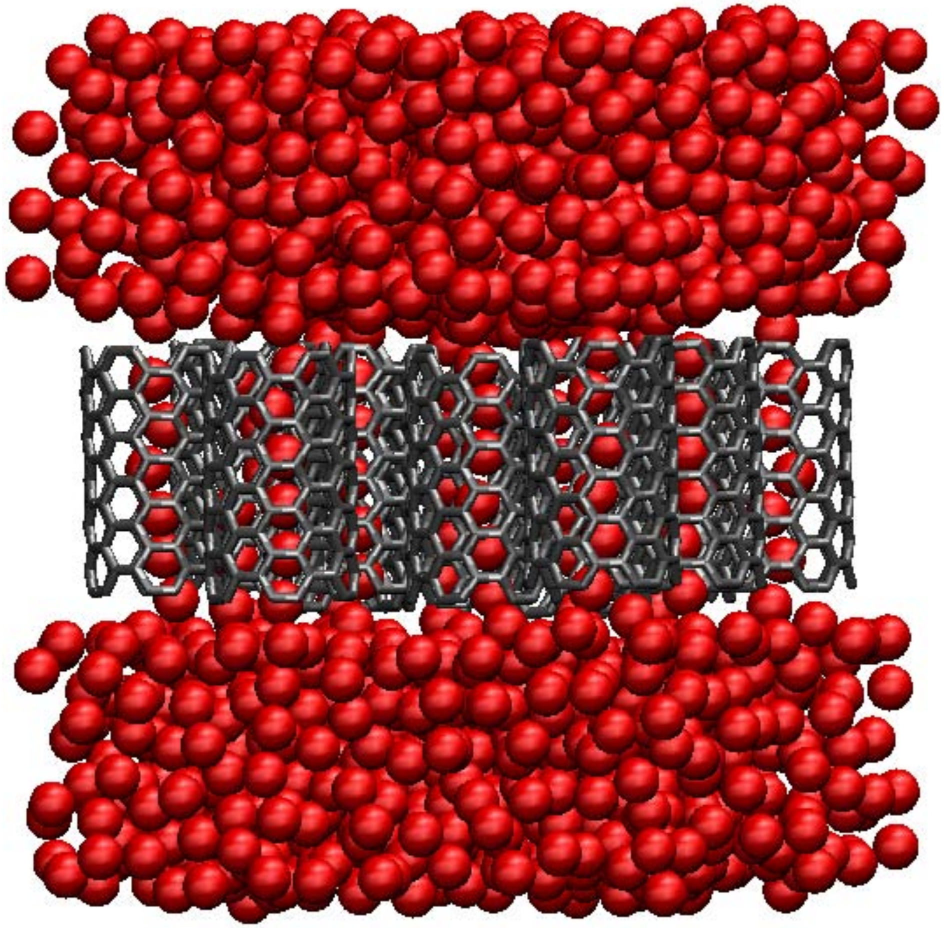
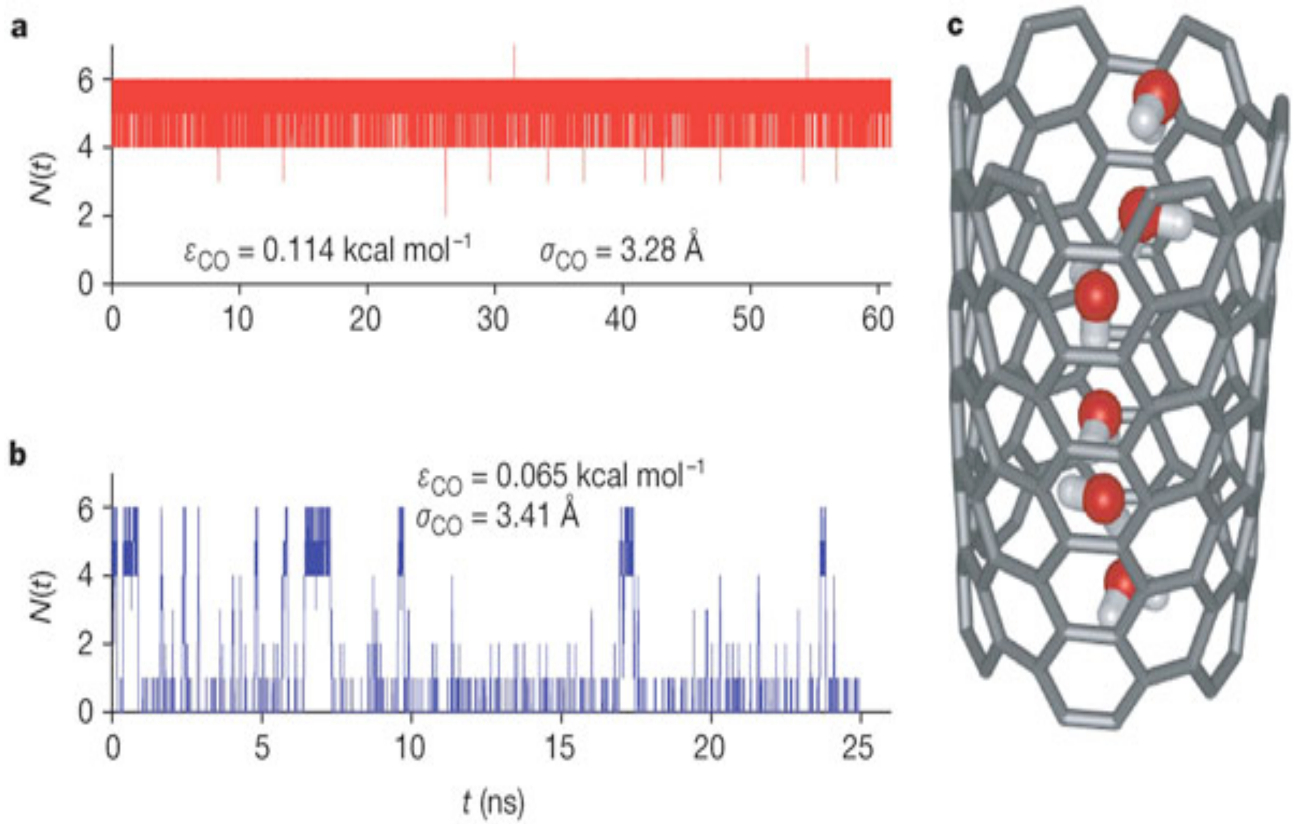
Carbon Nanotubes
Hydrophobic channels - Perfect Models for



A balance between the size and hydrophobicity

Water-nanotube interaction can be easily modified



Modifying charges
Modifying vdW parameters

Hummer, et. al., Nature, 414: 188-190, 2001

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Hydrophobic channels - Perfect Models for

- Much better statistics
- No need for membrane and lipid molecules

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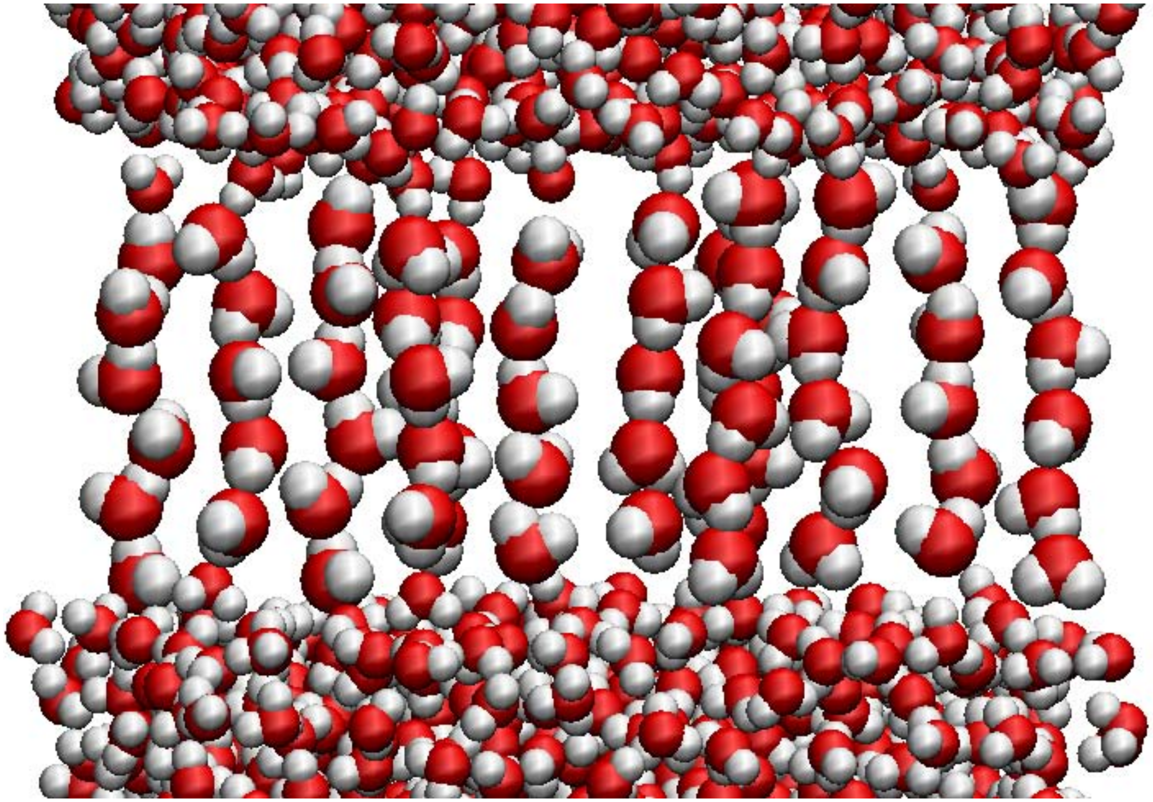
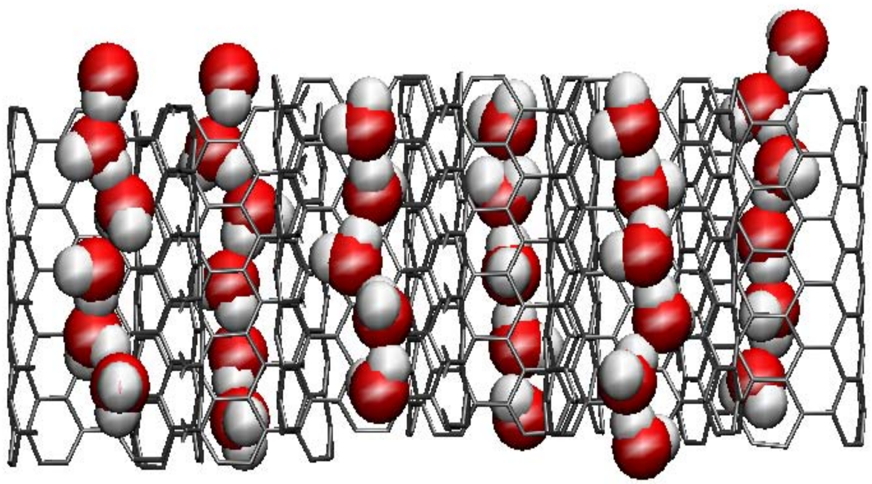
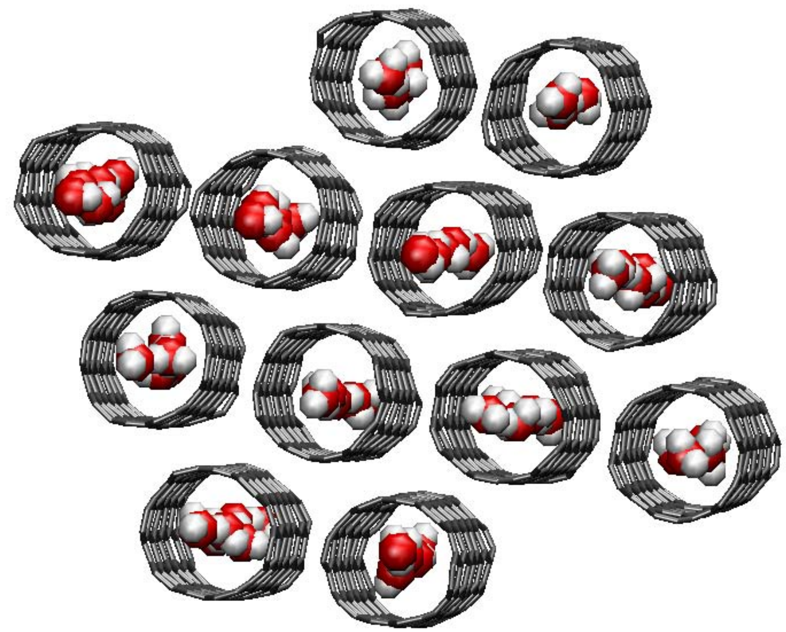
Hydrophobic channels - Perfect Models for



- Much better statistics
- No need for membrane and lipid molecules

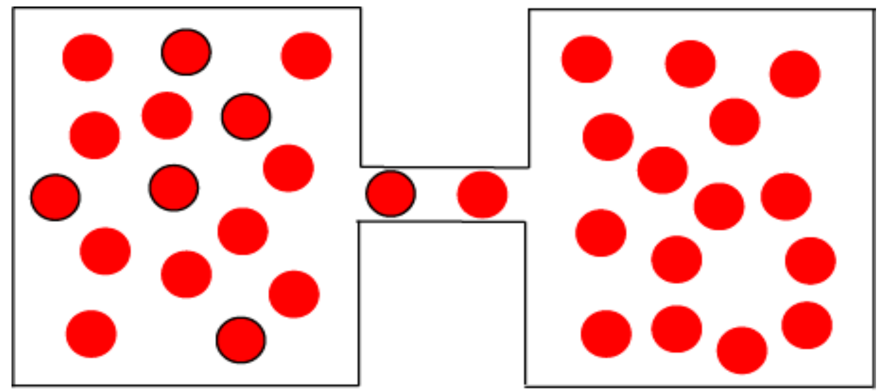
Water Single-files in Carbon Nanotubes





Water files form polarized chains in nanotubes

Calculation of Diffusion Permeability from MD



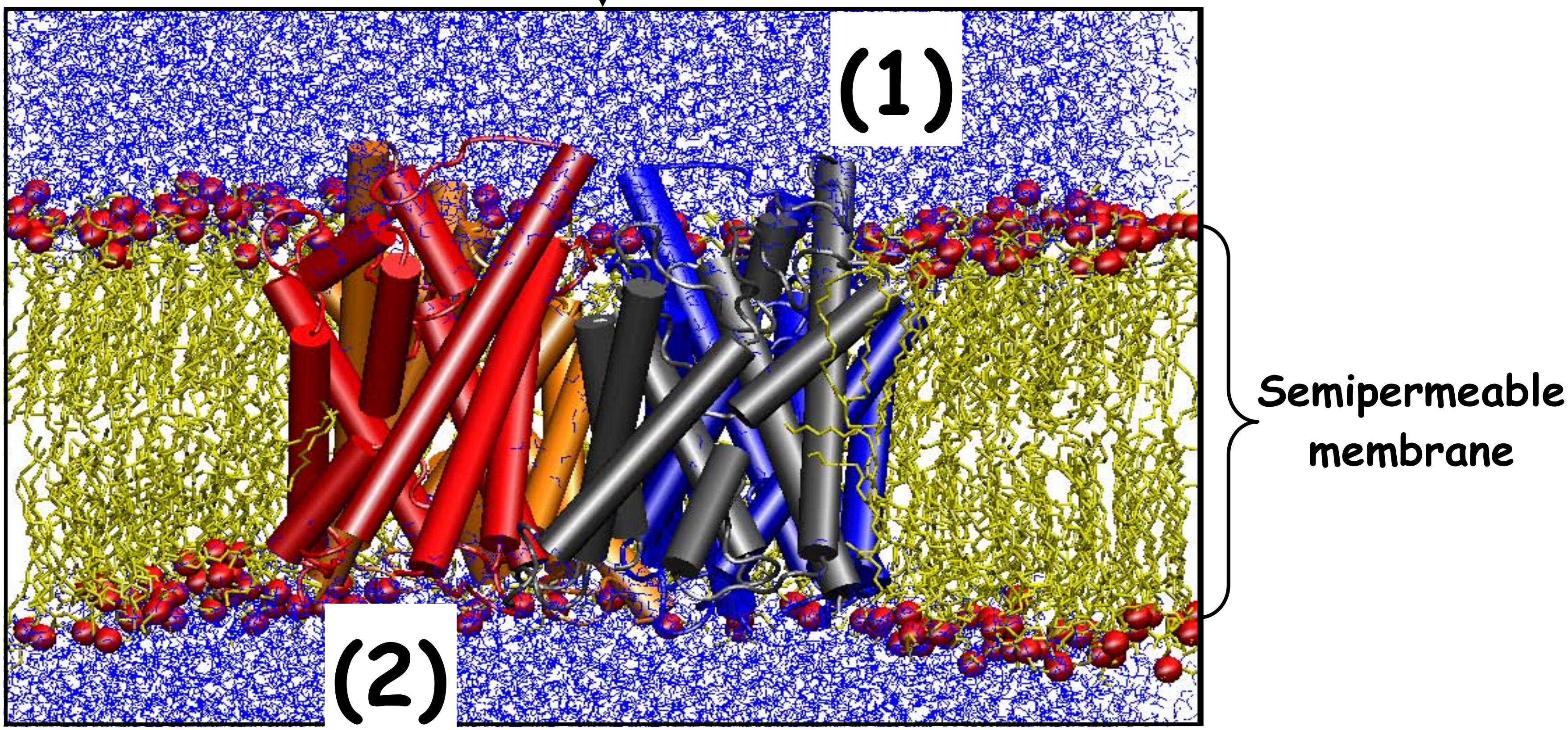
Φ_0: number of water molecules crossing the channel from the left to the right in unit time

$$p_d = \frac{V_w}{N_A}\Phi_0$$

Φ_0 can be directly obtained through equilibrium MD simulation by counting "full permeation events"

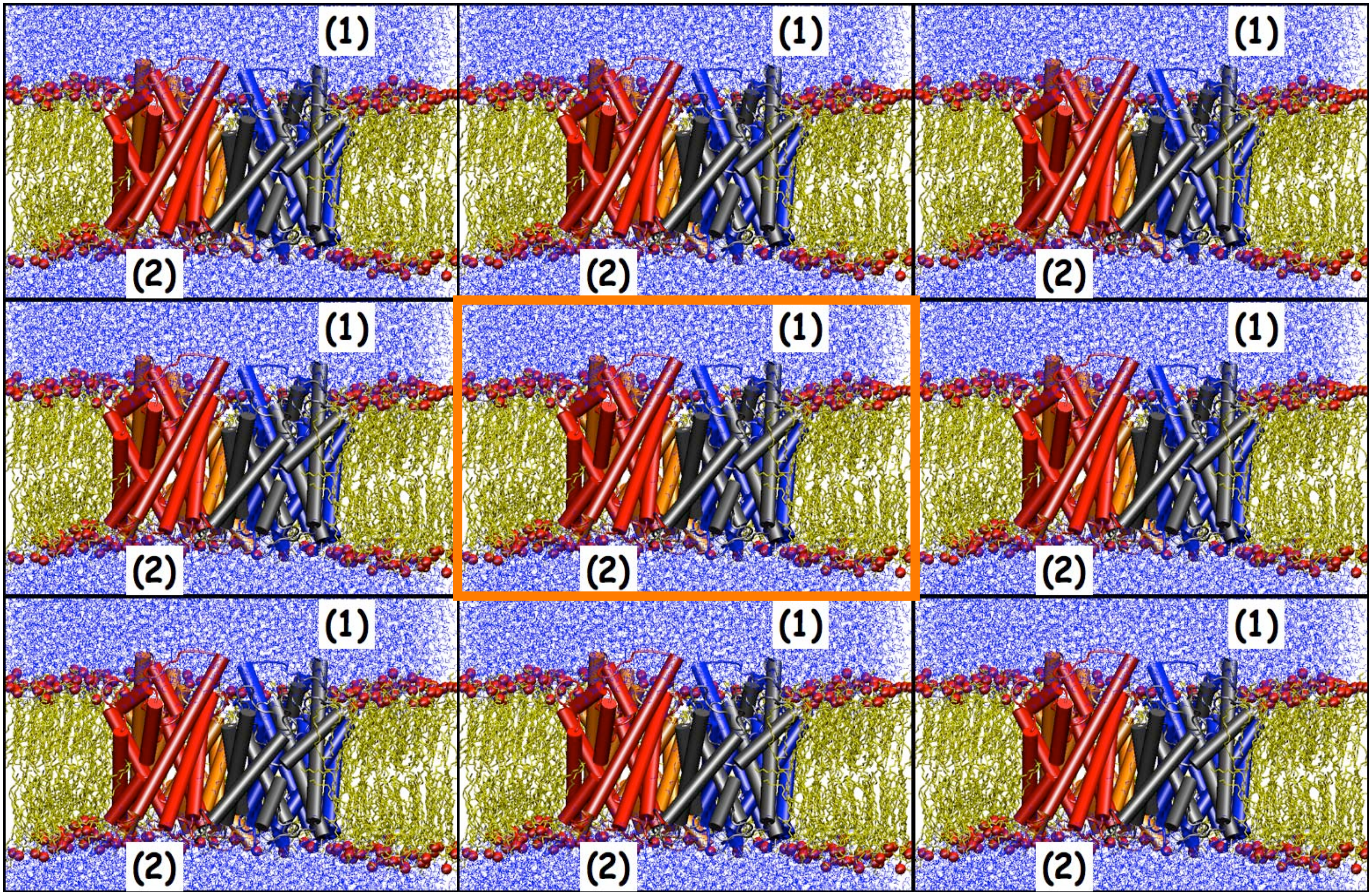
Simulation of osmotic pressure induced water transport may be done by adding salt to one side of the membrane.

$NaCl \rightarrow Na^{+} + Cl^{-}$

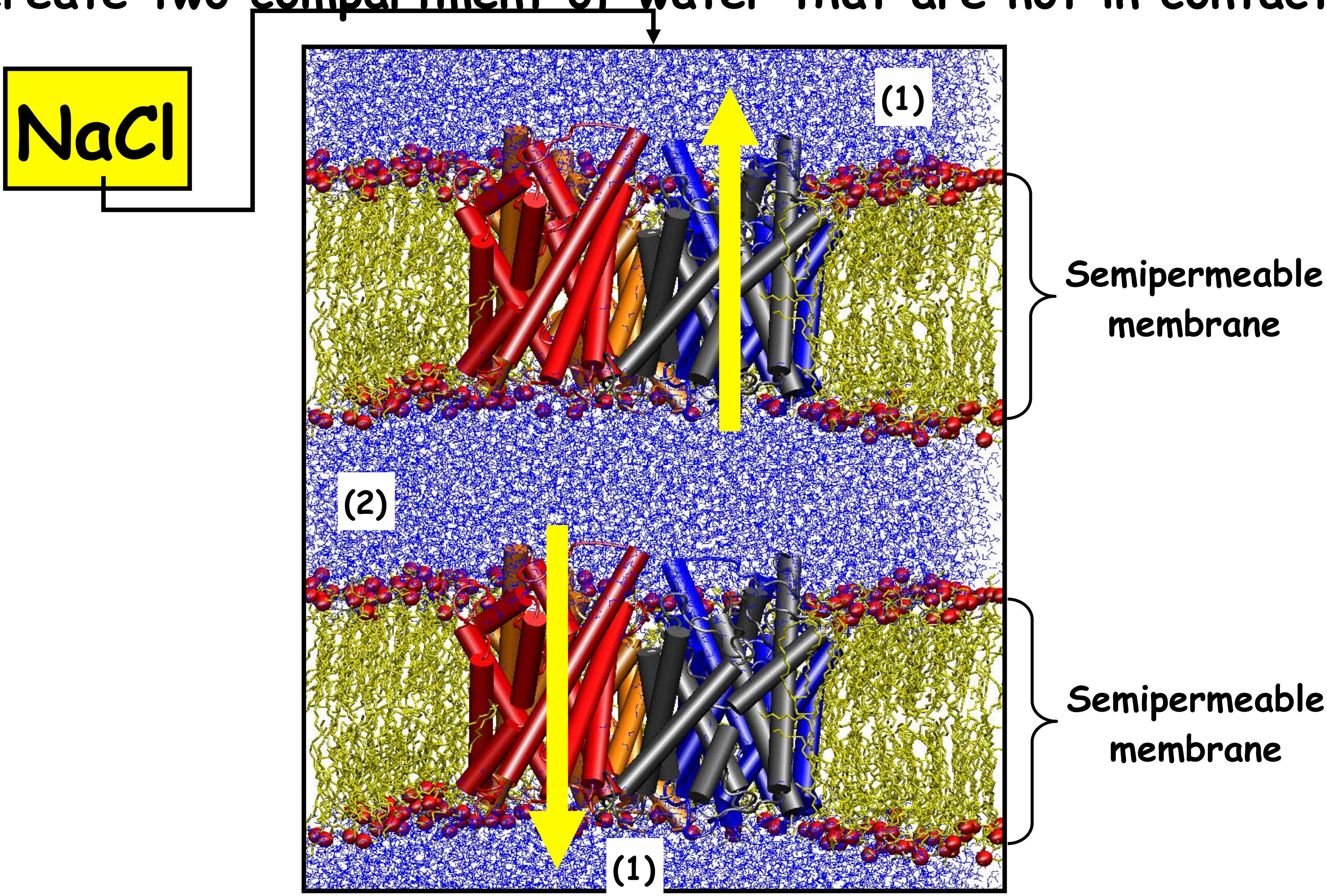


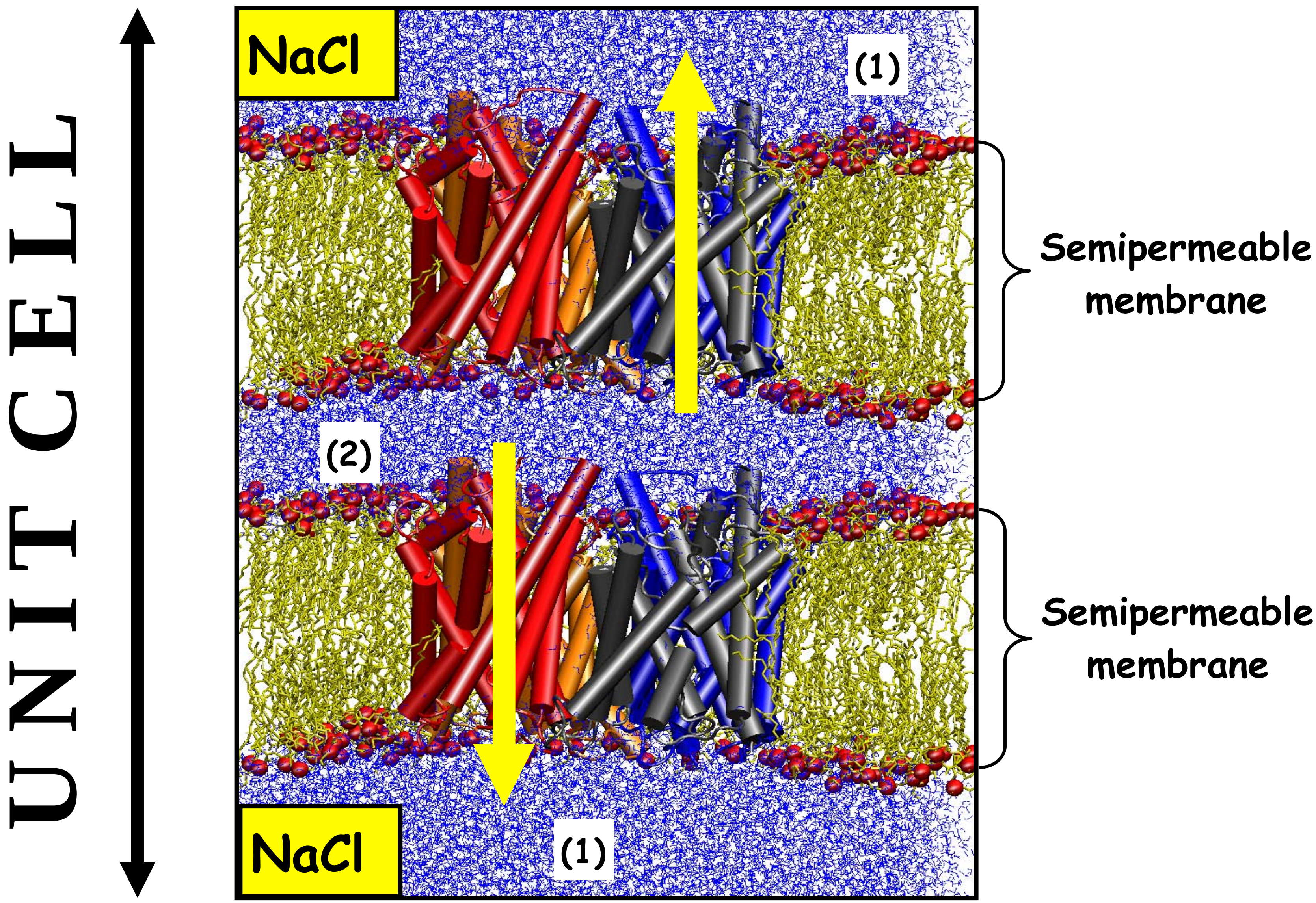
There is a small problem with this setup!

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 compartment of water that are not in contact




UNIT CELL
NaCl
(1)
(2)
Semipermeable membrane
Semipermeable membrane
NaCl
(1)

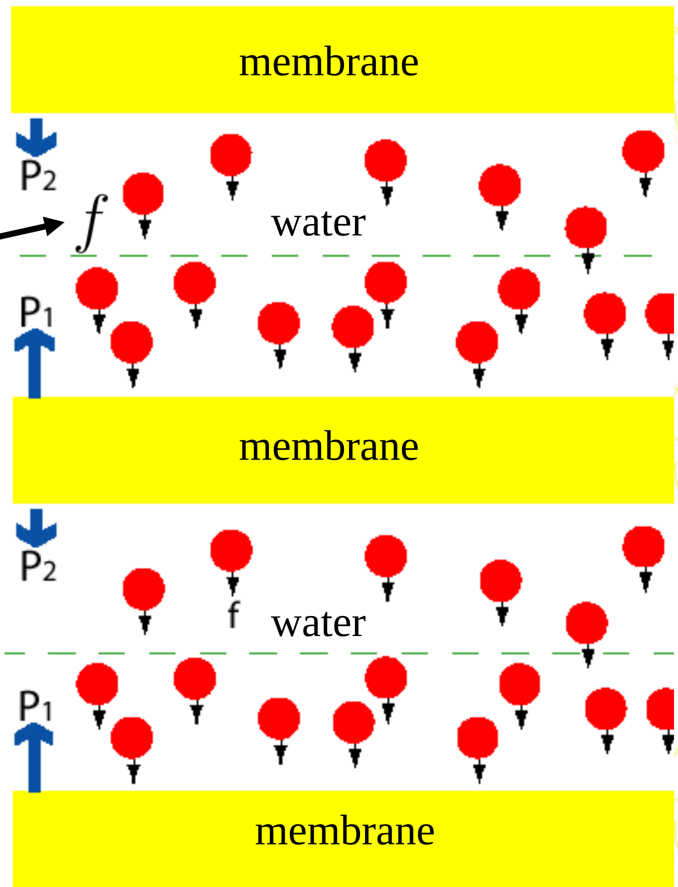
Realizing a Pressure Difference in a Periodic System

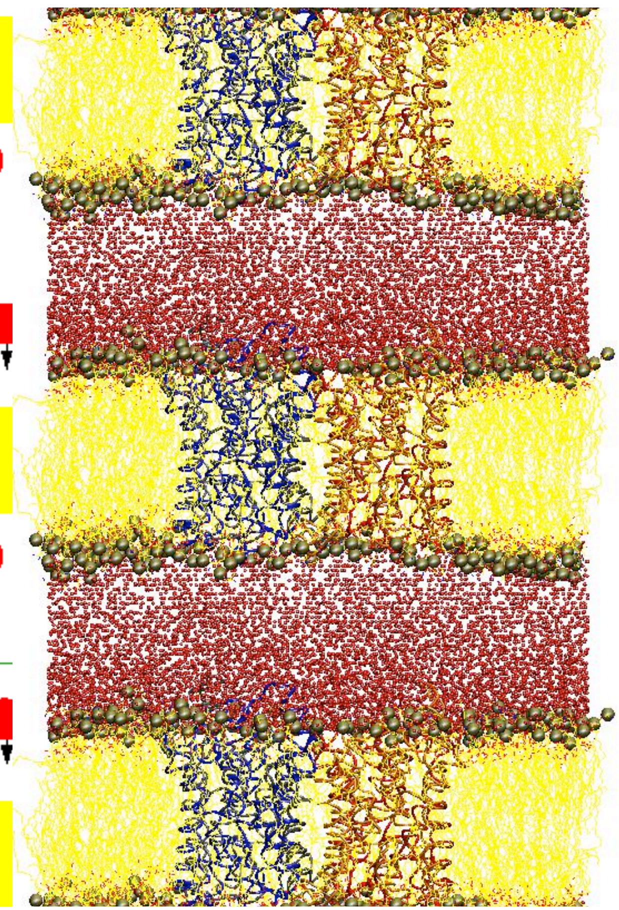
$$P_1 = P_2 + nf \Rightarrow \Delta P = nf / A$$

Fangqiang Zhu

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.

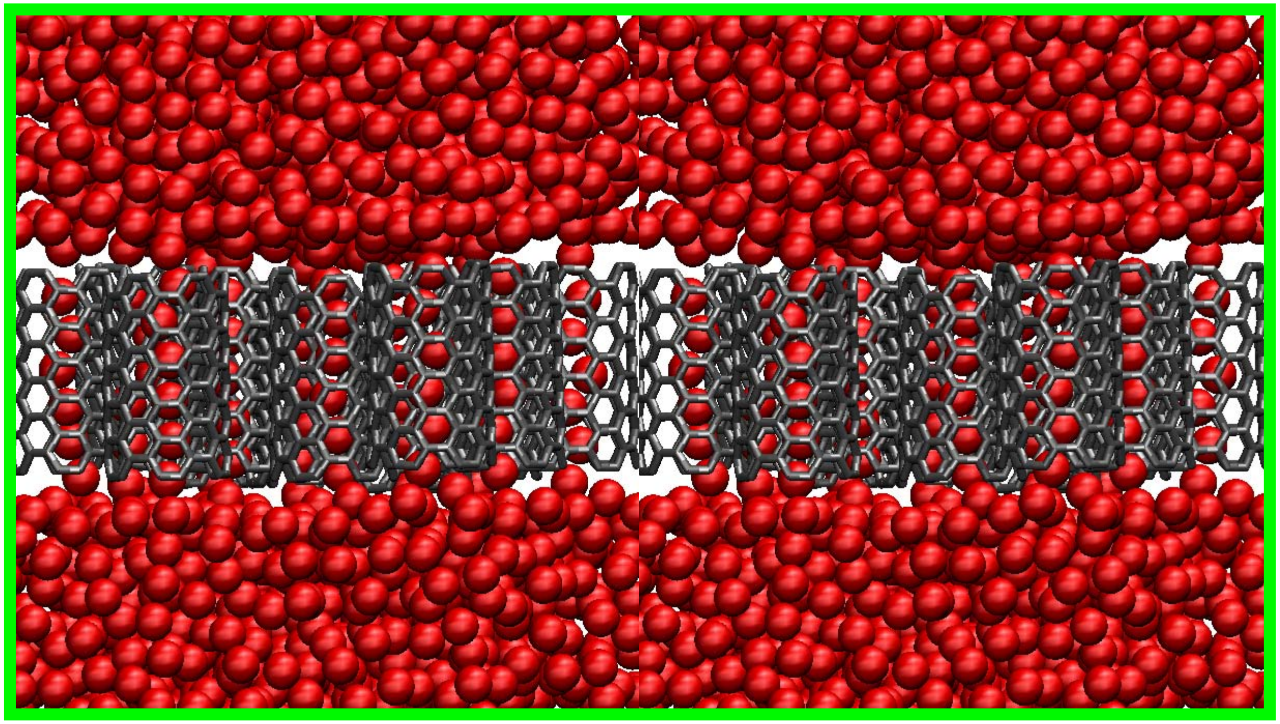




F. Zhu, et al., *Biophys. J.* 83, 154 (2002).

Applying a Pressure Difference Across the Membrane

$$\Delta P = nf / A$$

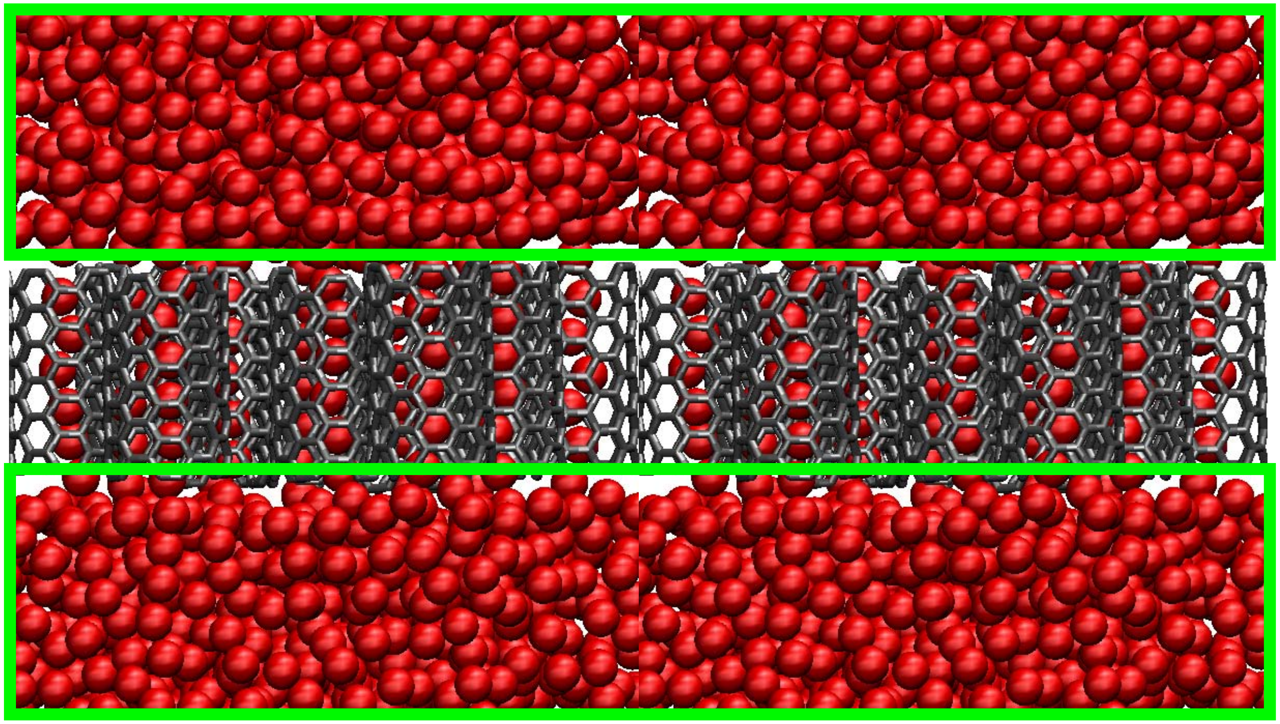


Applying force on all water molecules.

Not a good idea!

Applying a Pressure Difference Across the Membrane

$$\Delta P = nf / A$$

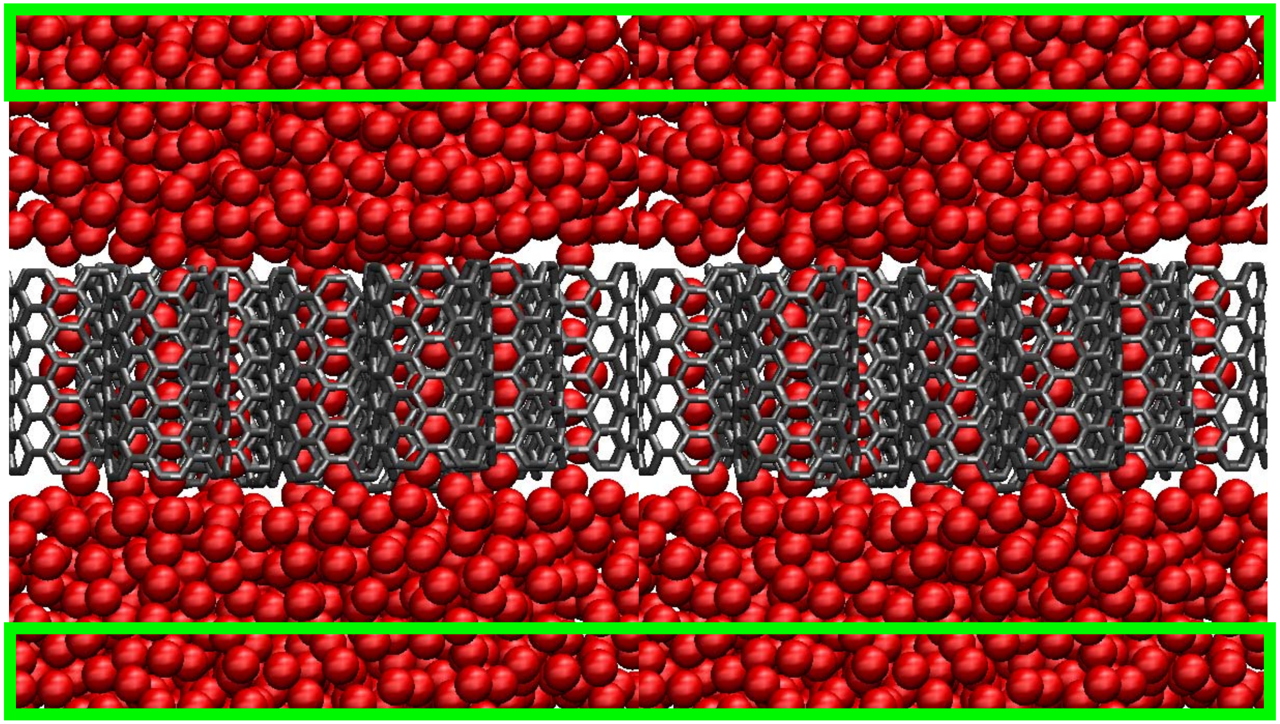


Applying force on bulk water only.

Very good

Applying a Pressure Difference Across the Membrane

$$\Delta P = nf / A$$



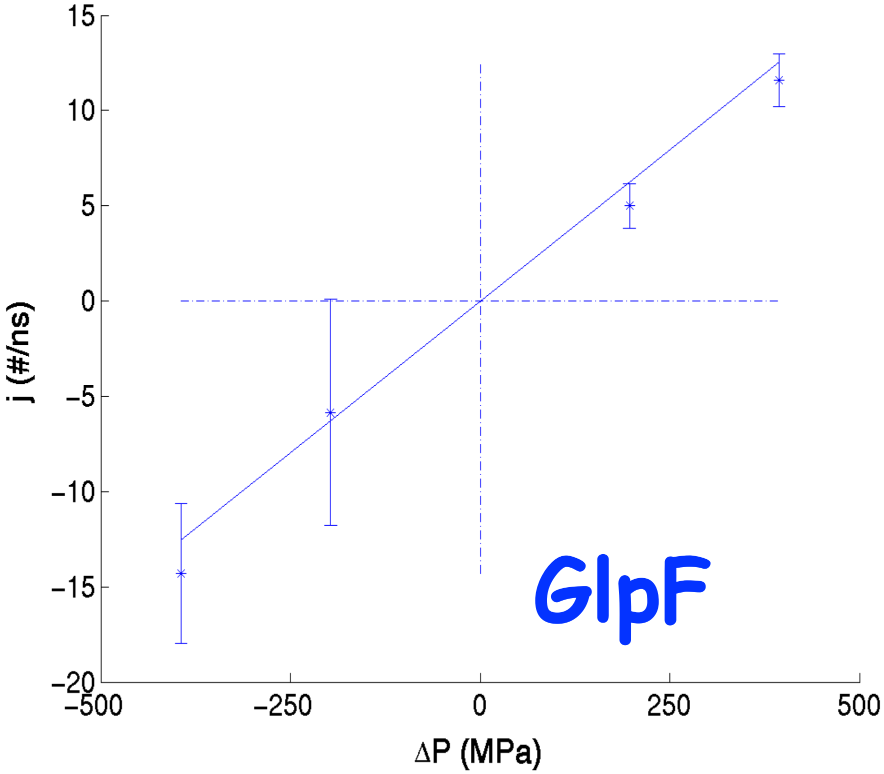
Applying force only on a slab of water in bulk.

Excellent

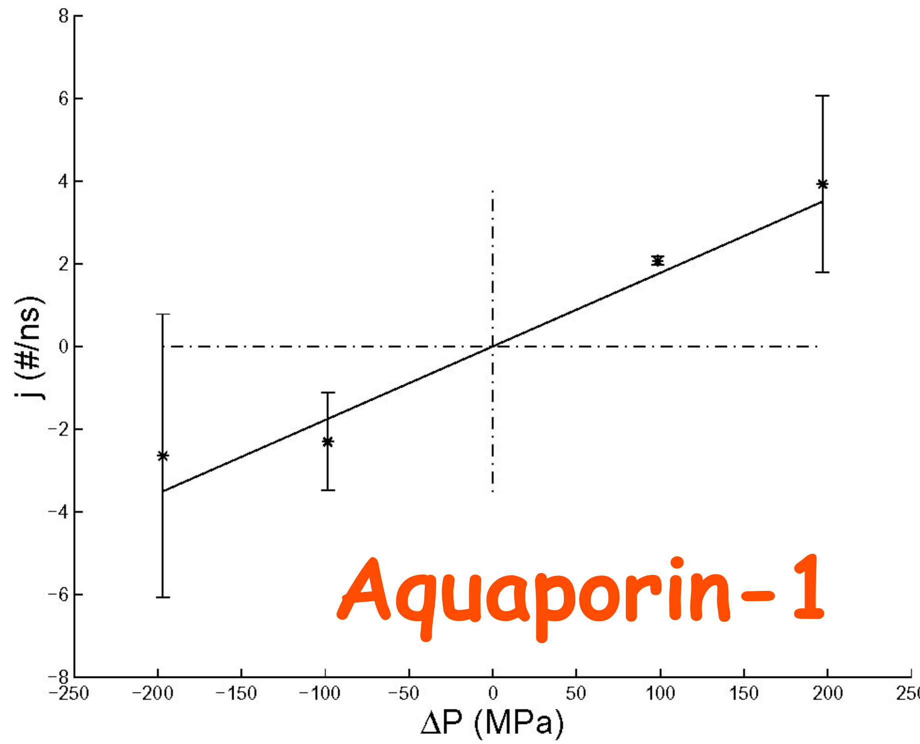
P_f can be calculated from these simulations

$$\Phi_w = P_f A(\frac{\Delta P}{RT} - \Delta C_s)$$

Calculation of osmotic permeability of water channels



p_f: 1.4×10^{-13} cm^3/s



p_f: 7.0 ± 0.9 × 10^{-14} cm^3/s

Exp: 5.4 – 11.7 × 10^{-14} cm^3/s