Institut de **C**himie **S**éparative de **M**arcoule

Postoctoral researcher position

STUDY OF THE INTERFACIAL LAYER AND OF THE ANISOTROPY OF WATER DYNAMICS WITHIN AUQEOUS SOLUTIONS CONFINED IN MODEL SILICA MATERIALS

Application submission before 15/07/2020

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Beginning: September or October **Duration** : 12 month

Subject

The understanding and the prediction of macroscopic behavior of nanoporous materials in aqueous solutions in the fields of geochemistry, construction, environment, effluent treatment, catalysis, and nuclear, require the use of geochemical modeling. This modeling is often carried out with softwares (PHREEQC, JChess, etc.) which take into account thermodynamic concepts and kinetics laws obtained from experiments performed in dilute media (concentration of dissolved ions, pH, kinetics and thermodynamic constants...). These nanoporous materials which can be cementitious materials, geopolymers, biomaterials, membranes, corrosion products, clay materials, secondary minerals… consist in a set of confined media of a few nanometers completely or partially filled with water and ions in which the validity of these concepts and laws has not been demonstrated. This validation is really important since the processes occurring in their nanoporosity such as ion sorption, phase precipitation, dissolution and recondensation, diffusion are different from those occurring with dense material in aqueous solution and are at the origin of their macroscopic properties.

In confinement (pores smaller than 5 nm) and in presence of ions, the behavior of water is modified by the strong interactions occurring between the pore surfaces and the ions structuring the water and slowing down its dynamics / transport from a nanoscale to a macroscopic scale. These effects can have significant consequences on chemical reactions since they are controlled by an interfacial layer. In this zone located between the solid and the liquid, the properties of the solution deviate from that of the "bulk". This interfacial layer is often described by the electric double layer or Poisson-Boltzmann model can be strongly modified if the solution is nanoconfined. Thus, it is essential to characterize both, this interfacial layer and the evolution of the pores of the material in contact with the solution in order to validate or invalidate the thermodynamic concepts and the kinetic laws used for predictive modeling.

The objective of this project is to study the interfacial layer and the anisotropy of water dynamics in aqueous solutions confined in model materials based on silica.

The study will be divided in several phases. During the first phase, the model systems based on oriented silica nanocylinders will be prepared and characterized. Then, the model systems filled with water and ions will be analyzed by SAXS and SANS in order to determine the electron density profiles within the nanocylinders. In parallel, the dynamics of water at the picosecond scale in its confined media filled with electrolytes will be characterized by QENS. To perform this work, several proposal will be written in order to obtain beam times on different diffractometers and time of flight spectrometers.

Candidate profile

The young doctor have to be independent, both in terms of materials synthesis and characterization. A good knowledge of scattering techniques is required (at least SAXS). Moreover, this project is a fundamental study which requires curiosity to carry out a bibliographic work and to communicate with the various collaborators. Finally, good writing skills are essential in order to publish articles.

Interest for the researcher

The ICSM is a dynamic institute, in which the young researcher will be able to work with specialists recognized worldwide in their scientific field and / or certain techniques (atomistic modeling, SAXS, X-ray diffraction and reflectivity, environmental microscopy, etc.). In addition to acquiring new scientific skills or improving those already existing, the young researcher will also be able to develop his contacts via the project himself, his participation in seminars (internal and external) and conferences (national and international).) as well as training.

Références

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M. Baum, D. Rébiscoul, C. Rey, F. Juranyi, F. Rieutord, *Dynamical and Structural Properties of Water in Silica Nanoconfinement: Impact of Pore Size, Ion Nature, and Electrolyte Concentration*, Langmuir, 35 (2019) 10780. 10.1021/acs.langmuir.9b01434

M. Baum, D. Rébiscoul, F. Juranyi, F. Rieutord, *Structural and Dynamical Properties of Water Confined in Highly Ordered Mesoporous Silica in the Presence of Electrolytes*, Journal of Physical Chemistry C, 122 (2018) 19857. 10.1021/acs.jpcc.8b02182

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