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The Open-Access Journal for the Basic Principles of Diffusion Theory, Experiment and Application

Dynamics of Electrolyte Solutions Confined in Nanopores

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Organic and inorganic nanoporous membranes, which are known to enhance the diffusion of certain species such as ions and to have a strong selectivity, are very attractive for nanofiltration and therapeutic applications. As a result, many experiments have been carried out to prepare and evaluate the performances of synthetic membranes that reproduce the characteristics of the natural ones. Nevertheless, despite an increasing number of fundamental studies on the subject, the physical mechanisms responsible for these properties remain to be clarified.

In this work, we report on a molecular simulation study of electrolytes confined in an inorganic membrane: sodium halides in water (electrolytes) in a carbon nanotube. Two nanotube diameters (1 and 3 nm) are considered for the carbon nanotube in order to address the effect of confinement. We also address the effect of the size of the ions by considering the following series of sodium halide electrolytes: NaX with X = F, Cl, Br, and I, at about 1.85 M. Special attention will be paid to the effect of polarizability as recent works have shown the crucial role played by this parameter. Finally, we will also consider the effect of the surface charge of the nanotube by considering host materials that are either neutral or charged. Grand Canonical Monte Carlo simulations (GCMC) are first employed to investigate the thermodynamical and structural properties of the confined electrolytes. In particular, concentration profiles as well as ion partition coefficients (defined as the ratio of ion within the tube and in the bulk reservoir) are presented to discuss the separation between the different species (water, anions and cations). Then, Molecular Dynamics simulations are used to determine the dynamical properties of the confined system such as the self-diffusivity. We also discuss the transport properties of the confined system, which is crucial for most of the practical applications involving nanoporous membranes.

diffusion-fundamentals.org 11 (2009) 20, pp 1-1