Understanding interface formation and extractant distribution at the liquid-liquid interface

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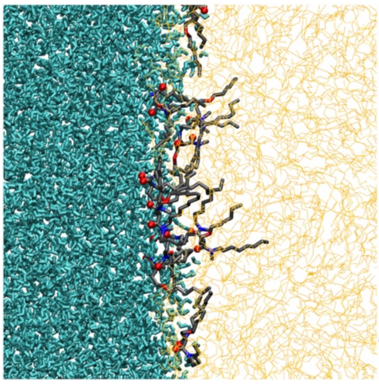

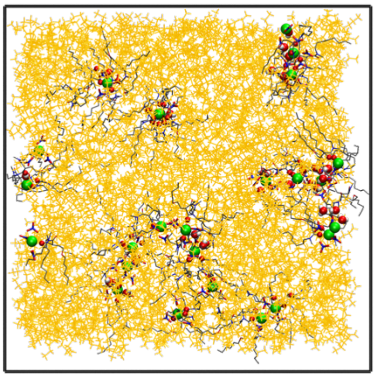

Lanthanide ions recycling has grown in importance in recent years as the demand for these elements has increased [1]. One of the approaches for recycling metals is liquid-liquid extraction, which selectively separates solutes based on the difference in their solubility between two immiscible liquids. In the nuclear industry, many processes based on liquid-liquid extraction are employed to recycle nuclear fuel, where lanthanide ions are separated from nuclear waste. DIAMEX (DIAMide Extraction) process is one such technique [2], where the reference molecule for separation of smaller lanthanides is N-N'-DiMethyl-N-N'dioctyl-2-hexylethoxymalonamide (DMDOHEMA) [2].

In our research, we use classical Molecular Dynamics (MD) to investigate the structural properties of the liquid-liquid interfaces between aqueous and organic phases with different amphiphilic extractant molecules. The main objective is to characterize and describe the species distribution at the interface and in bulk organic phase, comparing to the experimental results [3].

First, we investigated how the initial box configuration as well as the ratio between the two phases impacts the formation of the interface, the shape, and the structure of the interface in comparison with a theoretical thermodynamics model [4]. After validating the method for creating the interfaces by MD simulations, we studied the distribution of DMDOHEMA extractant molecules at the interface and in the bulk organic phase at various extractant concentrations. Additionally, our investigation extends to understanding the micelle formation with lanthanide cations (Eu^{3+}) and DMDOHEMA extractant within the bulk organic phase.

We extensively investigated the distribution and the structural properties of DMDOHEMA extractant at various concentrations, and we will apply the same approach to study TODGA extractant to compare the effect of structural differences on their behavior in the system. Furthermore, we will introduce Nd^{3+} cations into the system and explore the ion transfer from aqueous to organic phase, distribution of extractants, salts, and micelles formed in the system during extraction.

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