Supporting Information

Rapid Water Transportation through Narrow One-Dimensional Channels by Restricted Hydrogen Bonds

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Contents

1. TEM images

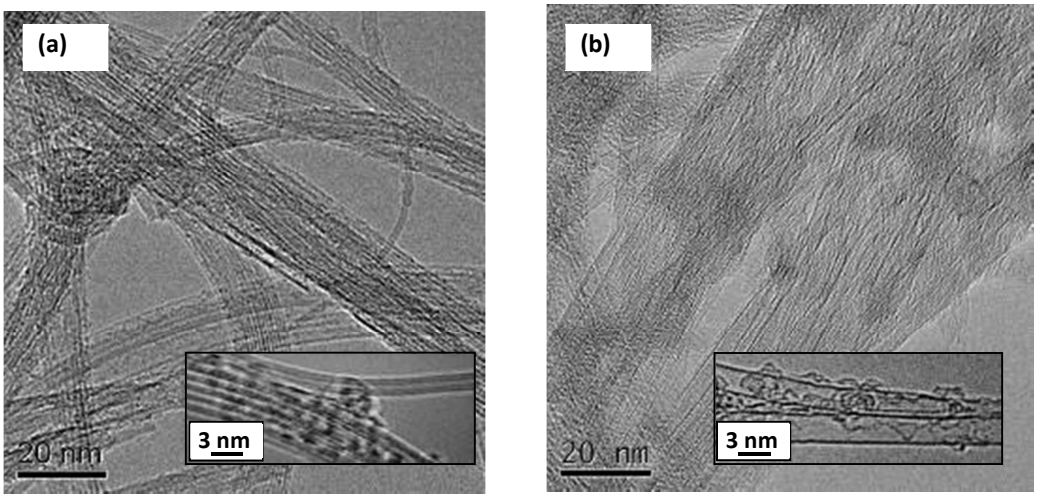

Figure S1. TEM images of **(a)** double-walled CNTs and **(b)** single-walled CNTs. The inserted images are high magnification.

2. MD simulation procedure

The initial configurations of 26 and 470 water molecules, which correspond to filling factor 0.25 in carbon nanotubes of MD simulation boxes, were determined by canonical ensemble Monte Carlo (CEMC) simulations for 1D channels of diameters 1 and 2 nm at 303 K. The number of calculation cycles was 3×10^6 steps, and the unit cell was $4 \times 4 \times 6$ nm^3. The calculated water configurations were used as the initial configurations of the subsequent MD simulations, as shown in Figure S2. The water configurations after CEMC simulation were divided into right and left 3-nm sides, and then were set on both edges of the unit cell in the MD simulations. Here, we assume that water vapor is stacked in the entrance of carbon nanotubes, because experimental water vapor adsorption was significantly slow rather than water vapor diffusion in bulk phase, as shown in Figure S4. Therefore, the initial conditions of MD simulations correspond with the start of the 2nd water adsorption step, as shown in Figure S4c, as mentioned later. The unit cell in the MD simulations was $4 \times 4 \times 12$ nm^3. The snapshots in the blue box depicted in Figure S2 are shown as insets in Figure 3. The filling factor of water in Figure 3 was determined by the number of water molecules in the blue box in Figure S2. The snapshots in Figure 3b were abstracted from the red box in Figure S2.

The five-site transferable interaction potential (TIP5P) model of a water molecule was used for simulating water adsorption, in combination with the Lennard-Jones interactions between oxygen atoms and the electrostatic interactions between partial charges on the sites of hydrogen atoms and lone pairs.

$$\phi_{ij}(r) = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right] + \sum_{i}^{4}\sum_{j}^{4}\frac{1}{4\pi\varepsilon_0}\frac{q_i q_j}{r_{ij}}$$

Here, ε_{ij} and σ_{ij} are the water potential-well depth (80.5 K) and the effective diameter (0.312 nm), respectively. The absolute value of the partial charge q_i is 3.86×10^{-20} C. Ewald summation was applied to long-range coulomb interactions between water molecules. We assume that a carbon atom is neutral and that the interaction between water and the graphitic carbon wall comes from the sum of the Lennard-Jones interactions. The intermolecular potential depth and collision diameter of a water molecule and a carbon atom of a 1D channel are 49.26 K and 0.3268 nm, respectively. One-dimensional periodic boundary conditions were adopted.

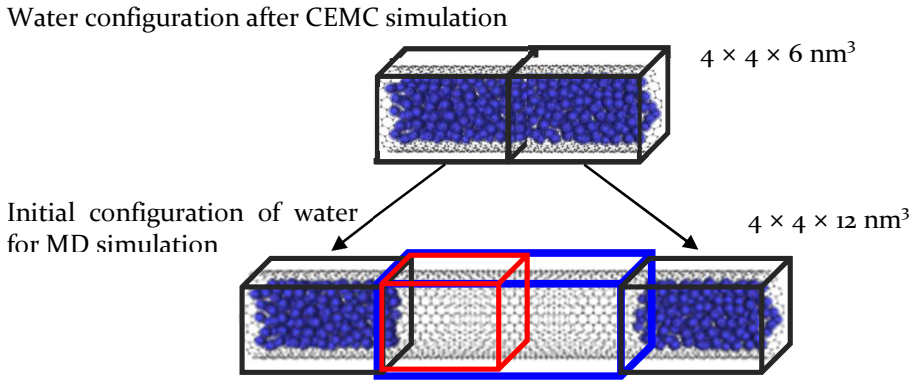

Figure S2. Schematic images of initial configurations in MD simulations. The blue box is for calculations of the filling factors in Figure 3a and average number of hydrogen bonds in Figure 4. The red box is for depicting snapshots of Figure 3b.

3. Characterization of nanospaces of narrow and wide 1D channels

The micropore volumes and average tube diameters of narrow and wide 1D channels were evaluated from the N_2 adsorption isotherms using the established α_S analysis.

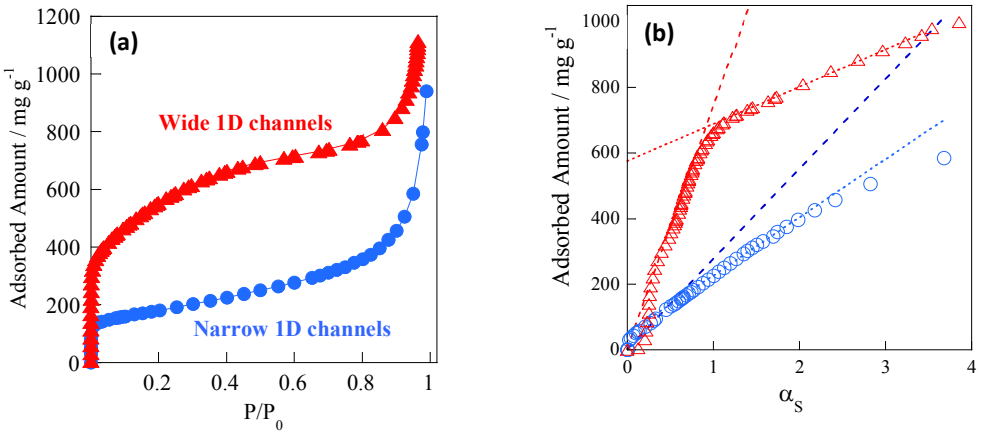

Figure S3. (a) N_2 adsorption isotherms at 77 K for narrow and wide 1D channels and **(b)** the α_s plots of N_2 adsorption isotherms.

Table S1. Structural analysis of narrow and wide 1D channels from α_s analysis.

	Micropore Volume / $cm^3\ g^{-1}$	Specific Surface Area / $m^2\ g^{-1}$	Average Tube Diameter / nm
Narrow 1D channels	0.06	580	1.2
Wide 1D channels	0.69	154	2.2

4. Water vapor adsorption rates of narrow and wide 1D channels

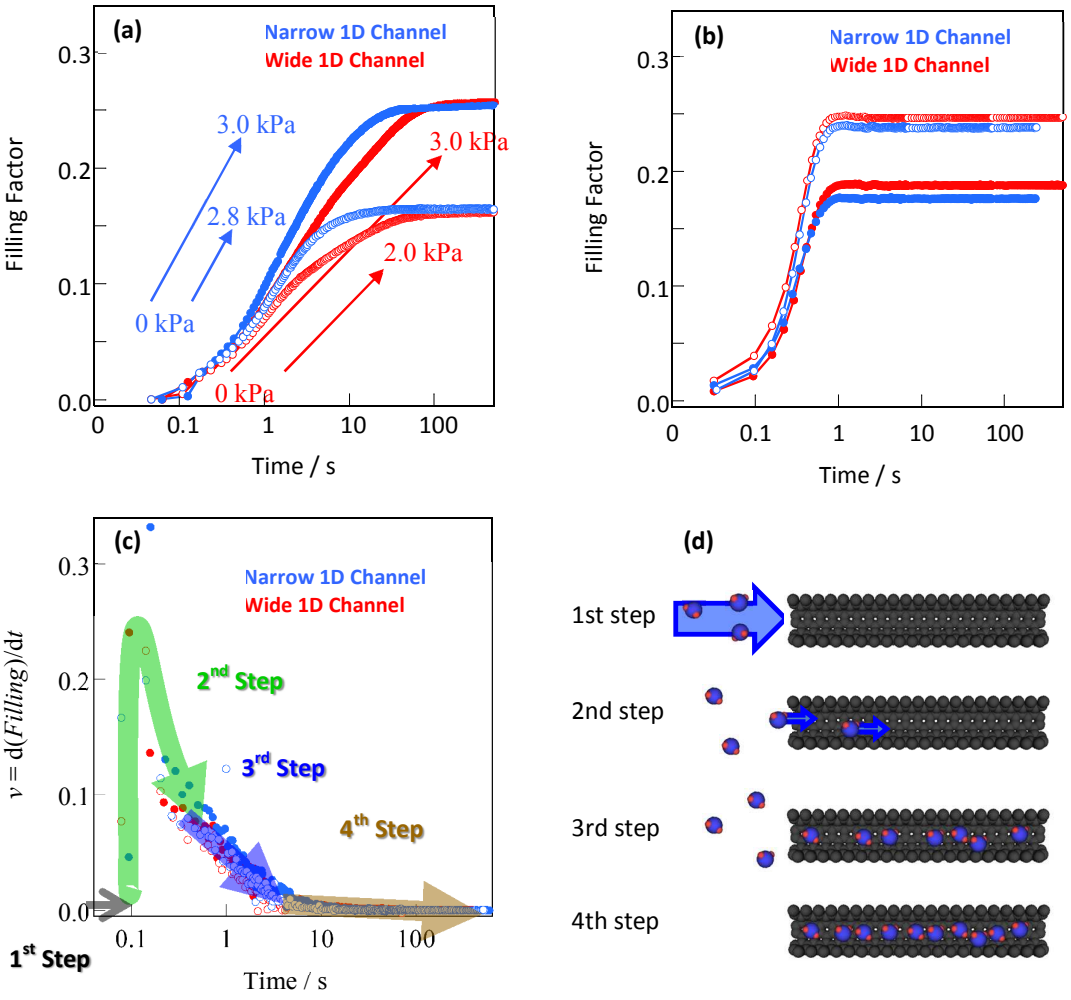

Figure S4. Changes of filling factors of water vapor **(a)** and SF_6 **(b)** in narrow and wide 1D channels. Adsorption rates of water vapor **(c)** and schematic images of water adsorption **(d)**.

5. Snapshots of water in the narrow and wide 1D channels, and transportation diffusion coefficients

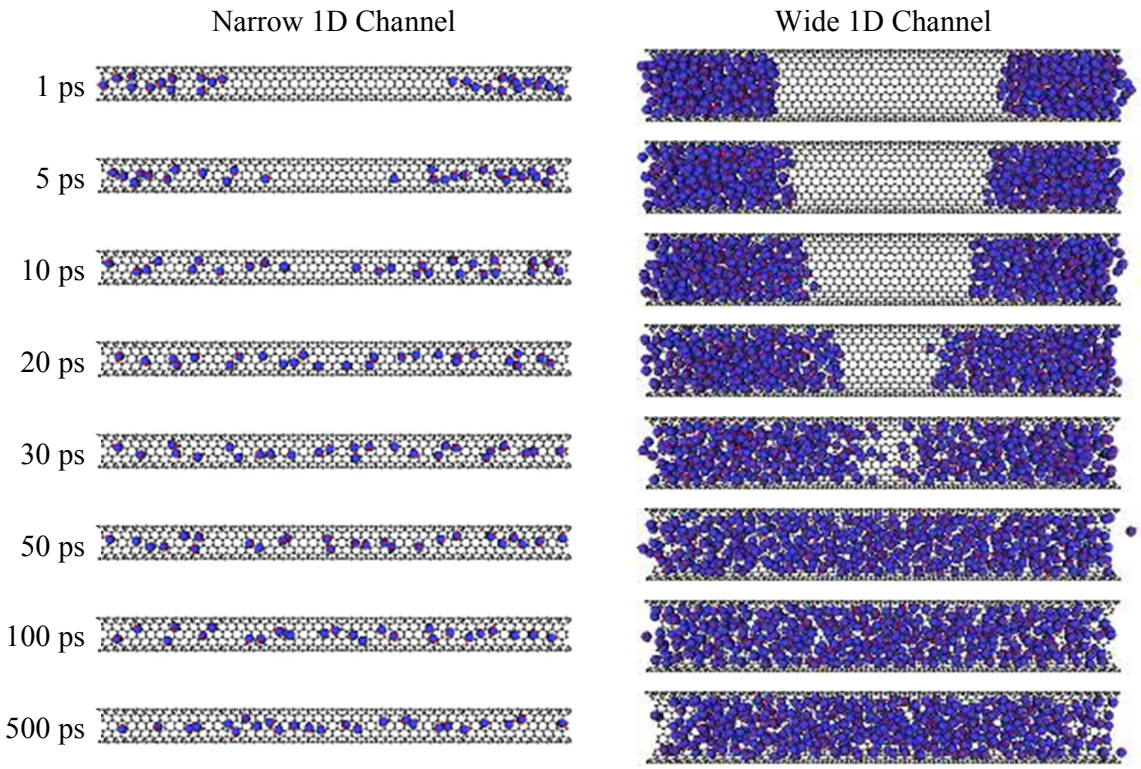

Figure S5. Snapshots of water in both 1D channels from MD simulations.

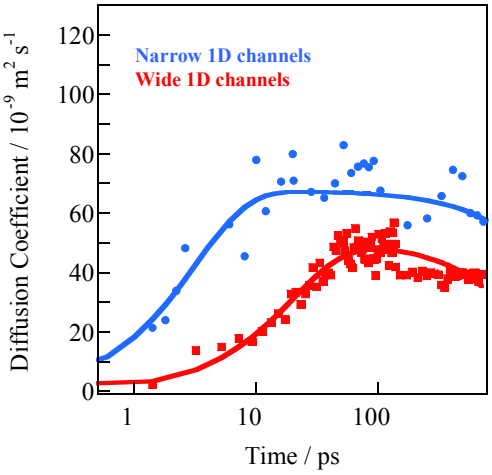

Figure S6. Transport diffusion coefficient of water in both 1D channels from MD simulations.