

Relation between Structure and Dynamics of water with BaCl₂ confined in nanoporous silica and the dissolution of the silica nanoconfinement

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Understanding the dissolution processes occurring in silica nanoconfined media is of interest to explain geochemistry earth system behavior. Particularly, in confinement and in presence of salt, water behavior is modified due to strong interactions with pore surface and ions. The determination of the consequences of such modifications on dissolution is a scientific challenge since the characterization of these processes in nanoconfinement is sophisticated.

In this study, we propose an innovative approach. We relate the water structure determined by Infrared spectroscopy and the water dynamics at a picosecond scale characterized by QENS (FOCUS, T=300 K, $\lambda=4.32$ Å) in highly ordered nanoporous silica (SBA-15; pore size 6.6 nm) filled of BaCl₂ solutions (0.01, 0.2, 1 M) with the kinetics of nanopore wall dissolution characterized by in-situ Small Angle X-ray Scattering (see Figure). The residence time of water, the fraction of less coordinated water and the dissolution kinetics of silica nanopore wall increase with the ion concentration.

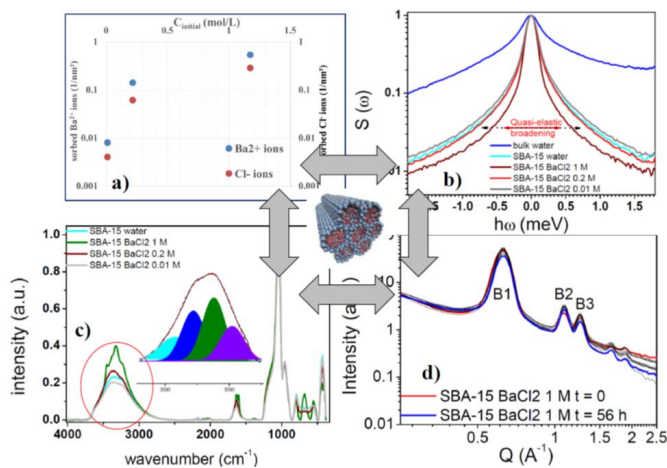


Figure: Sorption isotherms of BaCl₂ electrolytes at various concentrations in SBA-15 (a). Sum over Q of QENS spectra of SBA-15 filled of BaCl₂ electrolytes at various concentrations obtained at 300 K and $\lambda = 4.32$ Å (b). Infrared Spectra of BaCl₂ solutions in nanoconfinement (c). Evolution of the SAXS pattern during the dissolution of the nanoporous silica in BaCl₂ electrolytes (d).