

Structural and dynamical properties of water confined in highly ordered mesoporous silica in presence of electrolytes

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The understanding and the prediction of materials behavior regarding their interactions with aqueous solutions is of great interest in various fields, such as geochemistry, catalysis and nuclear wastes. Most of these materials are completely or partially nanoporous such as cementitious materials, clay materials, and amorphous nanoporous alteration layer of glasses. They consist of a set of confined media having a complex form and filled with water and ions. For instance, under confinement, the solvent behavior can be modified due to strong interactions between water molecules and pore surfaces, structuring water and slowing down its dynamics, from nanoscale to macro-scale.¹ Several parameters play a major role on this behavior changes such as pore size, surface composition, roughness and curvature.² Also, the presence of ions is expected to have a slow-down effect on the water mobility perturbing the hydrogen bond network through solvation and sorption.^{3,4} 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 surface ion excess with 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 with electrolyte solutions XCl_2 ($X = Ba^{2+}$, Ca^{2+} and Mg^{2+}) at various concentrations (see Figure). Depending on the present ions and with increasing electrolyte concentration, we found a decrease of water dynamics and an increase of less coordinated water population.

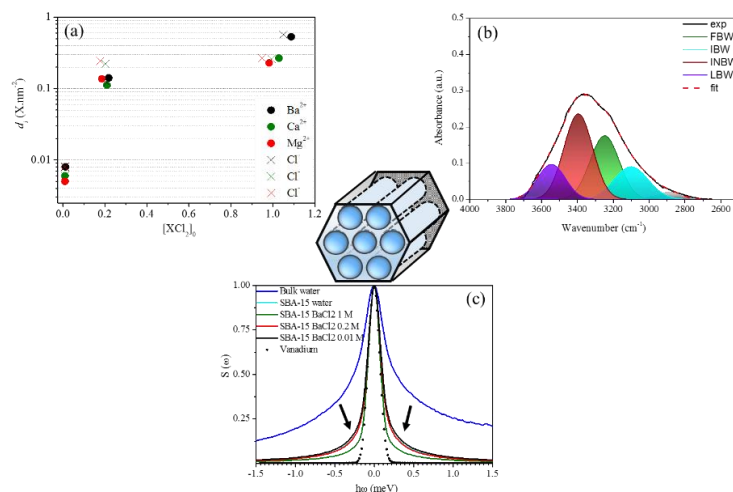


Figure: Sorption isotherms of XCl_2 electrolytes ($X = Ba^{2+}$, Ca^{2+} and Mg^{2+}) at various concentrations in SBA-15 (a). Sum over Q of QENS spectra of SBA-15 filled of $BaCl_2$ electrolytes at various concentrations obtained at 300 K and $\lambda = 4.32$ Å (b). Decomposition of O-H stretching band of $BaCl_2$ solution at 1 M in nanoconfinement (c).

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