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Water in nanotubes and proteins

Computer simulations are used to study the unusual structure, thermodynamics, and flow of water and protons in nanotubes and proteins. In the absence of strong interactions with the pore walls, water molecules tend to form wires or clusters held together by tight and long-lived hydrogen bonds. Simulations on classical and quantum energy surfaces show that 1D water wires in nonpolar pores facilitate rapid water flow and proton conduction. At ambient conditions, the water chains filling the tubes are continuous and dipole-ordered up to macroscopic dimensions. Implications on protein function and nanofluidics will be discussed.

Prof. Gerhard Hummer

香港科技大學
THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY