



Ph.D. defense

Institut de Chimie Séparative de Marcoule / CEA Marcoule
(UMR 5257, CEA, CNRS, Université Montpellier, ENSCM)

MICHAEL BLEY

will present his Ph.D. dissertation

Simulating Osmotic Equilibria by Molecular Dynamics – From Vapor-Liquid Interfaces to Thermodynamic Properties in Concentrated Solutions

The defense will take place on **Wednesday, November 21, 2018** at **2.00 pm**
in the ICSM Auditorium

The aim of this PhD thesis is the development of a new theoretical method based on the simulation of vapor-liquid equilibria by means of molecular dynamics (MD) simulation. This new method predicts thermodynamic properties such as solvent activities and solute activity coefficients of aqueous and organic phases used in liquid-liquid extraction systems. These thermodynamic properties are required for mesoscopic thermodynamic modeling approaches estimating the efficiency and selectivity of a given solvent extraction system up to an industrial scale. Thermodynamic and structural properties of aqueous electrolyte solutions and organic solvent phases including aggregates resulting from amphiphilic extractant molecules are reproduced in very good agreement with previously available experimental and theoretical data. The osmotic equilibrium MD approach provides a new and powerful tool for accessing thermodynamic data.

Keywords: Molecular Dynamics; Aqueous Electrolyte Solutions; Activity Coefficients; Aggregates in Organic Solvents; Separation Chemistry

