Carbon Nanotubes
Hydrophobic channels - Perfect Models for

A balance between the size and hydrophobicity
Water-nanotube interaction can be easily modified

Modifying charges
Modifying vdW parameters

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- Much better statistics
- No need for membrane and lipid molecules
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Water Single-files in Carbon Nanotubes

Water files form polarized chains in nanotubes
Calculation of Diffusion Permeability from MD

\[ \Phi_0: \text{number of water molecules crossing the channel from the left to the right in unit time} \]

\[ \Phi_0 = \frac{V^w}{N_A} \]

\( \Phi_0 \) can be directly obtained through equilibrium MD simulation by counting “full permeation events”
Simulation of osmotic pressure induced water transport may be done by adding salt to one side of the membrane.

\[ \text{NaCl} \rightarrow \text{Na}^+ + \text{Cl}^- \]

There is a small problem with this setup!
Problem: The solvents on the two sides of a membrane in a conventional periodic system are connected.
We can include more layers of membrane and water to create two compartments of water that are not in contact.
Semipermeable membrane

UNIT CELL

NaCl

Semipermeable membrane

(1)

(2)
Realizing a Pressure Difference in a Periodic System

\[ P_1 = P_2 + nf \Rightarrow \Delta P = nf / A \]

f is the force on each water molecule, for n water molecules.

The overall translation of the system is prevented by applying constraints or counter forces to the membrane.

Applying a Pressure Difference Across the Membrane

$$\Delta P = nf / A$$

Applying force on all water molecules.

Not a good idea!
Applying a Pressure Difference Across the Membrane

\[ \Delta P = n f / A \]

Applying force on bulk water only.

Very good
Applying a Pressure Difference Across the Membrane

\[ \Delta P = nf / A \]

Applying force only on a slab of water in bulk.

Excellent

\[ \Phi_w = P_f A \left( \frac{\Delta P}{RT} - \Delta C_s \right) \]

\( P_f \) can be calculated from these simulations.
Calculation of osmotic permeability of water channels

$\psi_f: 7.0 \pm 0.9 \times 10^{-14} \text{ cm}^3/\text{s}$

Exp: $5.4 - 11.7 \times 10^{-14} \text{ cm}^3/\text{s}$

$\psi_f: 1.4 \times 10^{-13} \text{ cm}^3/\text{s}$

GlpF Aquaporin-1