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## Molecular Dynamics Simulation of the Transport of Water Molecules through Nanochannels


Given the immense applications of nanoporous materials, such as their use in polluted water filtration or seawater desalination, it is crucial to understand the transport properties of water molecules through nanochannels. Despite considerable effort and progress, a controllable and unidirectional water flow through such channels is still difficult to achieve, and the underlying mechanism is far from being understood. In this talk, we discuss the transport properties of single-file water molecules through carbon nanotubes (CNTs) in the presence of external electric fields, via molecular dynamics (MD) simulations. First, it is found that the orientation of water molecules inside the CNT can be well tuned by the electric field, and is strongly coupled to the water flux. A critical field strength $E_c$ is observed, below which the water flux increases as $E$ increases and is almost unchanged for $E > E_c$. Even when the water dipoles inside the CNT are maintained along the field direction, a large amount of water molecules can still transport against the field direction for short CNTs, leading to a low unidirectional transport efficiency ($\eta$). As the CNT length increases, $\eta$ increases remarkably. These results provide some new physical insights into the biased transport of single-file water molecules, which show the feasibility of using CNTs to pump water in an electric field. This mechanism is important for designing efficient nanofluidic apparatus.


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