Electronic Supplementary Material (ESI) for Nanoscale Horizons.

Supporting Information for

Wetting hysteresis induces effective unidirectional water transport through a fluctuating nanochannel

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Other supplementary materials for this manuscript include the following:

- Movies S1 to S5

Similarity of the reversed Carnot cycle

To understand the hysteresis phenomena in the water pump system, we considered the correspondence between the hysteresis loop and the reversed Carnot cycle. Four processes exist in the reversed Carnot cycle: (a) adiabatic compression, (b) isothermal compression, (c) adiabatic expansion, and (d) isothermal expansion, as shown in Fig. S1A. The processes of the constant frequency water pump (Fig. 3B) could roughly correspond to these four processes: (a) adiabatic compression: contract without outflow, (b) isothermal compression: contract with outflow, (c) adiabatic expansion: expand without inflow, and (d) isothermal expansion: expand with inflow, as shown in Fig. S1B.

In the contraction process without outflow (a), the channel wall performs work on water molecules, thus increasing their kinetic energy. Conversely, in the expansion process without inflow (c), water molecules work on the channel wall, and their kinetic energy decrease. When no outflow and inflow occur, work is performed adiabatically, and the temperature should increase/decrease in the contraction/expansion processes, respectively.

In the contraction process with outflow (b), the channel wall performs work on the water molecules. Their kinetic energy momentarily increases; however, any increase in temperature is suppressed when a water molecule is pushed out from the channel. In this process, the temperature does not always increase, but increases and decreases repeatedly. Thus, this process can be associated to isothermal compression. Similarly, in the expansion process with inflow (d), the kinetic energy of water molecules decreases, but the temperature decreases and increases repeatedly because of the penetration of water molecules. This process could also be associated to the isothermal expansion.

The reversed Carnot cycle can produce a heat flow using energy provided from the outside, and its efficiency is the theoretical maximum. The nano water pump proposed in this study produces a flow of water molecules using a radius change of the channel. Because the flow of water molecules corresponds to the heat flow, the operating mechanism of the water pump is similar to that of the reversed Carnot cycle. Therefore, the water pump can be regarded as a nano scale heat pump. If the change in the kinetic energy of water molecules due to the radius change of the channel corresponds to the adiabatic temperature change, the water pump is expected to behave with a high energy efficiency as in the reversed Carnot cycle.

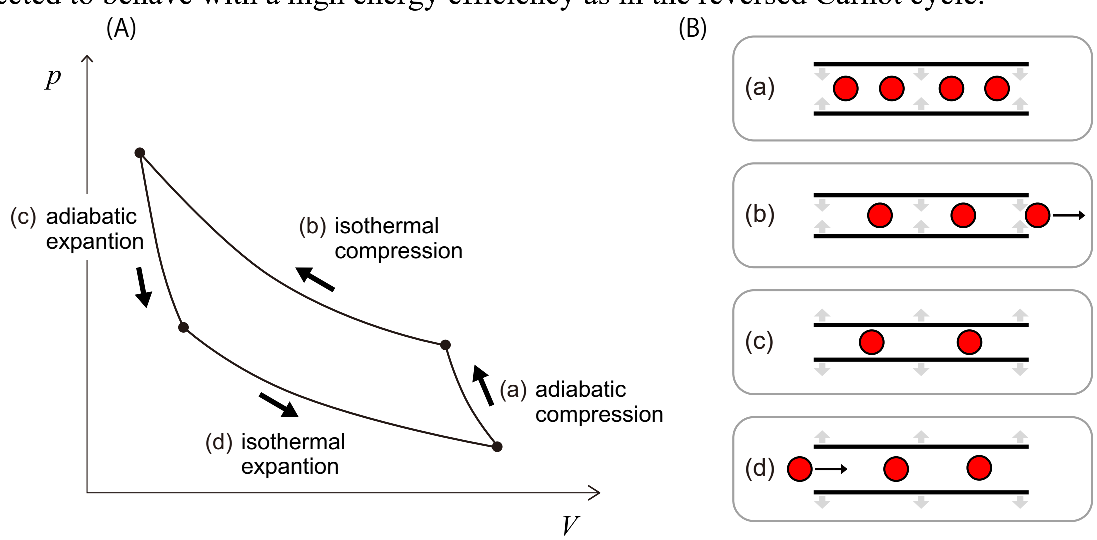

Fig. S1. Four processes of the reversed Carnot cycle (A) and corresponding behavior of water molecules in the channel whose radius changes at constant frequency (B).

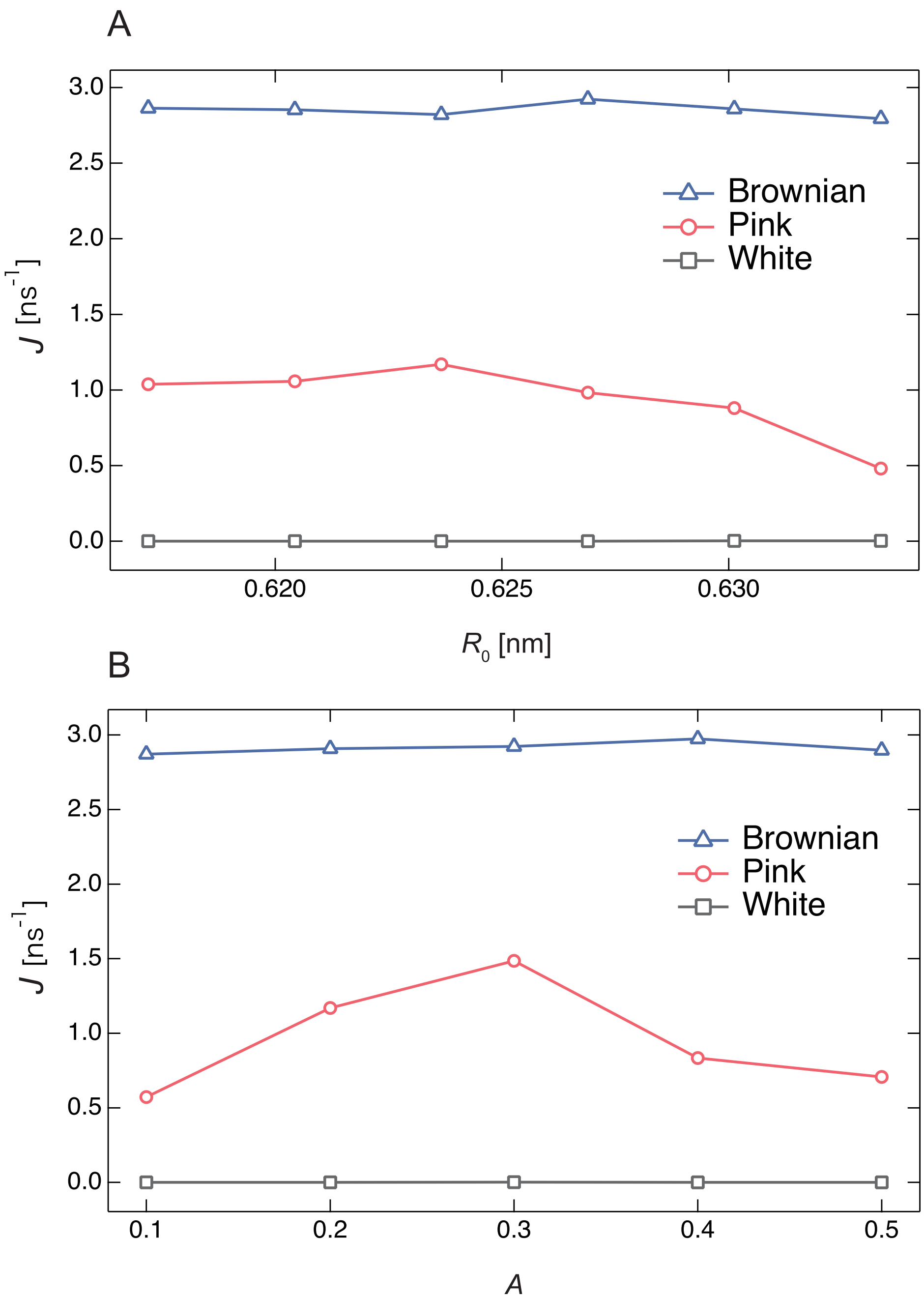

Fig. S2. Transport rate of water molecules depending on (A) average radius, R_0 and (B) noise amplitude, A.

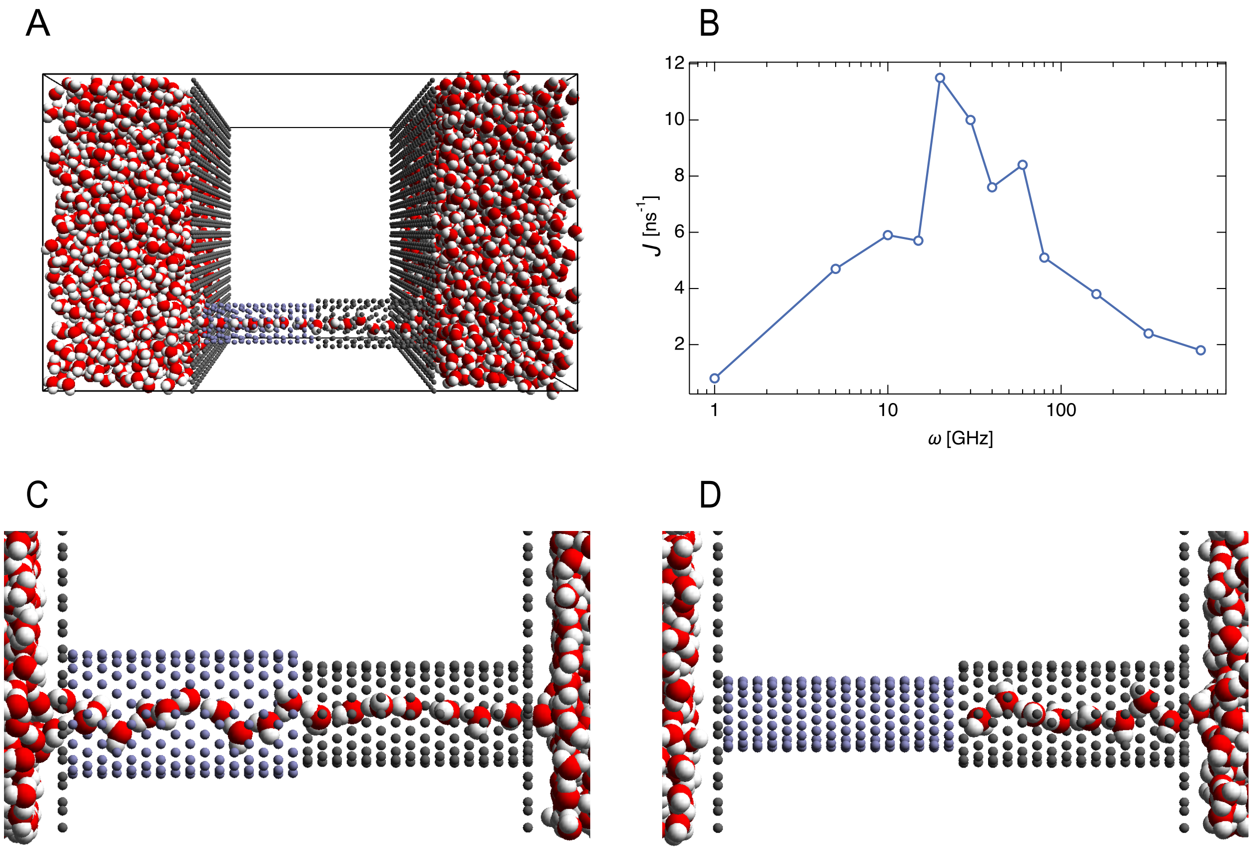

Fig. S3. (A) System of all atomistic (molecular dynamics) simulation. (B) Asymmetric transport rate of water molecules as nanochannel radius changes according to sine wave ($R = A\sin(\omega t) + R_0$). Vertical and horizontal axes represent the transport rate J in ns^{-1} unit, and frequency ω of sine curve in GHz unit, respectively. (C and D) Snapshots of wet and dry states in the nanochannel.

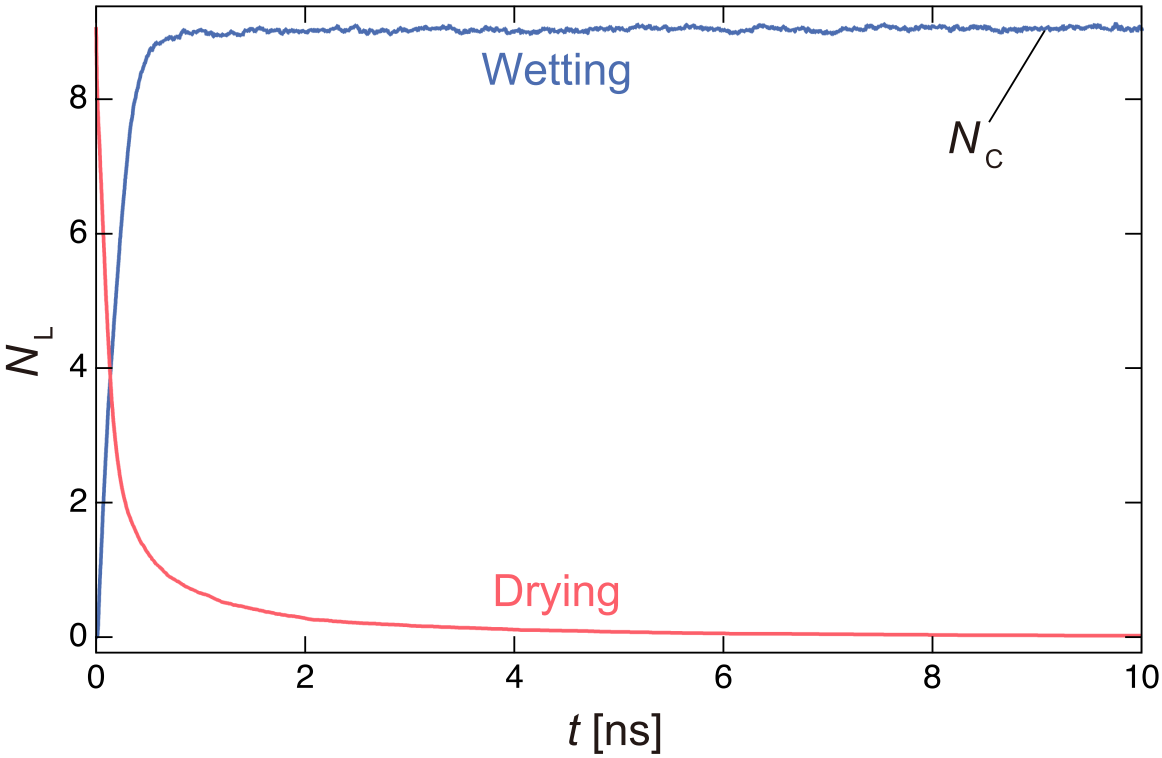

Fig. S4. Temporal change of water molecules in the left half of the channel immediately after a sudden expansion (Wetting) or contraction (Drying) of the channel radius. The number of water molecules in steady state in the wetting process is defined as N_c. Each curve is plotted based on the averaged data over five hundred independent simulations.

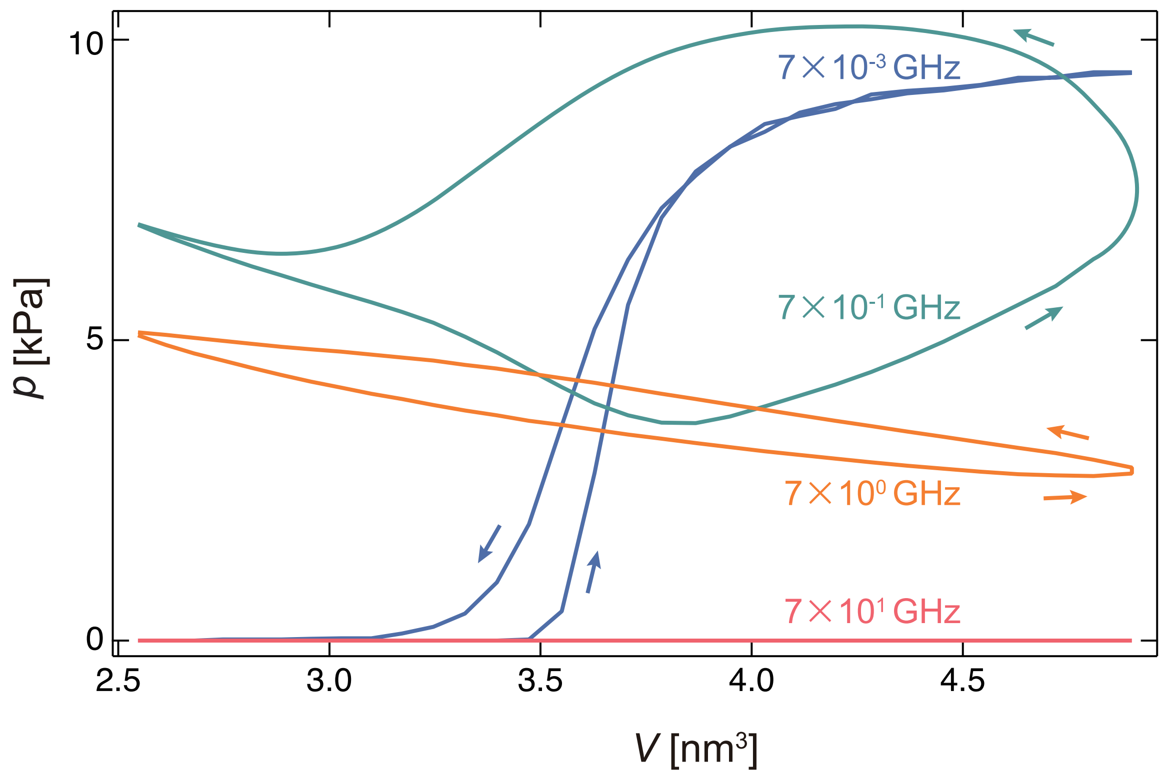

Fig. S5. Pressure-Volume phase diagram when the channel radius is controlled according to a sine wave. The perpendicular and horizontal axes represent the pressure and the volume of the nanochannel, respectively.

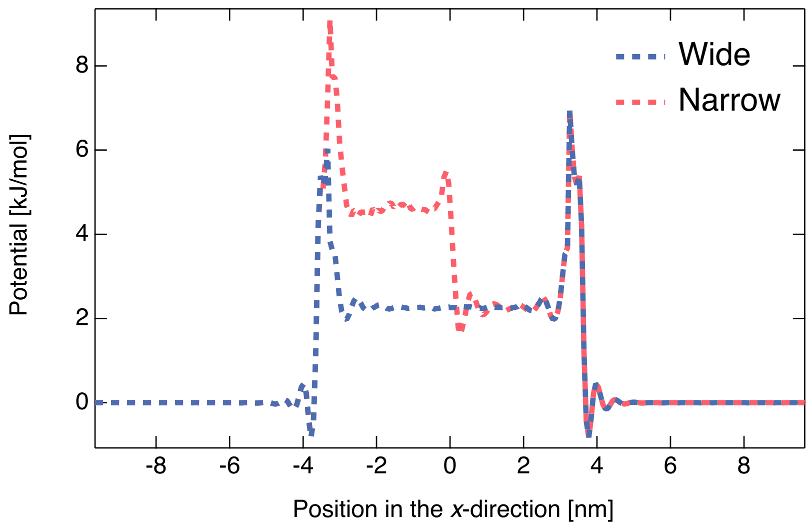

Fig. S6. Effective potential curves estimated by the water density distributions in the *x*-direction, $\varphi(x) = -k_B T \ln[\rho(x)/\rho_0]$ where ρ_0 is density in bulk.

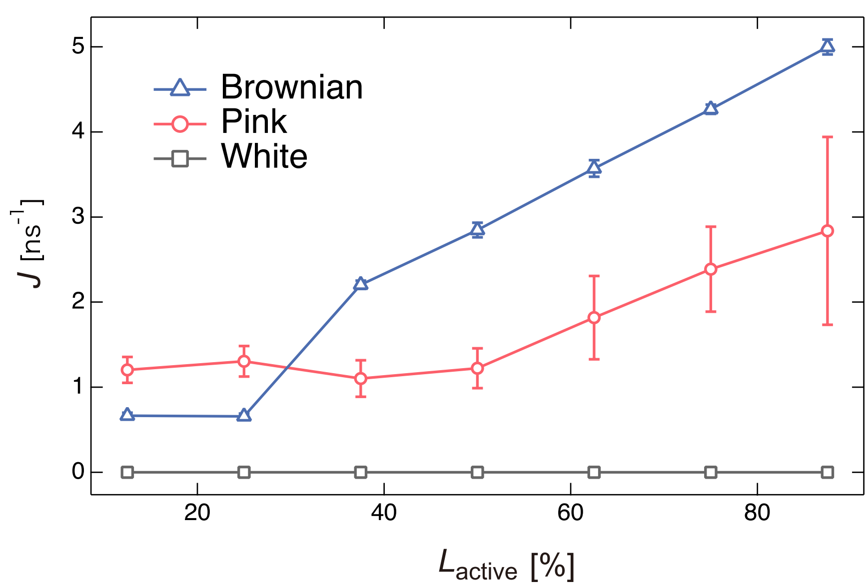

Fig. S7. Transport rate of water molecules depending on the active length (L_{active}) of channel.

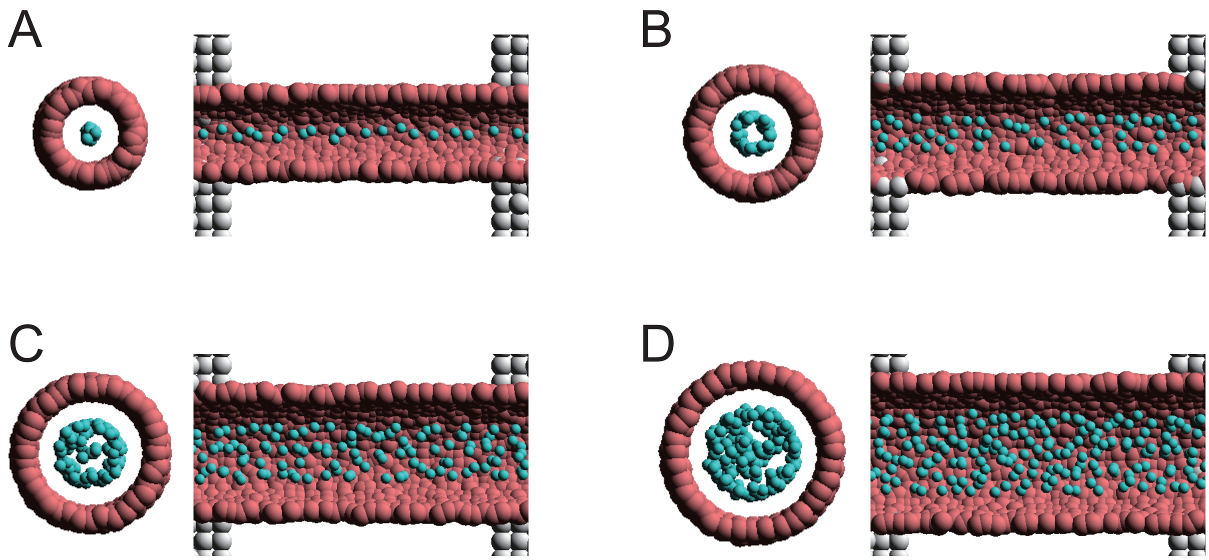

Fig. S8. Snapshots of equilibrium states inside nanochannels when the diameters are (A) 1.42 nm, (B) 1.81 nm, (C) 2.20 nm, and (D) 2.58 nm.

Movie S1.

Equilibrium state (passive mode) of our pump system.

Movie S2.

Water transport behaviour of an active pump model when the radius is varied according to $1/f^2$ (Brownian) fluctuation.

Movie S3.

Water transport behaviour of an active pump model when the radius is varied according to $1/f$ (pink) fluctuation.

Movie S4.

Water transport behaviour of an active pump model when the radius is varied according to white noise.

Movie S5.

Water transport behaviour of an active pump model when the radius is varied according to sine curve (ω = 3 GHz).