Microemulsion model: en route to prediction of solvent extraction

(ANR MULTISEPAR ANR18-CE29-0010)

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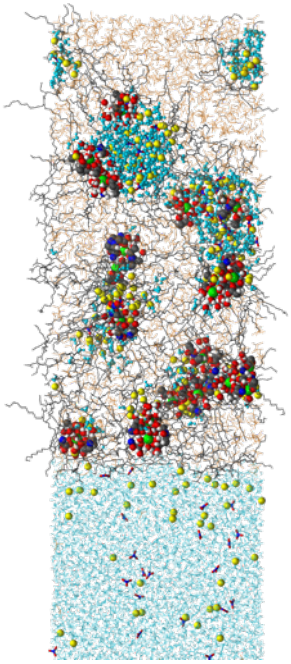
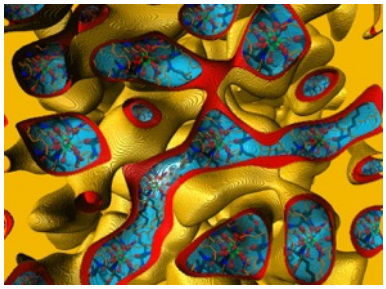
The proposed Ph.D. thesis aims at understanding the **separation methods** of rare earth metals commonly used in hydrometallurgy and recycling using a **multiscale approach** based on **molecular** and **mesoscopic modelling** techniques.

We will focus on **liquid/liquid extraction**: this method separates metals by performing a selective extraction of ions from an aqueous phase to an organized solvent phase. It is especially important for the ore treatment and for recycling of materials. Because of the cost, it is mainly used for relatively high value metals (such as strategic metals, rare earths, actinides (for nuclear waste treatments), etc....). Despite the importance of this separation technique the underlying **microscopic mechanism is still poorly understood**. The transfer of ions into an organic phase is possible thanks to the presence of extracting molecules (usually amphiphilic molecules), but the related exact mechanisms are mostly unknown. Typically, the organic phase exhibits a **supramolecular organization** [M. Spadina et al. **ACS Nano** *13*, 13745 (2019)]: aggregates of ions and water molecules surrounded by the extractant are obtained both from experiments and theoretical predictions, but the role of the various forces (complexation, solvation, electrostatic forces polarization) is not understood.



MD simulation of liquid-liquid extraction

The aim of this thesis project is to **derive mesoscopic models** in order to bridge the gap between molecular simulations and chemical engineering. This Ph.D. thesis will be mainly focused on **microemulsion theory** for characterizing the organic phase. We recently proved that this framework, in accordance with molecular dynamics, is a very good candidate for the description of liquid extraction [M. Duvail et al. **Soft Matter** *13*, 5518–5526 (2017)]. In that case, we will identify polar and organic phases of the system and see whether it can be described in terms of Helfrich Hamiltonian, by comparing the molecular dynamics simulations with Monte-Carlo simulations of microemulsions based on a two level-cuts Gaussian Random Field (GRF) model.



Monte-Carlo modelling of a microemulsion

The systems will be characterized in terms of **interface parameters**: bending constant, Gaussian rigidity, spontaneous curvatures. The role of the ions will be estimated by determining how they influence these effective parameters, and especially how they modify the aggregation or ordering process (since they change the physical-chemistry of the interface). More precisely, the Gibbs energy of the system will be typically considered as the sum of several terms, i.e., adsorption, bulk, complexation and a microemulsion term calculated from the GRF model. This latter term will be derived from the molecular dynamics simulations.

In addition, **intensive molecular dynamics simulations** will be performed with various extractants and ion concentrations. The result will be analyzed in terms of colloidal science.

In a context of separation chemistry in an attempt of recycling strategic metals and in connection with the research area developed in the Mesoscopic Modelling and Theoretical Chemistry Laboratory of the Institute for Separation Chemistry in Marcoule, the Ph.D. thesis will focus on organic solvent extraction phases whose aggregates are composed of lanthanide salts in the presence of diamide extractant molecules. The **theoretical and numerical methods** developed during the Ph.D. thesis could be **adapted and transferred** to other industrial applications for which solvent extraction is relevant.

Candidate profile: The candidate must have a Master 2 or an engineering degree with a recognized knowledge of physical chemistry.

How to apply: Interested candidates should email their CV and a (short) application letter to:

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