

**Research field:**

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**Title:**

Hydration forces and ionic specificity in complex media

**Abstract:**

We propose to study by modelling the origin of hydration forces between surfaces in complex media, and their link with the specific adsorption of ions. This theoretical work will be based on a multi-scale approach. The idea consist in understanding the origin of surface phenomena who couple electrostatic force and hydration. This work is all the more significant since these phenomena drive many of the numerous applications of silicas, i.e. in separation chemistry as a nanoporous material.

More precisely, an atomic model of silica, depending on the pH and of the ions in solution will be proposed. Molecular dynamics and Monte Carlo simulations will allow the deduction of a coarse-grained model, which will be solved by density functional theory. Together with dynamical (electrokinetic phenomena) and equilibrium (ion exchange) experiments performed in ICSM, we will determine how the various ions modify the surface and drive the behaviour and the one of the solvent. In a longer term, it should be possible to propose a theory which is quantitatively in agreement with experiments, and which takes into account molecular effects.

**Location:**

Institut de Chimie Séparative de Marcoule

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Centre : Marcoule

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**DSM**

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