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Water diffusion in carbon nanotubes under directional electric fields: Coupling between mobility and hydrogen bonding

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ABSTRACT

Molecular Dynamics simulations of water confined in carbon nanotubes subjected to external electric fields show that water mobility strongly depends on the confining geometry, the intensity and directionality of the electric field. While fields forming angles of 0° and 45° slow down the water dynamics by increasing organization, perpendicular fields can enhance water diffusion by decreasing hydrogen bond formation. For 1.2 diameter long nanotubes, the parallel field destroys the ice-like water structure increasing mobility. These results indicate that the structure and dynamics of confined water are extremely sensitive to external fields and can be used to facilitate filtration processes.

1. Introduction

The characterization of the molecular transport phenomena is relevant for the study of pure liquids, mixtures and complex systems such as gels, liquid crystals, and polymers. For simple liquids, the diffusion coefficient, D , at a constant temperature usually decreases with the increase of density. This is not the case of water. The isothermal mobility of water at low temperatures increases with density and exhibits a maximum [1] at the temperature of maximum diffusion. This unexpected behavior is related to another water unusual behavior, the water structural anomaly. While most materials at constant temperature become more structured as density increases, water becomes less structured and the translational order parameter which measures the organization exhibits a maximum for a certain density [2]. In the case of water, the structural anomaly takes place in the same region of the pressure versus temperature phase diagram in which the density and the diffusion anomalies are present [3,4].

The link between the thermodynamic, dynamic and structural anomalies in water goes as follows. The density of water increases with the increase of temperature by breaking the hydrogen bond (HB) network which decreases the structural order parameter and enhances mobility. In the case of confined water, the link between mobility and structure is affected because the water HB network can be frustrated [5,6], and the water-surface interaction rises as a decisive factor, often

determining the fluid structural and dynamical behavior [7,8]. For example, inside carbon nanotubes (CNTs) water flows four to five orders of magnitude faster than would be predicted from conventional hydrodynamic theory [9]. The high flux depends on the nature of the confining medium [10], the number of water layers [11,12], structural transitions [13–15], and local viscosity [16], to name just a few of the parameters affecting the flow enhancement factor. For CNTs with diameter smaller than 1.2 nm, the diffusion mechanism depends on the competition between wall repulsion and HB formation [17–22] creating a two stage process.

Although the high flux of water inside CNTs is an alternative for separating water from salt ions in desalination processes, this strategy faces the challenge of introducing water inside hydrophobic nanochannels [10,23,7]. One alternative is the application of external electric fields. For instance, in small capillaries the electrostatic boundary conditions strongly influence the permeability of charged species. The electrostatics of a small channel embedded in a medium of very low dielectric constant leads to a large self-energy barrier for ions to enter the confined region [24]. In the case of water entrance in CNTs, fixed charges outside the tube affect the pressure-driven passage of water [25]. Additionally, CNTs filled with water exhibit electro-osmotic flow when an electric field is applied [26].

The idea behind using external electric fields to fill CNTs with water is that the field induces orientation in the water dipole moment which

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overcomes the dielectric barrier at the nanotube [27]. Charge magnitudes between zero to 1.0 e /atom were applied along different lengths of nanotubes to show that the electric charging can be used to manipulate the resistance along the nanotube and the resistance to flow at its entrance [28]. Two complementary effects contribute to the flow. The water dipole orientation inside a CNT is tuned by the electric field, which results in a pumping effect [29]. The dipole orientation also makes water's dielectric constant to be lower in the interface than in the center of the tube [30]. Even though the field is relevant for the water entrance, it also impacts other aspects of water inside the nanotube such as blocking temperature (required for water to escape from the nanotube) and frictional energy barrier [31]. The presence of an electric field can induce phase transitions [32] and the formation of solid ice-like structures inside CNTs [33]. It also affects mechanical properties of water-filled CNTs, as highlighted in recent MD simulations by Ye et al. [34]. They found a divergent effect depending on the electric field direction: longitudinal fields enhance, but transverse fields reduce the elastic modulus and critical buckling stress. The phenomenon is attributed to a competition between the axial and circumferential pressures induced by the polar nature of the water molecules in response to the applied field. For instance, this effect can be used in CNT membranes for separation of multicomponent gas mixtures [35].

In spite of the entrance and mobility of water in CNTs being affected by the introduction of an electric field [36–38], the specific correlation between the nanotube size, direction of the field and HB network is still missing. Here, we address this question by computing through Molecular Dynamics (MD) simulations the diffusion coefficient, the radial distribution function and the number of HBs of water molecules inside CNTs of various diameters. In our simulations we apply the field parallel, transverse and perpendicular to the tube axis. The remainder of the paper is organized as follows. In the next section, the computational details and methods are described. In section III, the main results on the confined water properties are discussed. Summary and Conclusions are presented in the last section.

2. Model and methods

We used the LAMMPS package [39] to perform MD simulations of water confined in CNTs under electric fields. A uniform field was applied in three different directions with different intensities. We considered (n, n) CNTs, with $n = 7, 9, 12, 16, 20$ and 40. We used the rigid four-point TIP4P/2005 [40] water model due to its good performance for computing the water mobility [41,42]. Our simulations indicate a bulk diffusion coefficient of 2.3×10^{-9} m²/s which is in good agreement with theory [43] and experiments [44].

The TIP4P/2005 water is modeled as masses at oxygen and hydrogen sites, where positive charges are placed in the H atoms and the negative charge is placed in a site M along the bisector of the H-O-H angle, coplanar with O and H atoms. The water-water interaction potential is given by Lennard-Jones (LJ) and Coulomb terms, namely:

$$U_{\alpha\beta}(r) = 4 \epsilon_{\alpha\beta} \left[\left(\frac{\sigma_{\alpha\beta}}{r} \right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r} \right)^6 \right] + \frac{1}{4\pi \epsilon_0} \frac{q_\alpha q_\beta}{r}, \quad (1)$$

where α and β represents oxygen, hydrogen, or the fictitious site M . The equilibrium distance between O and H atoms is 0.09572 nm and each hydrogen carries a positive charge $q_H = 0.5564e$. The equilibrium distance between O and M is 0.01546 nm and the negative charge, $-1.1128e$, which neutralizes the molecule is located at M .

For water-CNT interactions, we used O-C LJ parameters defined in a previous work [45]: $\epsilon_{CO} = 0.123$ kcal/mol and $\sigma_{CO} = 0.326$ nm. The LJ and Coulomb interactions' cutoff was set to 1 nm. In all simulations the geometry of the water molecules was constrained by the SHAKE algorithm [46]. Long-range Coulomb interactions were handled using the Particle-Particle Mesh (PPPM) method.

The simulations were conducted in the canonical NVT ensemble

Table 1

Nanotube chirality, diameter (d), length (L_z) and the average amount of water molecules inside each nanotube.

CNT	d (nm)	L_z (nm)	H ₂ O
(7,7)	0.957	123.465	901
(9,9)	1.22	50.66	908
(12,12)	1.63	22.63	901
(16,16)	2.17	11.07	911
(20,20)	2.71	10.33	1440
(40,40)	5.425	7.87	5221

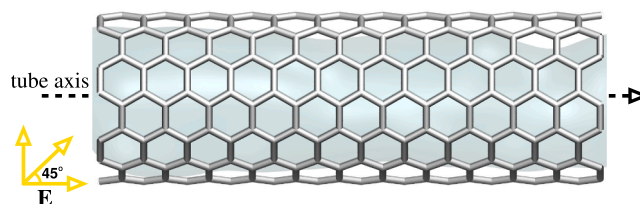


Fig. 1. Schematic depiction of the computational framework: side view of a CNT (7,7) filled with water under an electric field E . The field can be either parallel (0°), perpendicular (90°) or forming an angle of 45° to the nanotube axis.

with temperature T set to 300 K by a Nosé-Hoover thermostat [47]. Initial geometry and number of particles were based on previous works [15,22,45,48]. The amount of water molecules and nanotube details are given in Table 1. Periodic boundary conditions were applied in the axial direction of the tubes, as shown in Fig. 1, which results in isolated infinite nanotubes. In order to keep things as simple as possible, positions of the carbon atoms were fixed, i.e., not integrated during the simulations. The system was equilibrated for 10 ns with timestep set to 1 fs. Finally, simulations of 10 ns of data accumulation were performed.

We analyzed the diffusion mechanism of water by the scaling behavior between the mean squared displacement (MSD) and time:

$$\langle |\vec{r}(t) - \vec{r}(0)|^2 \rangle = ADt^n \quad (2)$$

where the angular brackets denote an average over time origins and all water molecules, $\vec{r}(t)$ is the displacement of a molecule during the time interval t , A is a constant equal to 1 and D stands for the diffusion coefficient. The n exponent refers to the diffusion regime: $n = 1$ for the linear Fickian diffusion, $n > 1$ for superdiffusive and $n < 1$ for subdiffusive regime. The statistical error in diffusion measurements could be reduced by averaging over all MSD components, but the nanopore confinement in x and y directions hinders molecules' radial displacement. Therefore, radial diffusion is almost zero for all the cases studied here and only the axial diffusion D_z is considered. Three sets of simulations with different initial thermal velocity distributions were averaged to build each MSD curve.

The number of HBs was computed using a geometrical criteria: $\alpha \leq 30^\circ$ and $|\vec{r}_{OO}| \leq 3.50\text{\AA}$, where α is the $OH \cdots O$ angle and $|\vec{r}_{OO}|$ is the distance between two oxygen atoms.

3. Results and discussion

First, we analyze the impact of the field strength and directionality in the water mobility. As a polar substance, water is not only susceptible to the electrical field magnitude, but also to the field direction inside the channel. Fig. 2(a)–(c) illustrates the diffusion coefficient as a function of the nanotube radius for $E = 0.5, 0.75$ and 1.0 V/nm. The field was applied in three different directions: parallel to the tube axis (referred as 0°), perpendicular (90°) and forming an angle of 45° with the tube axis. In the case of no electric field, the diffusion is not

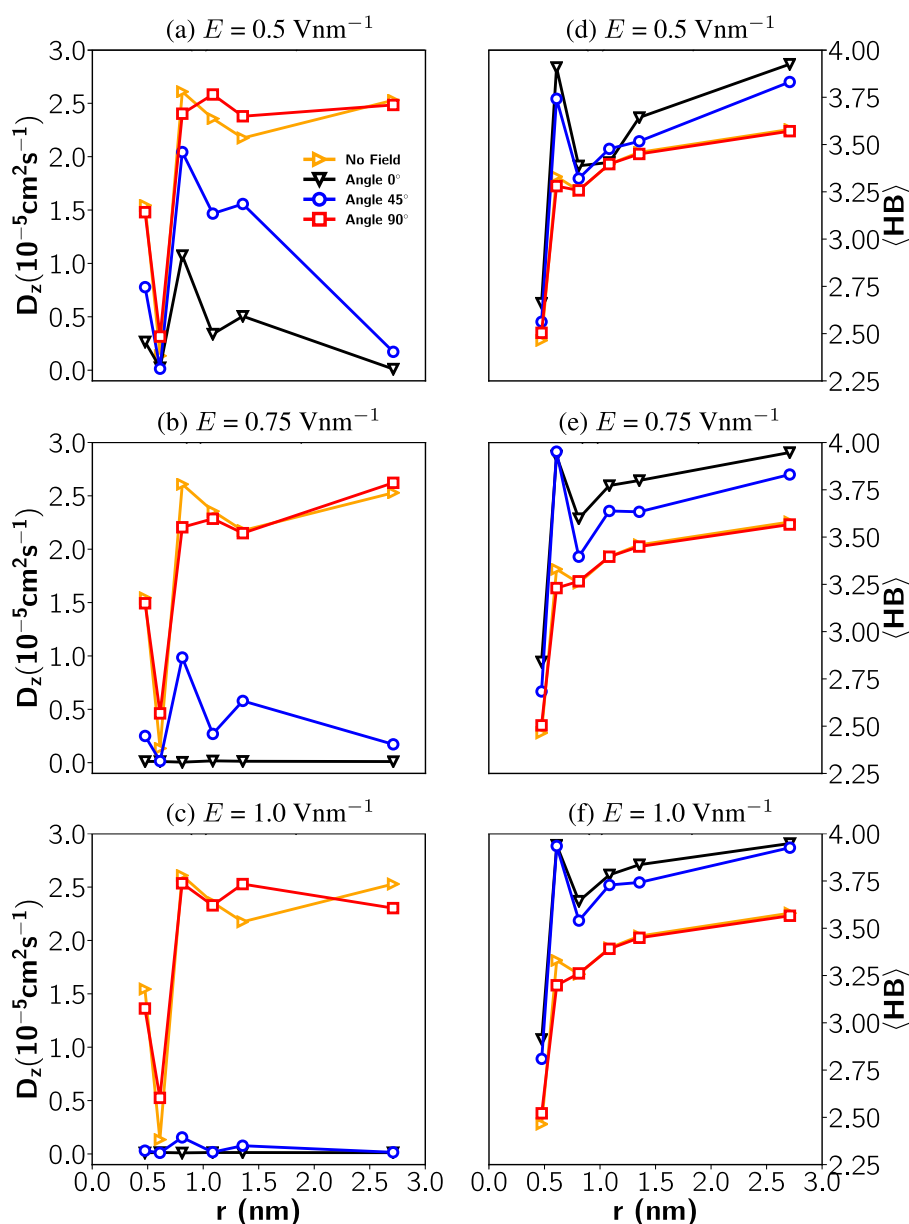


Fig. 2. Water diffusion coefficient (left) and number of HBs (right) as a function of the nanotube radius r under external electric fields $E =$ (a, d) 0.5 V/nm , (b, e) 0.75 V/nm , and (c, f) 1.0 V/nm applied in different directions.

monotonic with the nanotube radius. While water shows no diffusion inside 1.2 nm diameter long (9,9) nanotube, for larger nanotubes the diffusion increases with r and tends to the bulk value, which is in accordance with the work of Farimani and Aluru [19].

When the 0.5 V/nm field is applied perpendicular to the nanotube axis, the mobility behaves very similarly to the zero field case. Fig. 2(d)–(f) shows the number of HBs versus nanotube radius for different fields and orientations. In the case of the perpendicular field the number of HBs is almost identical to the zero field case, indicating a negligible impact in the water mobility. Remarkably, when the field is applied parallel to the tube axis (0°), the diffusion of water decreases drastically in agreement with previous theoretical works [33]. We found that the decrease in mobility goes along with an increase in the number of HBs. The electric field applied along the tube axis increases the connection through HBs and consequently hinders the water mobility.

For the 45° field, we observe intermediate values in the mobility between the parallel and the perpendicular case, with a decrease in the diffusion and an increase in the number of HBs.

If we increase the field magnitude to 0.75 V/nm , Figs. 2(b) and (e)

show that even for 45° field water forms a HB network and mobility decreases. The same effect is observed for 1.0 V/nm field. The comparison between the diffusion and the number of HBs is consistent with the idea that as the HB network is formed the diffusion decreases.

In order to understand how the increase and direction impacts the mobility of water for specific nanotubes, in Fig. 3 we present the water diffusion coefficient as a function of the applied field intensity for each direction and fixed nanotube radius. For the field applied perpendicular to the nanotube axis, the particles diffuse as in the zero field case with the exception of the (9,9) nanotube. In this case, the diffusion increases almost linearly with E and becomes ~ 3 times larger than the zero field case. For other directions (0° and 45°) the water diffusion is decreased as we increase E and becomes almost zero for $E = 1 \text{ V/nm}$. In this case the field perpendicular to the axis disrupts the perfect HB network present for the zero field system where the mobility is zero since the system forms an ice-like structure. By laterally stressing the HB's the system forms a state that is no longer ice-like.

An important aspect regarding the mobility of confined water is the close relation between structural and dynamical behavior [7,15,8,49,50]. By applying an electric field, we have observed

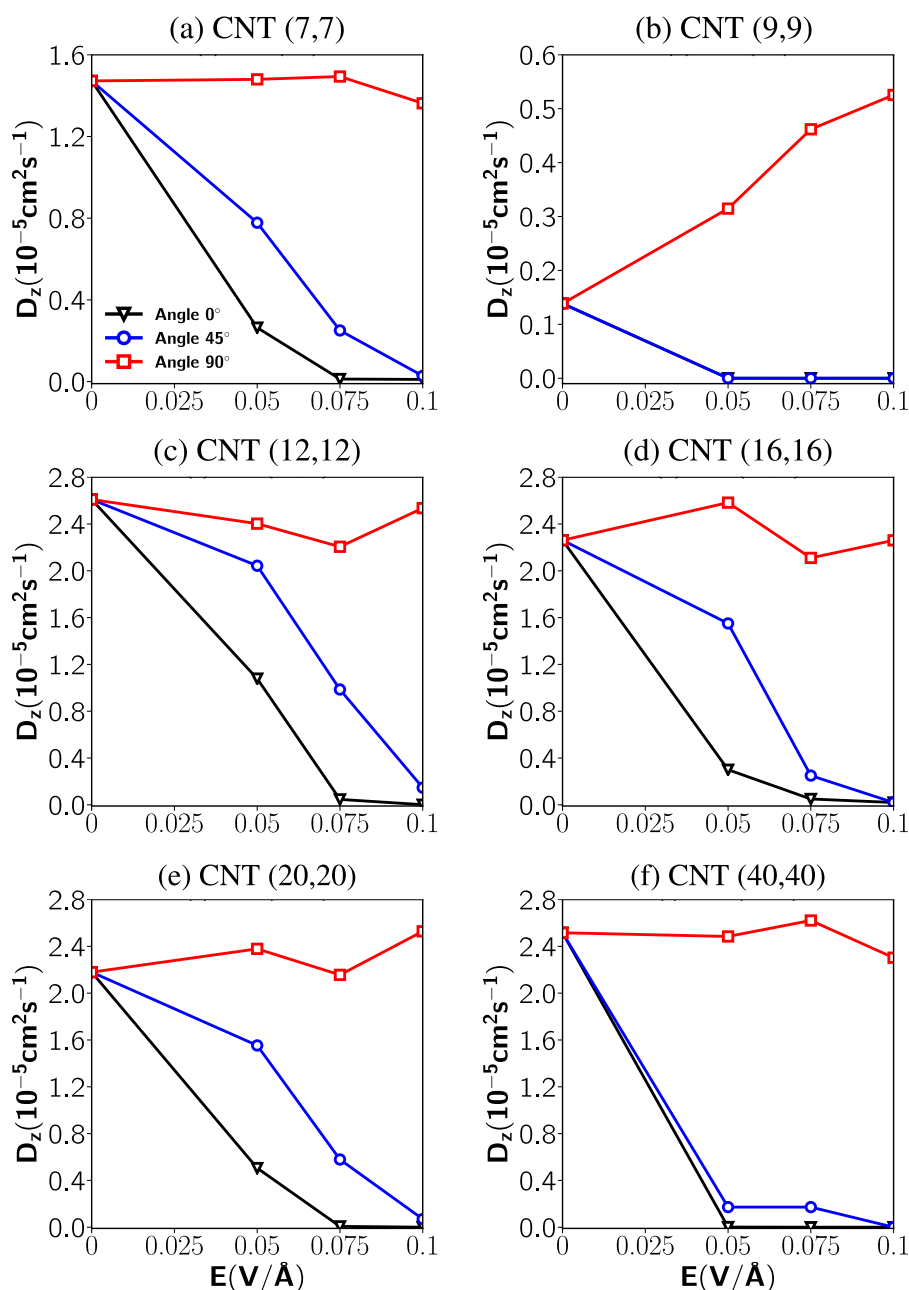


Fig. 3. Water diffusion coefficient as a function of the electric field's magnitude.

dynamical modifications that can be related to structural transitions of water molecules inside the tube. For instance, Winarto et al. [33] found that the water dipole moments can align with the electric field inside the nanotube to increase water density and form ordered ice-like structures. This mechanism induces a transition from liquid to ice nanotubes in a wide range of CNT diameters.

In order to clarify the influence of field direction in the water structure, we show in Fig. 4 the radial density profile of the oxygen atoms as a function of r for the CNT (9,9). This quantity is calculated by dividing the inner of the CNT in concentric cylindrical shells and averaging the number of oxygen atoms in each shell along the simulation. We can observe that the parallel electric field (0°) induces water molecules to occupy positions closer to the center of the tube as compared to the no field case. Additionally, we observe highly ordered ring-like structures, as shown in the inset featuring a frontal snapshot of the system. This strongly packed structure can be linked to an ice-like phase, in accordance with the work of Winarto et al. [33], which can

explain the lowering in water diffusion. It is also interesting to note that as the oxygen atoms aligns with the parallel field, they are carried away from the wall. This distance from the wall, also recognized as a “de-wetting” transition, can lead to a decrease in the dielectric constant as suggested in experiments with planar confinement [30].

On the other hand, as we apply the electric field perpendicular (90°) to the tube axis, the water molecules are pushed closer to the hydrophobic CNT wall, breaking the ring structure and increasing the mobility, as shown in Fig. 3(b). The mechanism behind this enhanced diffusion can be understood in terms of the energetic stability, since it is energetically unfavorable for water to be closer to the wall. Particularly, in this case the field affects the water's dipole moment melting its ordered structure at the nanotube wall, leading now to a “wetting” state [51]. As a result, the water-wall repulsion increases water's mean displacement. In other words, in the search for a more stable structure the water molecules experience an increment in mobility.

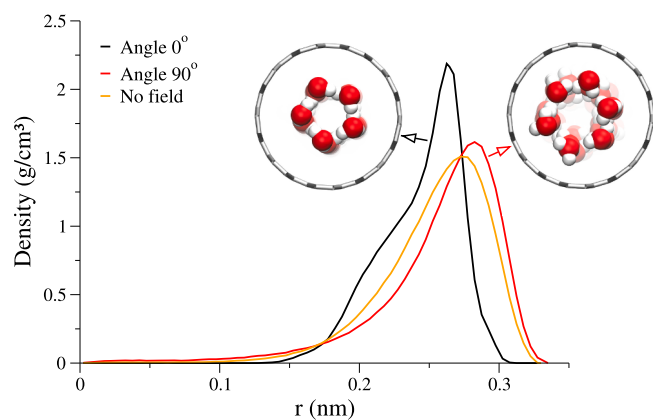


Fig. 4. Radial density profile of oxygen atoms inside CNT (9,9) for $E = 1.0 \text{ Vnm}^{-1}$ applied parallel (black line) and perpendicular (red line) to the tube axis. The orange line stands for no applied field and $r = 0$ is at the center of the tube.

4. Summary and conclusions

We studied the influence of electric fields in diffusion, HB network and structure of water confined in CNTs through MD simulations. We found size-dependent diffusion of water under several electric field directions and intensities. There is always a local maxima in diffusion for intermediate nanotubes ($r = 0.8\text{--}1.0 \text{ nm}$).

We also found that large fields induce the orientation of water's dipole moment and in the case of fields applied parallel to the tube, the network becomes more organized and the diffusion decreases. For fields applied perpendicular to the nanotube axis, water dynamics is similar with the no field case for most of the CNTs. The exception is the CNT (9,9) where the diffusion is enhanced by a factor of 3 when we increase the perpendicular field from 0 to 1 V/nm.

These results open the possibility of tuning the water flux inside a CNT by only varying the direction of the applied electric field. It is particularly relevant for application in nanotube membranes, where the water's dipole moment can constitute as an important factor for flux control.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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