

Ph.D. defense

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

MARKUS BAUM

will present his Ph.D. dissertation

The role of water properties and specific ion effects on the evolution of silica nanoconfinement

The defense will take place on **Friday, November 9, 2018 at 10.00 am**
in the ICSM Auditorium

In this study, we investigated the water properties in the presence of ions in silica nanoconfinement. The main objective is to relate these water properties to the evolution of silica mesoporous materials in aqueous solutions. To reach this goal, we used an original approach, consisting in the use of electrolyte solutions having more or less kosmotropic properties XCl_2 ($X = Ba, Ca, Mg$) confined in model systems such as two parallel and plane silica surfaces spaced of 3 and 5 nm (nanochannels) and highly ordered mesoporous silica materials represented by SBA-15 (6 nm pore size and microporous pore wall) and MCM-41 (3 nm pore size and dense pore wall).

The obtained results indicate that the filling kinetics in nanochannels are driven by the size of the confinement, the nature of ions and the salt solubility of electrolytes. In some cases, the incomplete filling of the nanochannels may be explained by a decrease of water dynamics associated to the saturation of XCl_2 salts into the interfacial layer. The possible precipitation of XCl_2 phases may explain an incomplete filling by a nanochannels clogging.

Thereafter, the water properties in nanoconfinement made of silica concave surface such as cylinders were studied. The water structure and dynamics at a picosecond scale in presence of ions were respectively characterized by infrared spectroscopy and quasi-elastic neutron scattering. The results suggest that the structural and dynamical water properties are strongly affected by the size of the confinement, the kosmotropic properties of ions and the surface ion excess in the interfacial layer.

Finally, we characterized the evolution of two mesoporous silica in electrolyte solutions using in-situ small-angle X-ray scattering. For 3 nm pore size and dense pore wall (MCM-41), the slow dynamics at a picosecond scale probably lead to a supersaturation of ions in the interfacial layer and thus, to a reprecipitation of XCl_2 salts and/or silica phases. In that case, the evolution of the MCM-41 is driven by a dissolution-recondensation/precipitation process. In the bigger mesopores of SBA-15, due to the microporosity in the pore wall, the alteration process is different. During a first stage, an alteration layer is formed and the pore size increases until the silica saturation. Afterwards, a similar recondensation/precipitation process as observed in MCM-41 occurs into the microporosity. These two types silica evolutions could persist until the formation of a thermodynamic stable silica phase.

