Abstract Submitted
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**Carbon nanotubes as molecular conduits: flow of water, protons, ions, and nucleic acids** GEHARD HUMMER, National Institutes of Health — The transport of water, protons, ions, and nucleic acids through carbon nanotubes was studied with all-atom molecular dynamics simulations. Water is found to fill even narrow pores of sub-nanometer diameter, but the filling is sensitive to the strength of attractive pore-water interactions and local electric fields. Motions of water through nanotubes is fast on a molecular scale. Protons were also found to move rapidly along one-dimensionally ordered water chains inside nanotubes. The transport of nucleic acids through nanotube membranes is dominated by polymer conformational dynamics during entry, and hydrophobic attachment to the pore walls during exit.

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