

Supporting Information

Ultraconfinement of Aqueous Electrolytic Solutions within hydrophilic Nanotubes

Richard Renou,[†] Anthony Szymczyk,[†] and Aziz Ghoufi^{*,‡}

*Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS, Université de Rennes 1,
263 Avenue du Général Leclerc, 35042 Rennes, France; Université Européenne de
Bretagne, France., and Institut de Physique de Rennes, IPR, CNRS-University of
Rennes 1, UMR CNRS 6251, 35042 Rennes, France*

E-mail: aziz.ghoufi@univ-rennes1.fr

Abstract

*To whom correspondence should be addressed

[†]Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS, Université de Rennes 1, 263 Avenue du Général Leclerc, 35042 Rennes, France; Université Européenne de Bretagne, France.

[‡]Institut de Physique de Rennes, IPR, CNRS-University of Rennes 1, UMR CNRS 6251, 35042 Rennes, France

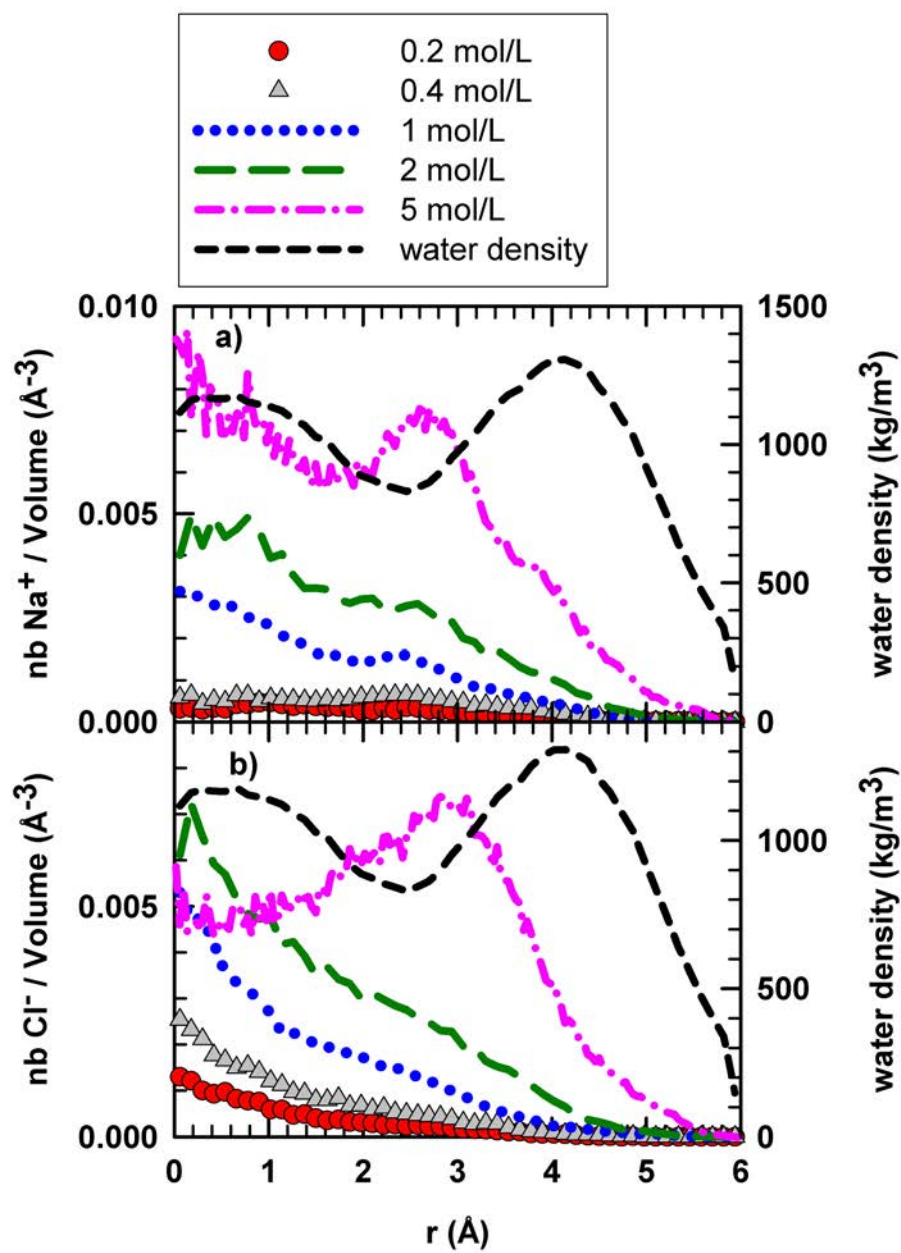


Figure S1: Radial distributions of Na^+ (a) and Cl^- (b) for 0.2, 0.4, 1, 2 and 5 mol/L NaCl solutions. Radial water density corresponding to the NaCl concentration of 0.2 mol/L can be read on the right axis. Water density

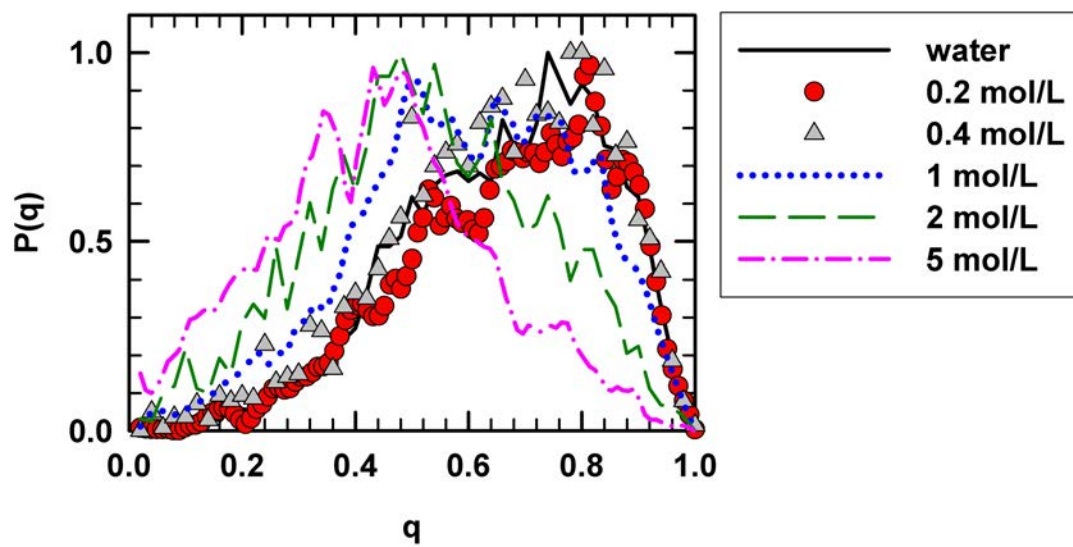


Figure S2: Tetrahedral order distribution of water molecules in bulk phase as function of the NaCl concentration

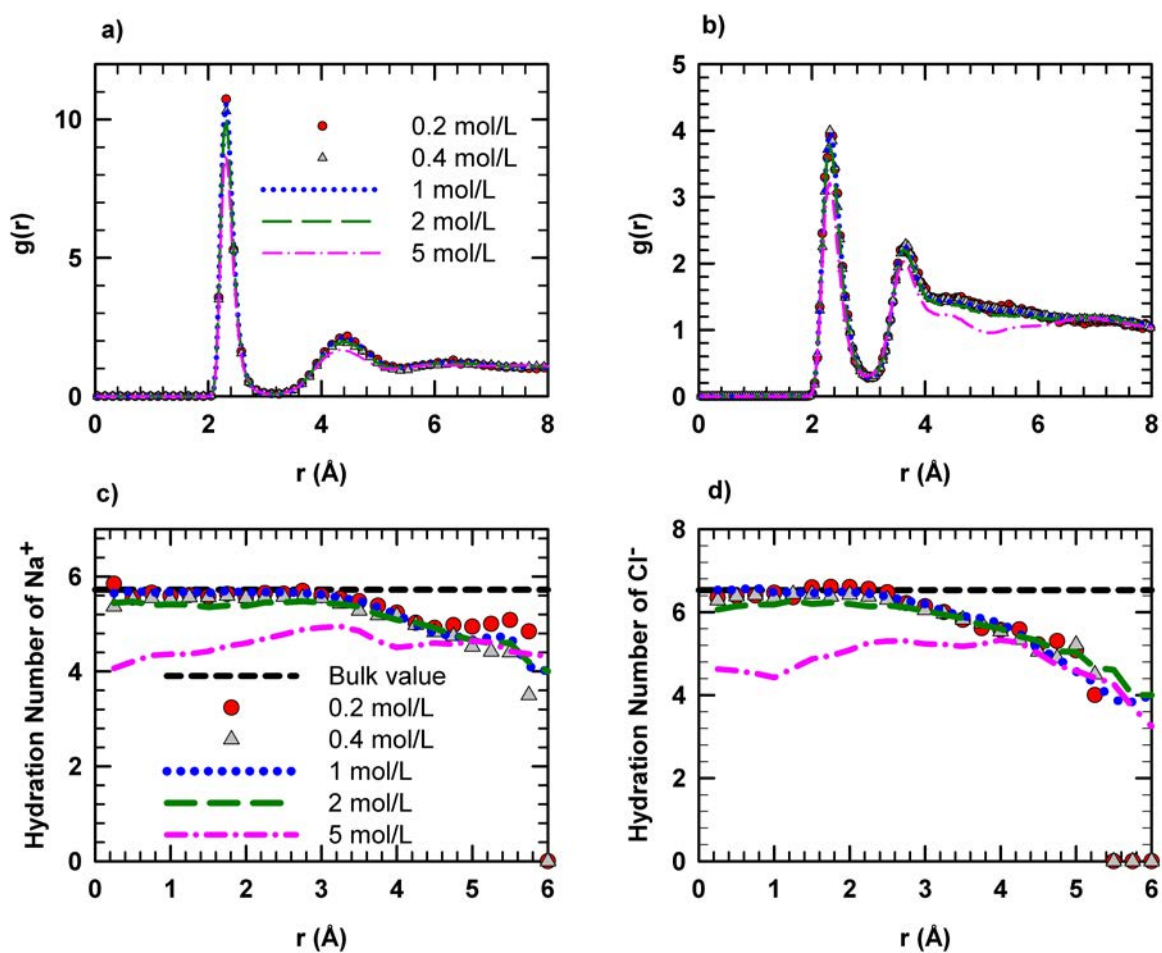


Figure S3: Radial distribution function a) between the oxygen atom water and Na^+ ion and b) between the hydrogen atom of water H and Cl^- ion as function of the NaCl concentration. Radial profile of hydration number of c) Na^+ and d) Cl^- as function of the NaCl concentration.

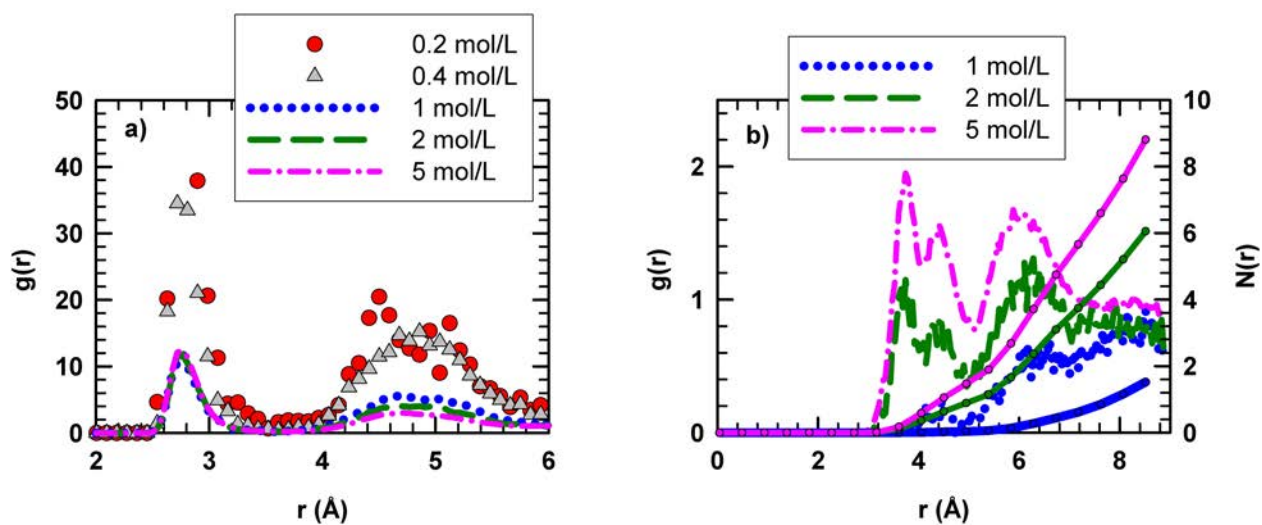


Figure S4: Radial distribution function a) between Na⁺ and Cl⁻ ions and b) between Na⁺ and Na⁺ ions as function of the NaCl concentration. In b) the coordination number of Na⁺ can be read on the right axis. Coordination numbers were calculated from the integration of the radial distribution functions and correspond to the solid lines in b).

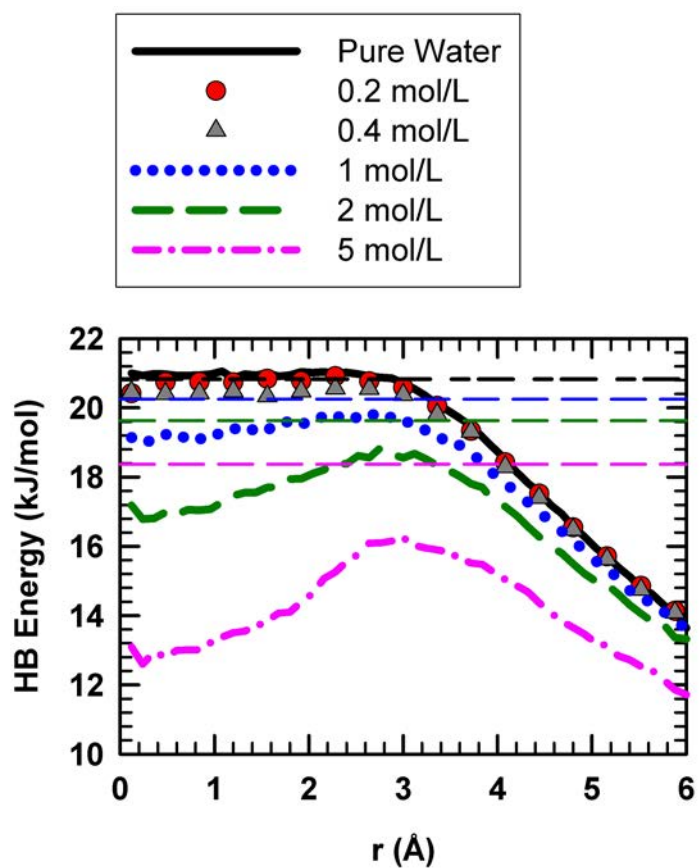


Figure S5: Radial HB energy as function of the NaCl concentration. Energy was calculated by considering electrostatic and Van der Waals interactions between two water molecules. The horizontal lines correspond to the HB energy in bulk phase.

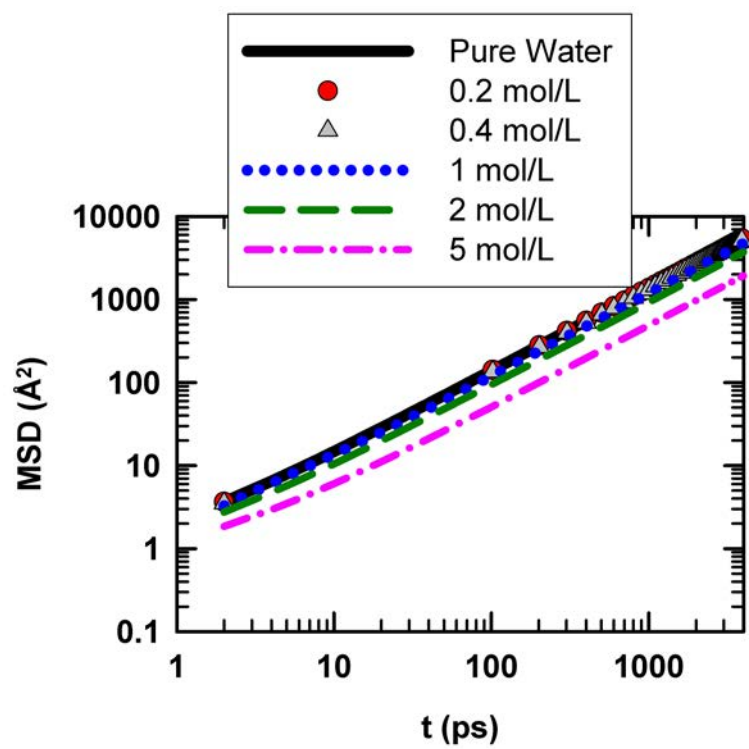


Figure S6: Mean square displacement (MSD) of water molecules in bulk phase as function of the NaCl concentration.