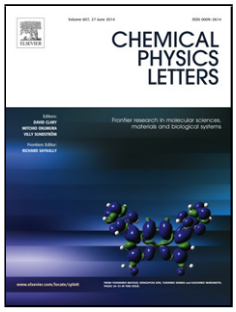

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Fast Transport of Water Molecules across Carbon Nanotubes Induced by Static Electric Fields

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Water permeation across a single-walled carbon nanotube has been studied in the presence of static electric fields (SEFs) with different directions under hydrostatic pressures. With the angle between the SEF direction and tube axis increasing from 0 to 90 degrees, the water flux decreases gradually until almost vanishes, and the maximum value at 0 degrees is approximately four times the case without SEFs. The phenomenon is attributed to the alignment of the polar water molecules along the SEF direction. We also show that water permeation properties are dependent on the field strength due mainly to thermal fluctuations of water molecules.

Introduction.— Water, as a key constituent in cell biology [1], plays an important role in biological activities [2, 3, 16]. It is well known that the ability of living cells to transport water molecules across their cell membrane is mediated by proteins which function as transporters and channels. Water permeation through membranes can be controlled by pH [5], solute concentration [6], and charge distribution [7]. In spite of this, it is still not easy to acquire a clear insight into the intrinsic mechanism for the sake of the complex biological channels structure. Single-walled carbon nanotubes (SWCNTs), due to structural simplicity, have been used to investigate dynamical properties of confined water in the past [8–12]. It has interestingly been revealed that SWCNTs can hopefully be used for building novel nanofluidic devices or machines, and reproducing a number of interesting dynamical properties of water molecules in biological channels: the single-file ordered chain [12, 13], vapor-liquid transitions [14, 15], wavelike density distributions [16, 17], wet-dry transitions [9, 18], and so on.

Water transport in nanochannels is of great importance in many applications, including drug delivery [19], flow sensors [20], desalination of seawater [21], biomolecule separation [22], etc. It has been confirmed that hydrostatic/osmotic pressures [21, 23], AC electric fields [24], Coulomb dragging [25], temperature gradients [26], and mechanical vibration [27] can drive water unidirectional transport through nanochannels. In addition, electro-osmosis technology using to realize controllable flows in nanochannels is recognized as very convenient and promising approaches [24, 28, 29]. Nevertheless, there is some dispute about whether the static electric fields (SEFs) can pump water through the nanochannel or not [30, 31]. Some reports show that the pumping may arise in SEFs due to the problematic setup of the computation program [31, 32]. we also basically agree that the steady EF cannot cause the unidirectional flow of water molecules, because the energy acquisition and spatial asymmetry are necessary to generate pumping, which can not fulfilled for electroneutral polar water molecules in the SEF. As we know, although it is still a controversial topic that whether or not a SEF can drive a continuous flow, the SEF really is able to remarkably affect the water intermolecular structures [33–36] in nanochannels. Recently, Ren *et al.* demonstrated that the structural and wetting properties of water droplets on a graphene substrate are aslo highly sensitive to the SEFs [37]. It has been reported that water transport properties are closely dependent on water structures inside the nanochannel [36, 38–40]. However, excluding the studies on electro-osmosis pumps [30, 34, 35], the electrostatic field as a controllable condition does not draw enough attention to the research of water transport properties in the nanochannels. The structure and permeation properties of water molecules across nanochannels under the effect of SEFs remains inexplicit up till now. Moreover, it is also unclear how to effectively manipulate the transport of water using the SEF in nanometer scale. In this Letter, we thus use MD simulations to investigate the dynamic behavior of water permeation through (6,6) SWCNTs with hydrostatic pressures in the presence of SEFs. We have observed that water permeation properties can greatly be affected due to the realignment of the polar water molecules along the EF. The flux increases gradually as the angle between the SEF direction and tube axis decreases from 90 to 0 degrees. This result suggests that SEFs are promising to develop high-flux nanofluidic devices and explore possible implications for the biological water channelling.

Computational Methods.—A sketch of the MD simulation model built with the molecular visualization program [41] is displayed in Fig. 1. To mimic the biological water channels in membranes, an uncapped (6,6) armchair SWCNT with a length of 1.34 nm and a diameter of 0.81 nm is embedded along the z direction in two parallel graphite sheets which subdivided the water box into two equal parts. The distance in z-direction between the bottom end of the SWCNT and the graphite sheet is 2 $\mathring{A}$. MD simulations are carried out using the NAMD2 [42] in the canonical (NVT) ensemble with the initial box sizes of $3.5\times3.5\times6.3\ nm^3$, constant temperature (300 K) regulated by Langevin dynamics with a 1 ps^{-1} dumping constant, and periodic boundary conditions in all direc-

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