Water and proton transport through narrow pores

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A one-dimensional (1D) dipole lattice model is developed to study water confined into molecularly narrow pores such as carbon nanotubes [1,2]. By re-summing the Hamiltonian and expressing it in terms of dipole-ordered segments of water molecules, dipole defects, and gaps, this model allows us to investigate the structural and thermodynamic behavior of 1D-confined water up to macroscopic system sizes. The dipole lattice model is parameterized and validated by using detailed atomistic simulations. The model is then applied to study water inside long carbon nanotubes, in grand-canonical equilibrium with a water bath (or vapor). At ambient conditions, the water chains filling the tube are essentially continuous up to macroscopic dimensions. At reduced water vapor pressure, we observe a 1D Ising-like filling/emptying transition without a true phase transition in the thermodynamic limit. In the filled state, the chains of water molecules in the tube remain dipole-ordered up to macroscopic lengths of about 0.1 mm, and the dipole order is estimated to persist for times up to about 0.1 s. The observed dipolar order in continuous water chains is a precondition for the use of nanoconfined 1D water as mediator of fast long-range proton transport, e.g., in fuel cells. For water-filled nanotube bundles and membranes, we expect anti-ferroelectric behavior, resulting in a rich phase diagram similar to a 2D Coulomb gas.

[1] C. Dellago, M. M. Naor, G. Hummer, Phys. Rev. Lett. **90**, 105902 (2003),
[2] C. Dellago, G. Hummer, Phys. Rev. Lett. **97**, 245901 (2006).