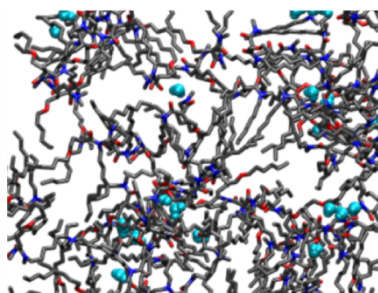


Open PhD position

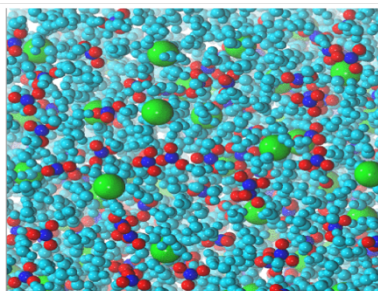
Institut de Chimie Séparative de Marcoule (ICSM), Bagnols-sur-Cèze, France
 Ecole doctorale 459 Sciences Chimiques Balard (Université de Montpellier)

Molecular prediction of ion transfer for extraction

Starting date: October 2022



Organic phase



Aqueous phase

Liquid/liquid extraction is the experimental method of choice for the recycling of metallic elements. Molecular simulation of this technique remains a novel challenge due in particular to the different scales and systems (aqueous and organic) involved. This thesis aims at **predicting for the first time this method** by calculating the **free enthalpies of ion transfer** from one phase to another. This quantity quantifies the efficiency and the selectivity of the process.

In this context, **two systems will be simulated**, one **aqueous** and the other **organic** with different solutes. Two advanced simulation methods will be used:

- the first one will be based on Jarzynski equality,
- the second one will use a "replica exchange" procedure.

It will be possible to couple thermodynamically the two phases and to **calculate the difference of free enthalpy** during a transfer and thus to predict it. The result will be directly related to the partition coefficients and selectivity measured experimentally. The effects of the concentration of the extractant, which is the molecule allowing the transfer, will be explicitly predicted.

The system studied here will be the extraction of rare earths by diamides. This atomic modeling aims to change the era of molecular modeling, since we will finally simulate directly the phase transfer, the ultimate goal being to arrive at predictive codes of the extraction.

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 Physics or Chemistry, engineering school, ENS. You 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.

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 Pr. Jean-François Dufrêche (jean-francois.dufreche@icsm.fr) and Dr. Magali Duvail (magali.duvail@cea.fr).

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