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Research field:

Chemistry / Solid state physics, chemistry and nanosciences
Soft matter and complex fluids / Solid state physics, chemistry and nanosciences

Title:

Multiscale modelling for separation chemistry: aggregates in organic phase for separation chemistry

Abstract:

Separation processes performed for recycling of heavy metals commonly use liquid-liquid extraction for which ions are selectively transferred from an aqueous to an organized organic phase. The description of the aqueous phase is being relatively well established, but for the organic phase nothing exists from a predictive point of view. This thesis will study the physical chemistry of liquid-liquid extraction from a theoretical approach. The main goal is the understanding of the various effects (solvation, electrostatic and Van der Waals forces, entropy), which drive the transfer from one aqueous phase to an organic organized phase. A method based on density functional theory (classical DFT) will allow the calculation of the ion distribution in the various inverse micelles. Then the various thermodynamical properties of the system will be obtained. The experimental support will be first the extraction of Europium nitrate thanks to DMDOHEMA for which experimental data have been measured. Molecular modelling will allow the checking of this mesoscopic approach and it will provide some physical parameters, specially for the solvation effects.

Location:

Institut de Chimie Séparative de Marcoule

Modélisation mésoscopique et chimie théorique
Starting date: 01/10/2011
Centre : Marcoule

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