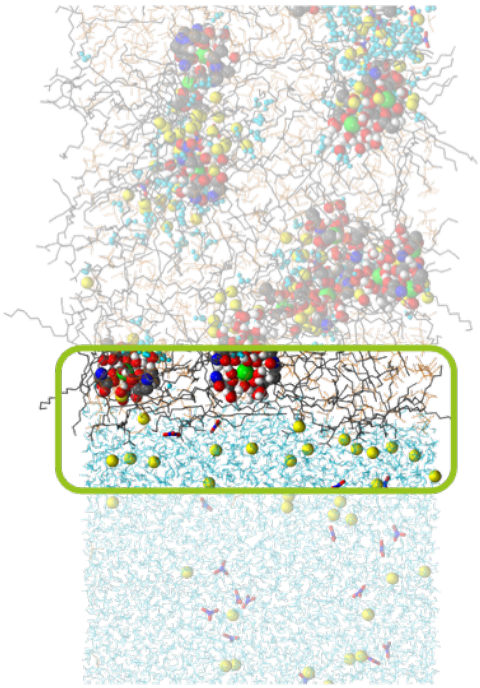
Internship proposal M2 2021-2022 at
Institut de Chimie Séparative de Marcoule (ICSM), Bagnols-sur-Cèze, France

Simulation of ion adsorption at the liquid/liquid interfaces

This project may be a preliminar internship before a 3-years PhD



The proposed internship aims at **describing and understanding the extraction mechanisms** occurring at the **liquid/liquid interfaces** and more particularly the water/oil interfaces such as those involved in the separation chemistry. The recycling of metals is commonly done by **liquid-liquid extraction** where various ionic metal compounds are selectively transferred from an aqueous phase to an organic phase. The last few years have seen the development of new molecular modeling methods that allow describing more precisely these complex systems[1,2]. The speciation in the aqueous phase and the supramolecular organization in the organic phases have been especially characterized. Simulations of the adsorption and the ion transfer at the interfaces, and the corresponding kinetics, remain a difficult task due to the complexity and time scale at which the process takes place[3]. The aim of this project is to **model** these **transfer properties** using a theoretical approach based on **molecular dynamics simulations** in an attempt of understanding the transfer mechanisms and predicting the transfer properties of the ions.

During this internship, we will study the **adsorption of ions at interfaces** by molecular dynamics simulations. We will be able to verify whether this simulation method allows to spontaneously observe the adsorption and transfer of ions, and to understand how the interface is organized and modified according to the presence of ions. Different surfactant molecules (monoamides, diamides, etc.) can be used to observe the influence of the nature of the molecule on these properties. We will also be able to observe how the presence of ions in the aqueous phase (lanthanides and/or uranyl) modifies these properties. These theoretical approaches at the **molecular scale** will be implemented while keeping a **link with the experiments** carried out these last years at the ICSM to characterize the interfaces (surface tension, neutron and X-ray reflectivity, SHG...).

This project of fundamental importance and using innovative methods may lead to publications in scientific international journals.

Profile: You are a student in your third year of engineering school or in master 2, you are rigorous and have solid theoretical knowledge in in chemistry-physics. You have a strong interest in programming and computer science, and ideally you already have a basic knowledge of code (Python, Fortran, … languages, Linux environment, Shell scripts ...). You also have good written and oral communication skills. You have the ability to work in a team while having the necessary autonomy to carry out your own research topic.

Further information: The successful candidate will join the LMCT group of ICSM.

Contact: To apply, please send a cover letter, a detailed CV, and references to Dr. Magali Duvail (magali.duvail@cea.fr) and Dr. Philippe Guilbaud (philippe.guilbaud@cea.fr).

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[1] M. Duvail et al., Soft Matter 13, 5518–5526 (2017). DOI: 10.1039/C7SM00733G
[2] M. Vatin et al., J. Phys. Chem. B 125, 3409–3418 (2021). DOI: 10.1021/acs.jpcb.0c10865
[3] M. F. Ruiz-Lopez et al., Nature Reviews Chemistry 4, 459–475 (2020). DOI: 10.1038/s41570-020-0203-2