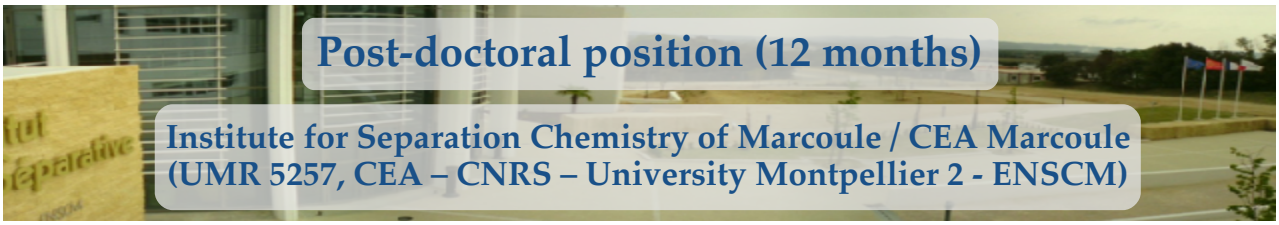


Post-doctoral position (12 months)

Institute for Separation Chemistry of Marcoule / CEA Marcoule
(UMR 5257, CEA – CNRS – University Montpellier 2 - ENSCM)

ORGANIC PHASES MODELLING FOR THE LIQUID – LIQUID EXTRACTION: A MOLECULAR APPROACH

Description

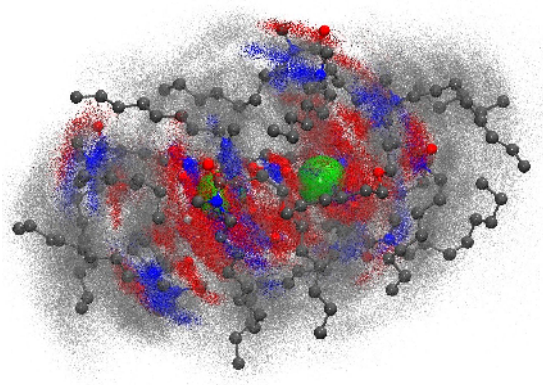
This post-doctoral researcher position will take place in the Mesoscopic Modelling and Theoretical Chemistry Group (LMCT) of the Institute for Separation Chemistry in Marcoule (ICSM), in collaboration with the teams of the French Atomic Energy Commission (CEA / RadioChemistry & Processes Department) of Marcoule. ICSM is a mixed unit composed of CEA, French National Center for Scientific Research (CNRS), University Montpellier 2 , and ENSCM. Both laboratories (LMCT and DRCP) are located in the research site of Marcoule (south-east of France, near Avignon).

The separation of metallic ions, such as lanthanides, is a crucial step for the recycling, and especially for the treatment of the spend nuclear fuel. CEA Marcoule is a prominent player in researches in this field, from fundamental studies to their implementations in the industrial processes. The Institute for the Separation Chemistry is an international institute involved in the research and development of new separation processes for energy, and sustainable development.

Institute for Separation Chemistry of Marcoule

Context

Separation processes performed for **recycling of heavy metals** commonly use **liquid-liquid extraction** for which ions are selectively transferred from an aqueous to an organised organic phase. Modelling such processes remains quite difficult since many phenomena occur: complexation, solvation, electrostatic interactions, polarisation forces, *etc.* Furthermore, these interactions occur at different length sizes.



Snapshot issued from molecular dynamics simulations representing a supramolecular aggregate.

Recently, experiments and simulations pointed out the presence of **supramolecular aggregates,** similar to reverse micelles, and having characteristic sizes of several nanometers. This suggests that the extraction process may be complex since it relies on the **selective formation** of such compounds. In each aggregate, a polar core is surrounded by a more or less stretched interface composed of extractant molecules.

Therefore, modelling such processes makes necessary the calculation of the **aggregates free energies**. An important term to consider is the free energy of the carbon chains which impose the spontaneous and stretched curvature of the surfactant film. However, a lack remains concerning its role, as well as its intensity.

Project

We propose to determine the carbon chains free energy in small molecular aggregates with small ions in organic phase by means of **molecular dynamics simulations.** This project aims at **proposing a model aggregate** for which the size of the polar core will change.

Using a method based on **thermodynamics integration**, the free energy will be calculated. Simulations in implicit and explicit solvent will be performed. The most stable conformation will be deduced, as well as the free energy cost needed to deform the aggregates. Then, it will be possible to compare the results obtained using such approach with mesoscopic theories based on phenomenological packing parameters or based on the concepts of Gaussian curvatures, *e.g.* the Helfrich free energy model. The role of the chain lengths and sizes will be studied. Such theoretical modelling already exists in literature since 20 years for detergents and lipids. However, it has never been used for extractant molecules. These results are the base of the detergent formulation and the membrane transport. In our case, the results will be used to **model the transfer of ions through phases**.

A new expression for the carbon chain energy term in extraction process will be proposed. The prediction of the global phenomenon will done using different approaches:

- ✔ from a **mesoscopic theory** where the results obtained at the molecular scale will be used,
- ✔ from **molecular modelling**, taking into account explicitly the polar core, for which this work will be a first needed step.

Beyond the publications, the calculation codes developed during the post-doc will be integrated to the simulation platform dedicated to the modelling of the liquid – liquid extraction process by evaluating the **transfer energies through phases at the mesoscopic scale**.

Practical information

Salary

The post-doctoral researcher will be employed by CEA for 12 months (extensible), with a salary of about 2100 € (ref. 2012)

Candidate profile

Ph.D. In Chemistry, Chemical Physics, Physics

Contacts

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LMCT on the web: http://www.icsm.fr/icsm_engl/lmct_en.html

Do not hesitate to contact them for further information.

Collaboration

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