9. Aqueous electrolytes confined within functionalized silica nanopores

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Molecular dynamics simulations have been carried out to investigate structural and dynamical characteristics of NaCl aqueous solutions confined within silica nanopores in contact with a "bulk-like" reservoir. Two types of pores, with diameters intermediate between 20 Å and 37.5 Å, were investigated: The first one corresponded to hydrophobic cavities, in which the prevailing wall-solution interactions were of the Lennard-Jones type. In addition, we also examined the behavior of solutions trapped within hydrophilic cavities, in which a set of unsaturated O-sites at the wall were transformed in polar silanol Si–OH groups. In all cases, the overall concentrations of the trapped electrolytes exhibited important reductions that, in the case of the narrowest pores, attained 50% of the bulk value. Local concentrations within the pores also showed important fluctuations. In hydrophobic cavities, the close vicinity of the pore wall was coated exclusively by the solvent, whereas in hydrophilic pores, selective adsorption of Na+ ions was also observed. Mass and charge transport were also investigated. Individual diffusion coefficients did not present large modifications from what is perceived in the bulk; contrasting, the electrical conductivity exhibited important reductions. The qualitative differences are rationalized in terms of simple geometrical considerations.