Supplementary information

Simulation Methods

A. Nanotube structures

We considered two open-ended finite length (5,5) BNNT and CNT with both ends saturated by hydrogen atoms. The tubes are 14.2 Å long and 6.9 Å in diameter. The initial C-C and C-H bond lengths were 1.42 Å and 1.09 Å, respectively. The initial BN bond length was 1.446 Å. The N-H and B-H bond length was 1.09 Å. The nitride atoms were then moved slightly outwards (by ~ 0.032 Å) and the boron atoms were moved slightly inwards from the tube center (by ~ 0.032 Å) to make a buckled BNNT, which is consistent with previous ab initio calculations on BNNT geometries.\textsuperscript{S1, S2} We then obtained geometry optimized structures for both tubes by the AM1 semiempirical method using HyperChem 7.51.\textsuperscript{S3} For BNNT geometries, AM1 method reproduces the large cBN cluster in good agreement with experimental structure.\textsuperscript{S4} For the CNTs, Han and Jaffe\textsuperscript{S5} found good agreement in carbon nanoconic tip energies and geometries obtained from using AM1 and DFT/B3LYP method. Furthermore, the CNT geometry obtained from the B3LYP/3-21G method has been found to be in good agreement with experiments.\textsuperscript{S6}

B. Molecular dynamics simulation

MD simulations were performed using modified GROMACS 3.2.1.\textsuperscript{S7} The initial simulation box was $2.8 \times 2.772 \times 6.3$ nm$^3$. The systems were replicated periodically in all the three dimensions. The reservoirs were initially filled with approximately 900 water molecules. The Nosé-Hoover thermostat\textsuperscript{S8} with a time constant of 0.1 ps was employed to regulate the temperature at 300K. The Parrinello-Rahman\textsuperscript{S9} piston-coupling scheme with a time constant of 2.0 ps and a compressibility of $4.5 \times 10^{-5}$ bar$^{-1}$ maintained the system at 1 bar. The Lennard-Jones parameters for carbon atoms, water molecules, and slab are summarized in the previous work.\textsuperscript{S10} The Lennard-Jones parameters for the boron and nitride atoms were taken from Ref. S11 ($\sigma_{B:B} = 0.3453$ nm, $\varepsilon_{B:B} = 0.3971$ KJ/mol, $\sigma_{N:N} = 0.3365$ nm, $\varepsilon_{N:N} = 0.6060$ KJ/mol), and parameters for the saturated hydrogen atoms were taken from Ref. S12 ($\sigma_{H:H} = 0.2813$ nm, $\varepsilon_{H:H} = 0.0683$ KJ/mol). Particle mesh Ewald (PME) method with a 10 Å real-space cutoff, 1.5 Å reciprocal space gridding, and splines of order 4 with a $10^{-5}$ tolerance was implemented to compute electrostatic interactions. The equations of motion were integrated by using a leapfrog algorithm and the simulation time step is 1.0 fs. The simulations were continued for 40 ns to obtain enough statistical sampling.

C. Diffusion coefficient

The self-diffusion coefficient was computed to evaluate water transport. The axial diffusion coefficient $D_z$ of water is related to the slope of the water mean-squared displacement (MSD) by the well-known Einstein relation,

\[
D_z = \lim_{t \to \infty} \frac{\langle r(t) - r(0) \rangle^2}{\Delta t} = \frac{1}{2} \lim_{t \to \infty} \frac{\langle \Delta r^2 \rangle}{\Delta t},
\]

where $r(t)$ is the position vector at time $t$.\textsuperscript{11}
D. Potential of mean force (PMF) analysis

The PMF of water was computed to obtain the energy barrier. When a water molecule $i$ moves along the axial direction from $z_0$ to $z$, the work done, $W_i(z) - W_i(z_0)$, is computed by integrating the mean force $<F_i(z)>$ acting on the water molecule along the nanotube axis contributed by all other atoms in the system averaged over all the configurations,\textsuperscript{S13} i.e.,

$$W_i(z) - W_i(z_0) = \int_{z_0}^{z} <F_i(z')> dz'$$

where $z_0$ is the reference position (taken as the end of the simulation box) where PMF is zero.\textsuperscript{S14} We obtained the mean force distribution by sampling the force experienced by the water molecules placed at various positions along the nanotube axis.\textsuperscript{S13}

REFERENCES

S3. HyperChem\textsuperscript{TM}, hypercube, Inc., 1115 NW 4\textsuperscript{th} Street, Gainesville, FL 32601, USA.