DYNAMIC PROPERTIES OF CONFINED WATER MOLECULES IN NANO-SCALE SYSTEMS

Guangchao Zuo, Rong Shen & Wanlin Guo [a)]
Institute of Nano Science, State Key Laboratory of Mechanics and Control for Mechanical Structures, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China

Summary Confined water molecules show different properties than bulk water. In this paper, we show the dynamic properties of single-file water chain in directional flow and propose a unique self-adjusted sustaining oscillation mechanism.

Water molecules are essential to life. In many technologically important situations, as well as in many biological processes, water molecules are confined in cavities at nano scale, rather than as bulk water. In recent years, water in confined environments has attracted considerable attention due to its important applications in directional drug transport, desalination, nano-filtration and flow sensor and so on. When confined in nano-scale systems, water molecules present unique dynamic properties quite different form bulk water [1]. Here, we study the dynamic properties of water molecules inside carbon nanotube for practical bionic design and application using dynamic simulations, first principle calculations and thermodynamic analysis; we study the dynamic properties of water molecules inside carbon nanotube for practical bionic design and application.

Aquaporins are membrane water channels that play critical roles in controlling the water contents of cells. In cell membrane, aquaporins can transport water molecules with high rate, which provides us an ingenious prototype for nanochannel design. Take the case of aquaporin-1, there are three asymmetrically distributed charged residues in the central pore, i.e., ARG197, ASN194 and ASN78 [2], which can reduce the local barriers for water transport and prevent proton passage across the membranes. The asymmetric water-protein interaction potential is considered as an intriguing driver for unidirectional water flow, based on which, a biomimic nanochannel is proposed. Our energetic analysis suggests that the water-water interaction, determined by dipole orientation configuration, influences the total interaction significantly, and no obvious unidirectional flow is exhibited [3]. Furthermore, the free energy profiles show that there is slight difference at the two ends of the biomimic nanochannel, which may be annihilated by thermal fluctuations outside the CNTs. Thus, it is demonstrated that, as in the aquaporins, asymmetrically positioned charges cannot generate robust unidirectional water flow in the CNT. Thermal fluctuation in bulk water competes with charge affinity to steer the water transport, resulting in nonmonotonic flow with intermittent reversal of transport direction. These findings can provide correct biomimic understanding of water transport properties and will benefit the design of efficient functional nanofluidic devices.

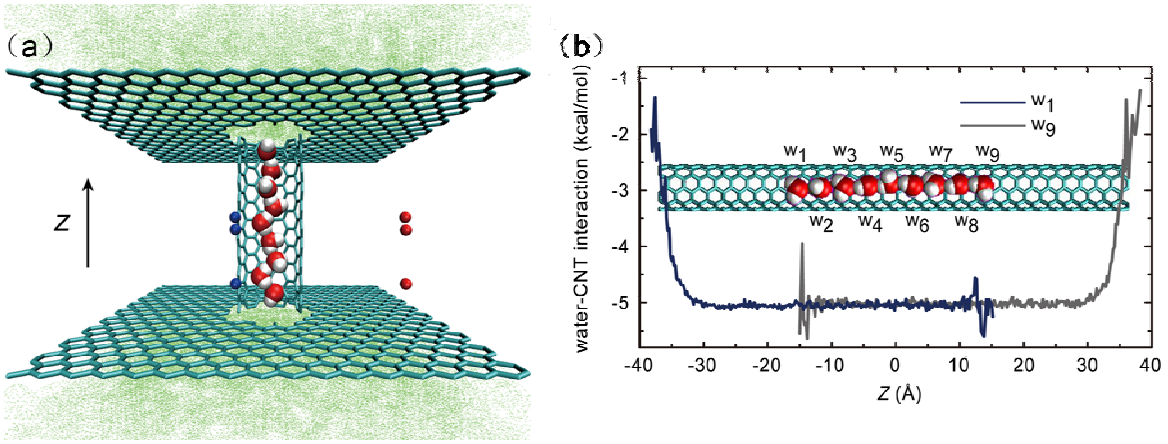

Figure 1. (a) Overview of the biomimic water channel. The carbon nanotube and graphite sheets are presented by cyan sticks. The blue spheres are the positive charges, and red spheres are the negative charges, while the electric quality is 0.5, 0.5, and 1.0e from top to bottom. (b) Schematic of the water-CNT oscillator. Interaction energies between water molecules w1 or w9 and the carbon nanotube.

[a)] Corresponding author. Email: wlguo@nuaa.edu.cn

Because of the growing emphasis on the energy shortage problem, creating molecular motors and nanofunctional systems driven by environmental energy is currently an area of immense research interest. Here, we demonstrate that a single-file water chain confined in carbon nanotubes can self-adjust into regular oscillation with remarkable lower entropy from random thermal motion with higher entropy (Figure 1b) [4]. The turning between the two phases is triggered by the orientation of the donor water molecule (w9) fluttering into or from the energy optimum configuration of the chain. Each of the lower entropy regular motions can only last for about 2 ns before turning back to the random motion phase, forming sustaining intermittent regular oscillation at tens of gigahertz at room temperature. According to the Boltzmann distribution law, it is demonstrated that the intermittent oscillating mechanism can greatly lower the escaping probability of the oscillating water molecules by overcoming the energy barriers at the open ends of CNT at room temperature. The characteristic frequency of the water chain in its regular phase is sensitive to tube diameter and chirality. The finding is helpful to understand the physics for thermal fluctuation driven regular motion and create novel nanodevices. New opportunities are made possible by the unique behavior of confined water molecules at the nano-scale.

References

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