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Title: Nanofluidics in Carbon Nanotubes

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Novel results, obtained by molecular dynamics simulations, concerning the ionic transport in aqueous solutions through carbon nanotubes are presented. Specifically, the effects of the nanotube radius, solute concentration, and applied external electric fields on the solution structuring are investigated in terms of spatial density distributions, pair distribution functions, and detailed electrostatics. The structural features are consistent with general theoretical results of nanofluidics (like, for instance, the Donnan-type voltages established at the channel apertures depending on the logarithm of the maximum ion concentration). The transport properties are characterized by mobilities, currents, and pairing times of the solute ions and corroborate, equally, general nanofluidics results (the linear log-log regime of the nanochannel conductance as function of the solute concentration and the current-voltage curve of the channel). Discontinuities in the partial ionic currents are explained on the basis of a recent theoretical model of quantized ionic conductance in nanopores. Correlations between the structural and dynamic properties are established, linking causally the highly structured spatial density profiles, the ion pairing phenomenon and the ionic currents. The simulated properties are based on averages over the largest data collection times reported in the literature (0.8 μs), providing unsurpassed accuracy.
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