

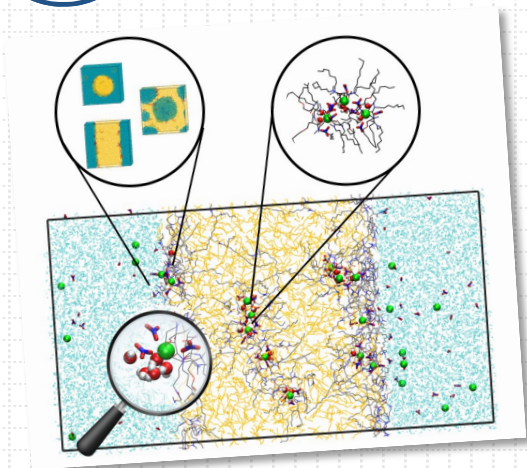


PhD DEFENSE

Lara ŽIBERNA

**Mesoscopic Modeling and
Theoretical Chemistry (LMCT)**

Simulation of the equilibrium and the transport of ions at the liquid-liquid interfaces



**Thursday,
November 20,
2025**



2:00 PM



**Auditorium
ICSM**

In this thesis, the structural organization in the bulk organic phase, at the interface, and the transport of ions in systems with the extractants DMDOHEMA, DMDBDMA, and TODGA were investigated using classical molecular dynamics. First, we demonstrated that using a demixing approach, i.e., starting from randomly distributed molecules, was the optimal approach to create interfaces. The analysis revealed different interfacial shapes depending on the ratio of the two immiscible liquids, with the organization of extractants directly influencing interfacial thickness. We then focused on bulk organic phases containing $\text{Eu}(\text{NO}_3)_3$ salt in the presence of the three extractants. To characterize the aggregates formed in the organic phase, the code `CoordDynA_MD` was developed. All extractants form reverse micelle-type aggregates, with compositions depending on the extractant used. We demonstrated that increasing the $\text{Eu}(\text{NO}_3)_3$ concentration impacts the number of aggregates comprising more than one cation but not the average oligomer stoichiometries. These oligomers arose from monomeric aggregates connected through hydrogen bonds involving water molecules, nitrate anions, and extractant molecules, which enabled the formation of bridges. Finally, the transfer of $\text{Eu}(\text{NO}_3)_3$ from the organic phase to the aqueous phase was studied. The mechanism, driven by nitrate-water H-bonding in the aqueous phase and the cation hydration, was independent of the extractant. However, distribution ratios and retention times varied, with shorter retention times for extractants that were able to form larger aggregates.

Keywords: *Liquid-liquid extraction; Interfaces; Molecular Dynamics; Lanthanides*



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