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Water flow in carbon nanotubes: The role of tube chirality

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1 Simulation details

In classical molecular dynamics (MD) motion of the atoms are described by Newtonian equations of motion. The equation of motion of a particle i with mass m and position r acted upon by a net force F is given by:

$$m_{\mathrm{i}} \frac{d^2 \boldsymbol{r}_{\mathrm{i}}}{dt^2} = F_{\mathrm{i}}(t) \tag{1}$$

where F_{i} can be expressed as the gradient of the potential energy (U):

$$F_{\mathrm{i}}(r_1, r_2....., r_{\mathrm{N}}) = -\nabla U(r_1, r_2....., r_{\mathrm{N}}) \tag{2}$$

The potential energy consists of bonded $U(\vec{r})$ and non-bonded $U(r_{\mathrm{ij}})$ interactions. In our study, we used the harmonic potentials for the bond stretching and angle bending interactions.

$$U(\vec{r}) = \sum_{\mathrm{bond}} \frac{k_{\mathrm{bond}}}{2} (r - r_0)^2 + \sum_{\mathrm{angle}} \frac{k_{\mathrm{angle}}}{2} (\theta - \theta_0)^2 \tag{3}$$

where k_{bond} and k_{angle} are the coefficients of the harmonic potentials of the bond stretching and angle bending, respectively. r_0 and θ_0 represents the reference bond length and angle. Non-bonded terms include van der Waals (vdW) and electrostatic interactions, which were modeled using 12-6 Lennard-Jones (LJ) and coulombic potentials, respectively.

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Table S1: Interaction parameters used for the study.

Parameter	Value
l_{OH} (nm)	0.1
θ_{OH}	109.47
$q_{\mathrm{H}}(e)$	0.4238
$q_{\mathrm{O}}(e)$	-0.8476
σ_{OO} (nm)	0.3166
ϵ_{OO} (kcal/mol)	0.15535
σ_{CO} (nm)	0.3190
ϵ_{CO} (kcal/mol)	0.09369

$$U(r_{\mathrm{ij}}) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \left(4\epsilon_{ij} \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] + \frac{q_{\mathrm{i}} q_{\mathrm{j}}}{4\pi\epsilon_0 r_{\mathrm{ij}}} \right) \tag{4}$$

We performed MD simulations using the LAMMPS software package. [1] Carbon-carbon interactions are modeled with the reactive empirical bond order (REBO) potential [2], which has been widely used to study graphene and CNTs. SPC/E model was used for water molecules, whose bulk property predictions agree well with experiments [3]. Fluid-wall Lennard-Jones interaction parameters were taken from Werder *et al.* [4], and the interactions were truncated at a distance of 1 nm. Long range electrostatic interactions were handled by the Wolf method, [5, 6] using a 1 nm cutoff and a damping parameter of 2.25 nm^{-1}. The parameters for the interaction potentials are given in TABLE I.

Simulations were performed in the NVT ensemble at 300 K temperature. We coupled the Nosé-Hoover thermostat to the CNT walls to maintain the average system temperature. The Nosé-Hoover thermostat modulates the kinetic temperature by coupling the system to a “fictitious” heat bath (η) of mass Q. The average system temperature approaches the target value by scaling the velocities of each particle by a factor P_η. The equation of motion of a particle can be written as:

$$\frac{d^2\boldsymbol{r}_{\mathrm{i}}}{dt^2} = \frac{\boldsymbol{F}_{\mathrm{i}}(\boldsymbol{r}_{\mathrm{i}})}{m_{\mathrm{i}}} - \frac{P_\eta}{Q}\frac{d\boldsymbol{r}_{\mathrm{i}}}{dt} \tag{5}$$

The net momentum of the CNT was set to zero at each time step to avoid drifting of the CNT due to the force imparted by the water.

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