Undergraduated training (24 weeks)

1. Subject details

Title Multiscale modelling of ion surface mobility in confined silca

Keywords Silica, Electrophoretic mobility, Confinement, Molecular dynamics, Theoretical chemistry, Mesoscopic modelling

Abstract This course takes place in the Mesoscopic Modelling and Theoretical Chemistry group of the *Institut de Chimie Séparative de Marcoule* (ICSM), which belongs to CEA, CNRS, Université de Montpellier 2 and ENSCM. This institute, located close to Avignon (South-East of France), is the reference place in France for strategic metals recycling.

The aim of the course is to model ion surface mobility in porous glass. This study is part of development of innovative methods for soil and water decontamination polluted by heavy metals.

Porous silica used in separation chemistry are made of subnanometric channels. When driven through this porous network, an aqueous solution exchanges ions with glass surface, and is decontaminated. The process is controlled by species surface mobility, which is the diffusion in the vicinity of surfaces.

The aim of this course is to model this phenomenon at the molecular scale for a series of monovalent ions.

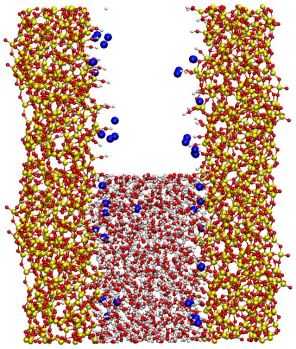

Figure 1 : An atomic model for porous glass

The method rests on Molecular Dynamics simulations, coupled with a thermodynamical analysis based on functional density. Linking models with experiments, the student will use electrokinetics models with boundary conditions.

This course will allow an outstanding student to get to know theoretical chemistry and simulations methods. Following the results obtained, this work can be the basis for a publication in an international scientific journal, and is also the start for a thesis supported 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.