

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 ion transfer at liquid/liquid interfaces

Starting date: October 2021

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. The last few years have seen the development of new molecular modeling methods that allow describing more precisely these complex systems. 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 (M. F. Ruiz-Lopez et al., Nature Reviews Chemistry 4, 459–475 (2020)). 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 (L2IA).

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 in 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.

<u>Skills:</u> Master degree (or equivalent) with a recognized knowledge in chemistry-physics. Programming skills are a plus (Fortran, python...).

Funding: The Ph.D thesis is funded by CEA DES (Direction des EnergieS).

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.

<u>Contact:</u> To apply, please send a cover letter, a detailed CV, and references to Dr. Magali Duvail (<u>magali.duvail@cea.fr</u>) and Dr. Philippe Guilbaud (<u>philippe.guilbaud@cea.fr</u>) before April 19th 2021.

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http://www.icsm.fr/icsm_engl/Imct_en.html