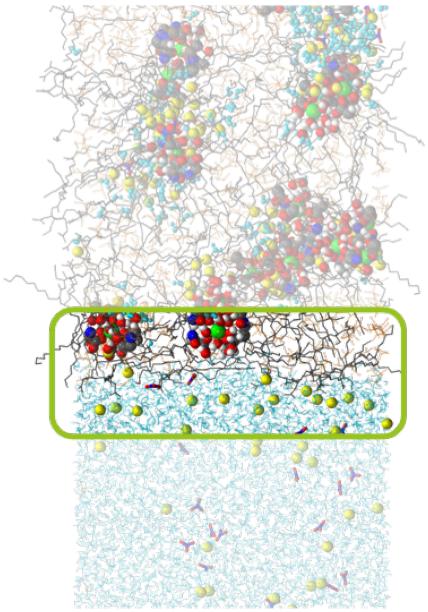
Open PhD thesis at
Institut de Chimie Séparative de Marcoule (ICSM), Bagnols-sur-Cèze, France
Ecole doctorale 459 Sciences Chimiques Balard (Université de Montpellier)

Simulation of the equilibrium and the transport of ions at the liquid – liquid interfaces

Starting date: October 2022



The proposed Ph.D. thesis 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 thanks to the presence of amphiphilic extractant molecules. 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. Simulation of the adsorption and the ion transfer at the interfaces, and the corresponding kinetics remains a difficult task due to the complexity and time scale at which the process takes place[3]. The aim of this thesis 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.

Theoretical approaches at the **molecular scale** will be implemented, with a strong **link with the experiments** conducted these last years at ICSM (surface tension, neutron and x-ray reflectivity, SHG, …).

Two numerical approaches will be proposed during the thesis:

1. **Study of the adsorption of ions at interfaces by molecular dynamics simulations** in order to understand how the interface is organized and modified according to the presence of ions.
2. **Biased molecular dynamics simulations** to assess the energy landscape of the **ion transfer** and to understand the differences of efficiency of various extracting molecules.

The theoretical and numerical methods developed during the thesis can be adapted and transferred to other industrial applications involving liquid – liquid interfaces. During the thesis, the Ph.D. student will be led to disseminate his/her scientific results through publications in scientific journals and communications in national and international conferences.

Profile: We are looking for a highly motivated Ph.D. student with a solid theoretical knowledge in physical-chemistry. You have a Master degree in chemistry, physical-chemistry, chemical-physics, theoretical chemistry or physics, or equivalent. 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.

Secured funding: The Ph.D thesis is funded by French Alternative Energies and Atomic Energy Commission (CEA).

Further information: The successful candidate will join the LMCT group of ICSM and will be register at the doctoral school ED459 Sciences Chimiques Balard of the University of Montpellier (France).

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) before May 6th 2022.

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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