

Supporting Information

Spontaneous Directional Motion of Water Molecules in Single-Walled Carbon Nanotube with a Stiffness Gradient

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S1. Calculation Details of Displacements

The trajectories of water molecules were stored every 1 ps. At every picosecond, the coordinates of five water molecules were recorded. The centre of the water molecules was used to represent the position of the water molecule chain, i.e. the average value of the coordinates of these five water molecules. The variation in the coordinates along the nanotube axis direction was calculated to be the displacement. For example, from simulation time 0, 1, ..., i , ... to 50 ps, the coordinate of the water-molecule chain along the nanotube axis direction was x_0, x_1, \dots, x_i to x_{50} Å, then the corresponding displacements were 0, $x_1-x_0, \dots, x_i-x_0, \dots, x_{50}-x_0$ Å.

S2. Displacements with Different Initial Positions

Figure S1 shows the displacements of the water-molecule chain as a function of time with different initial positions. It is seen that water molecules initially located at the soft region exhibit a slightly faster movement.

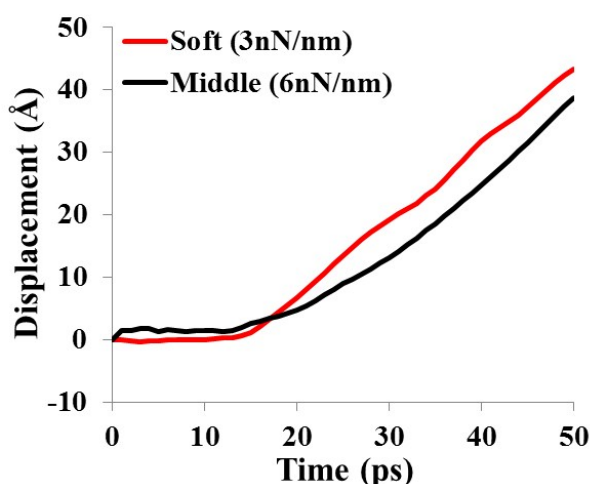


Figure S1. Displacements of the water-molecule chain as a function of time at different initial positions.

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S3. Friction forces in (6, 6), (7, 7), (8, 8) and (10, 10) CNTs

Figure S2 plots the friction forces in (6, 6), (7, 7), (8, 8) and (10, 10) CNTs. It is seen that the friction force in (7,7) CNT is comparable to that in (6, 6) CNT, while the friction forces in (8, 8) and (10, 10) are smaller than that in (6, 6) CNT.

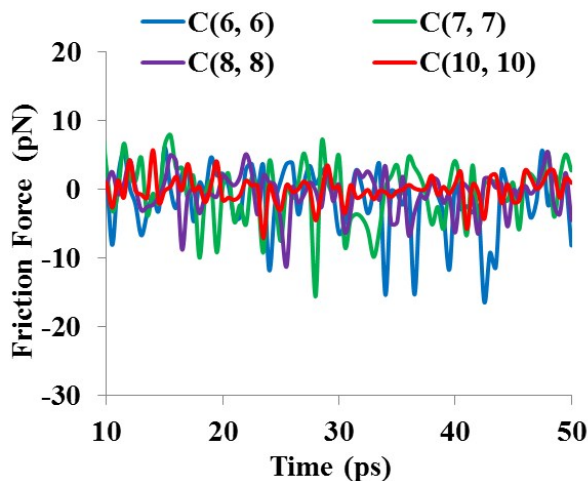


Figure S2. Friction forces in (6, 6), (7, 7), (8, 8) and (10, 10) CNTs.

S4. Description of movies.

Video S1-Gradient1: water transportation in (6,6) CNT with stiffness gradient of 1 nN/nm^2

Video S2-Gradient2: water transportation in (6,6) CNT with stiffness gradient of 0.7 nN/nm^2

Video S3-Gradient3: water transportation in (6,6) CNT with stiffness gradient of 0 nN/nm^2

Video S4-340K: water transportation in (6,6) CNT with stiffness gradient of 1 nN/nm^2 at the temperature of 340K

Video S5-360K: water transportation in (6,6) CNT with stiffness gradient of 1 nN/nm^2 at the temperature of 360K.

Video S6-(5,5)CNT: water transportation in (5,5) CNT with stiffness gradient of 1 nN/nm^2 .

Video S7-(7,7)CNT: water transportation in (7,7) CNT with stiffness gradient of 1 nN/nm^2 .

Video S8-(10,10)CNT: water transportation in (10,10) CNT with stiffness gradient of 1 nN/nm^2 .