Electronic Supplementary Information for

Concerted orientation induced unidirectional water transport through nanochannels

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Ps1: Net flux with respect to the simulation time

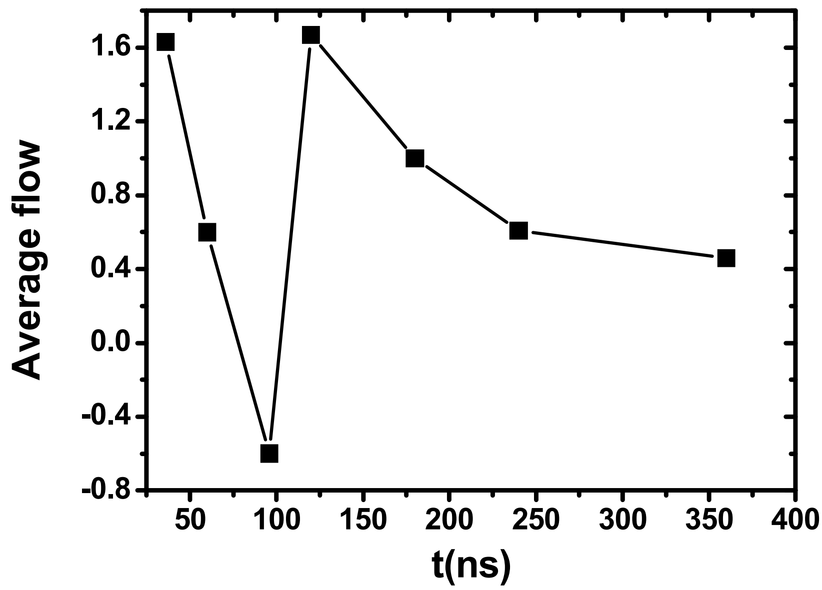

Figure S1. Net water flux with respect to the simulation time t. As the simulation time increases, the net flux decreases towards zero when the simulation time is larger than 200 ns.

Ps2: Transportation raised by asymmetrical potential

Early in 1993, Magnasco showed the unidirectional transportation of particle due to an asymmetrical potential in the environment of thermal noises [S1], where he used a piecewise linear potential (Fig. 1 in his paper) to illustrate his idea. We note that the water-water interaction for the + dipole state shown in Fig. 1(C) in our paper closely resembles the piecewise linear potential and our simulation results on the unidirectional transportation along +z direction are consistent with his analysis. For the - dipole state, which has a mirror symmetry potential of + dipole state, the induced flux is along -z direction.

Ps3: Different between our result of net flux and the burst of flow

We showed here the individual events of water molecules conducting through the nanotube with respect to time *t* in a + dipole state at 13.5ns and in a - dipole state at 15.5ns. The former has a pulse-like flow but a small net flux (Fig. (b)). The latter has a large net flux without any pulse-like flow (Fig. (c)).

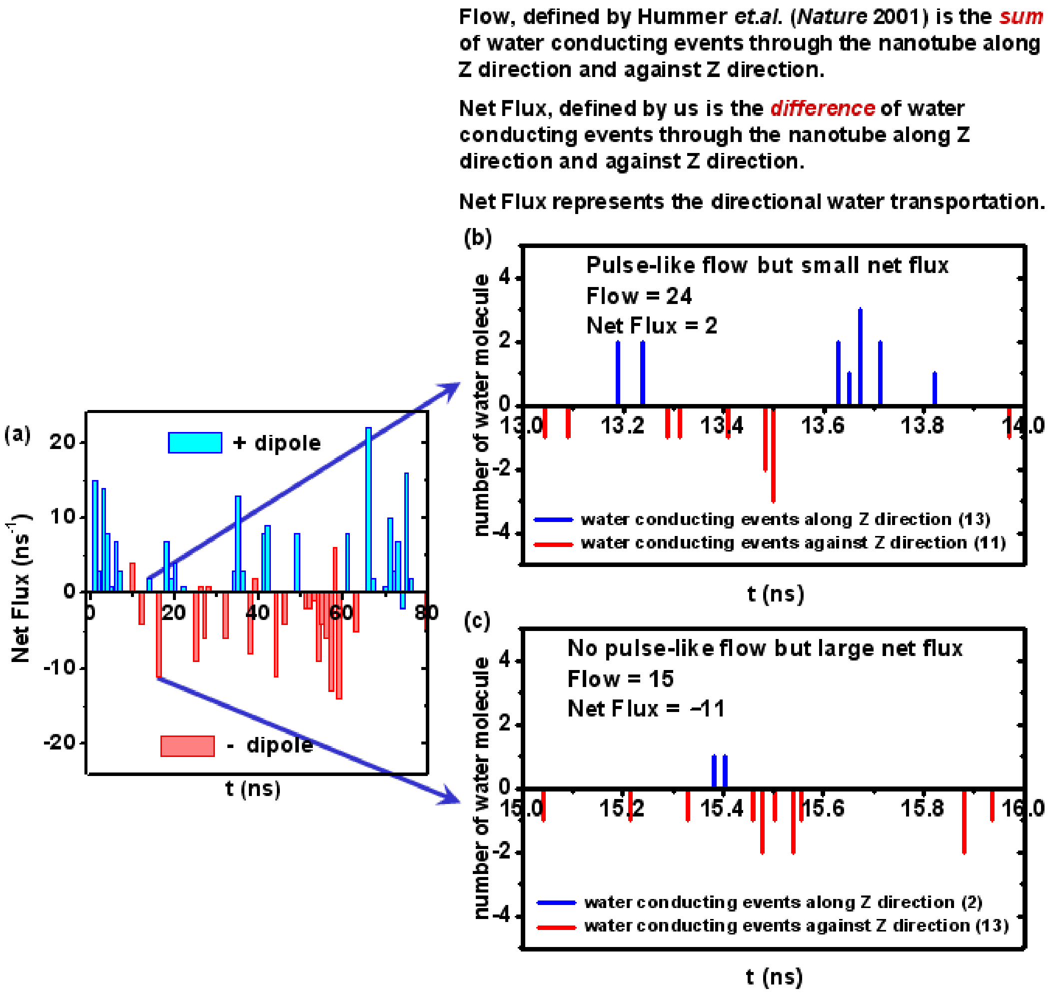

Figure S2. Net flux within each duration of each state (only the first 80 ns data are shown). Individual events of water conducting through the nanotube (b) in a + dipole state at 13.5 ns (c) in a - dipole state at 15.5 ns.

Ps4: Molecular dynamics simulation with artificial osmotic pressure

When two sides of a membrane have same hydrostatic pressure but different concentrations of an impermeable solute, an osmotic pressure difference is established and water flows from the side with lower solute concentration to the other side. In the simulation, we applied a force to each water molecule along $+z$ direction to obtain a pressure difference between two ends of the SWNT. This pressure difference is something like the osmotic pressure difference [S2, S3]. It was found that the pressure difference between two ends of the SWNT is 133 MPa for an additional acceleration of 0.1 nm ps^{-2} at each atom., Fig S3 showed the average flux value with respect to the simulation time.

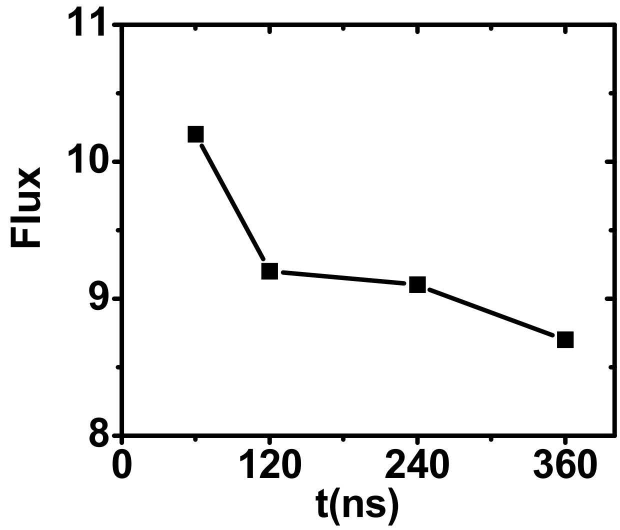

Figure S3 Average flux with respect to the simulation time. As time increases, the flux converges to a value about 8.7/ns.

References

S1. M. O. Magnasco, Phys. Rev. Lett. **71** 1477 (1993).

S2. F. Q. Zhu, E. Tajkhorshid, K. Schulten, Biophys. J. **83** 154 (2002).

S3. R. Z. Wan, J. Y. Li, H. J. Lu, and H. P. Fang, J. Am. Chem. Soc. **127**, 7166 (2005)