Talk

Effect of confinement on the solubility of salt in water: A simulation study on zeolites.

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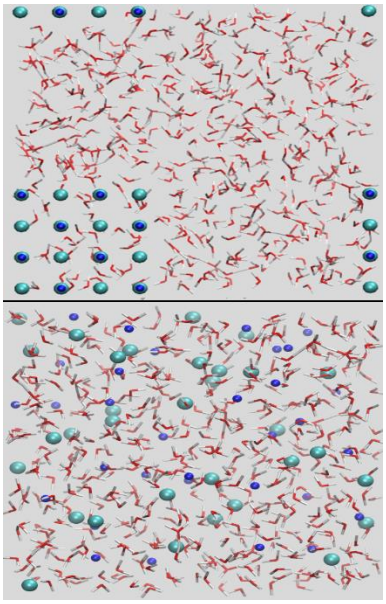
ABSTRACT

Motivation: Salinity is an important concept to understand the environmental conditions and organisms that can be found in water as well and depends on the solubility of salts in water. The effect of temperature and pressure on the solubility of salts (as sodium chloride) in water and other solvents has been widely studied. However, there is scarce studies on the solubility of salts in confined systems, and how the confinement affects to the solvation of salts. Zeolites are a group of crystalline porous solids based on silica and they exhibit high surface area, high thermal stability, and high exchange capacity. Pure silica zeolites are hydrophobic, but the presence of cations can change this nature making them suitable for a variety of applications such as drying of refrigerants, removal of atmospheric pollutants, separation of air components, recovering radioactive ions from waste solutions, catalysis of hydrocarbon reactions, and many others. In this work, we study the influence of the confinement of water in two types of zeolite on the solubility of sodium chloride.

Methods: To study the influence that confinement of water in zeolites has on the dissociation of NaCl clusters, we carry out molecular simulation using two techniques, Molecular Dynamics (MD) and Monte Carlo methods (MC). All simulations are performed using the RASPA simulation code and the force fields and models used for water and the ions are taken from the literature and previously validated. As initial step, we use MD to analyse the effect of temperature and system size on the dissociation of salt. Then, the effect of confinement is analysed using MC simulations. For this purpose we calculated the adsorption of water in two commercial zeolites (MFI and FAU) and after obtaining the adsorption capacity of water for these structures, we study the dissociation of salt in the adsorbed water. We focus on the effect exerted by the number of cations on the zeolites, the topology and the initial concentration of salt.

Results: Our results show that the size of the simulating box has an impact on the dissociation of ions, obtaining that the larger the box, the better the dissociation. In the confined systems, we found that in the pure silica MFI zeolite (longitudinal channels connected to zig-zag channels) dissociation is enhanced and the same occurs in the pure FAU zeolite (cages connected throw windows). Nevertheless, for the FAU zeolite with aluminium atoms, the dissociation of ions is hampered when increasing the number of Al substitutions. On the contrary, the presence of aluminium in the MFI does not alter the dissociation of ions.



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