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Computational study of water transport through carbon nanotubes and channel proteins

Water transport across cell membranes is facilitated by aquaporin (AQP) channel proteins. AQPs are ubiquitous in all existing life forms. More than ten different AQPs have been identified to date in human tissues such as kidneys, eyes, and brain and their dysfunctional forms have been implicated in several diseases. Recently determined high resolution crystal structures of several AQP proteins made possible all atom molecular dynamics studies of water (and other small molecules) conduction through these channels for understanding the underlying physical mechanism of this process. An important common feature of AQPs is that (at least in their constriction region) they conduct water in single file. Surprisingly, recent MD simulation studies showed that, in spite of their hydrophobic pore, single-walled carbon nanotubes (SCNT) can also conduct single file waters even with higher efficiency than AQPs. In this regard, SCNT can be regarded as simplified models of the much more complex channel proteins. Understanding the microscopic mechanism of the conduction through SCNTs may provide useful insight in the functioning of biological channels. Here we present MD simulation results for single file water transport in SCNT and AQPs. By using the potential of mean force (PMF) that guides the diffusion of water molecules through the nanopore, we generalize a previously proposed continuous time random walk model that successfully describes the concerted single file water transport through both SCNT and AQPs.