Undergraduated training (24 weeks)

1. Subject details

Title Modelling of the water/oil interface for the strategic metals extraction: a molecular approach

Keywords Molecular modelling, Liquid-liquid extraction, Microemulsion, Heavy metals

Abstract Element selective separation processes used for the recycling of strategic metals (lanthanides, actinides, *etc.*) rely on the liquid-liquid extraction principles. During this process, ions are selectively extracted from an aqueous phase to an organized organic phase. This is possible thanks to the presence of tensioactive molecules (surfactant molecule composed of a polar hydrophilic head, and an apolar hydrophobic tail) which are localised at the water/oil phase. Hence, a good understanding of the phenomena occuring in the aqueous phase, as well as in the organic phase is crucial to improve such process. Although, this last decade, many theoretical studies have been performed at the molecular scale to provide realistic pictures of aqueous solutions, a lack remains concerning the thermodynamics properties of ions in organic solutions and at the water/oil interface.

In this context, we offer a training position in molecular modelling. This training aims at determining the thermodynamics properties of ions at the water/oil/surfactant interface by using molecular modelling methods (molecular dynamics).

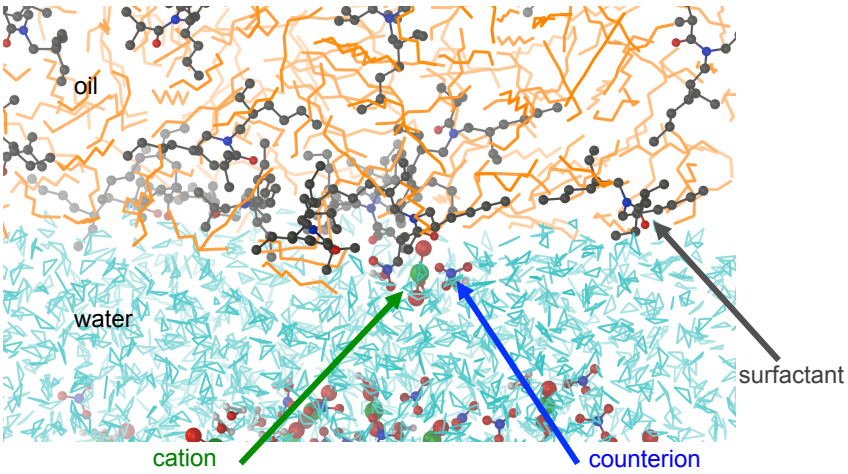

Figure 1: Snapshot of a molecular dynamics simulation box describing the water/oil interface with surfactant molecules, cations, and counterions.

First, we will focus on the elastic properties of the surfactant film (rigidity, curvature) that is localised at the water/oil interface. Different surfactant molecules (monoamides, diamides, *etc.*) could be simulated in order to observe the influence of the molecule's nature. Later, we may also observe how the presence of ions (lanthanides and/or uranyl) in the aqueous phase modify the surfactant film elastic and structural properties (hydration – dehydration of the polar heads of the surfactant molecule).

Modelling such systems at the molecular scale will improve our knowledge of the phenomena occuring during the liquid-liquid extraction process. At the end, this study will be used to better understand these systems (water/oil/surfactant) at the mesoscopic scale (several nanometers) already performed in the group. This training will be performed in collaboration with Dr. Philippe Guilbaud (CEA Marcoule / RadioChemistry & Processes Department).

This study, having a crucial importance, and using innovative methods may lead to publications in international scientist journals. This training may be also followed by a Ph.D. thesis funded by CEA.

2. Supervising details

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3. Training details

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4. Training benefits

Training salary	About 650 euros per month
Accomodation	About 200 euros per month

5. Additional comments

This training may be followed by a Ph.D. thesis funded by CEA.