 mois à partir du 22 janv 2018 / *5 months not earlier than January, 22nd 2018.*

grained models of the polyelectrolyte chain which account for its dynamical properties. Numerical simulations based on a simplified description of the solvent (Multiparticle Collision Dynamics) wilwill be used to compute the dynamic properties of the chain at the mesoscopic scale. A close collaboration with experimentalists working on the same kind of systems in the lab will enable to assess the relevance of the models.

2. Techniques ou méthodes utilisées / *Specific techniques or methods*

This internship consists in a theoretical work based on numerical simulations. Several simulation methods will be handled (molecular dynamics at the atomic scale, Multiparticle Collision Dynamics at the mesoscopic scale).

3. Références / *References*

[1] Caterina Dolce, Guillaume Mériguet. Ionization of short weak polyelectrolytes: when size matters. *Colloid and Polymer Science*, Springer Verlag, 2016, 〈10.1007/s00396-016-4000-x〉.
[2] M. Jardat, V. Dahirel, F. Carnal, Dynamics of ions in model charged porous media : Influence of polyelectrolytes, J. Mol. Liq. (2016), http ://dx.doi.org/10.1016/j.molliq.2016.10.054.
[3] V. Dahirel, X. Zhao and M. Jardat, Comparison of different coupling schemes between counterions and charged nanoparticles in multiparticle collision dynamics, Phys. Rev. E 94, 023317 (2016)