

# Nanofluidics in carbon nanotubes

Aleksandr Noya\*, Hyung Gyu Parka,b, Francesco Fornasieroa, Jason K. Holta, Costas P. Grigoropoulosb, and Olgica Bakajin†

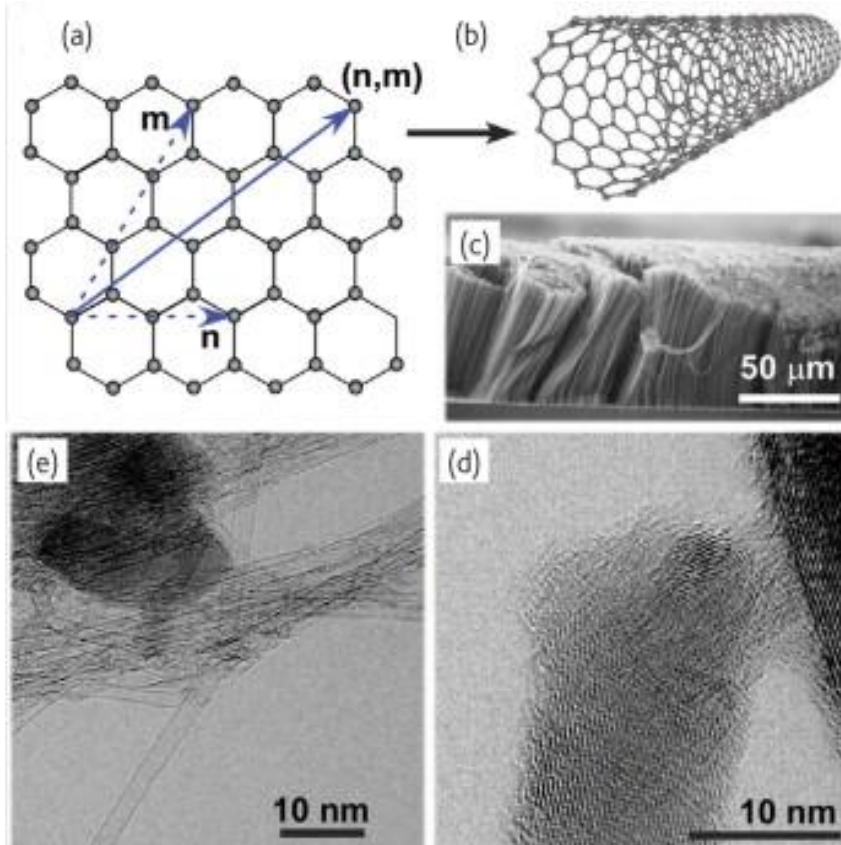
*aMolecular Biophysics and Functional Nanostructures Group, Chemistry, Materials and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA*

*b Department of Mechanical Engineering, University of California at Berkeley, Berkeley, CA 94720-1740, USA*

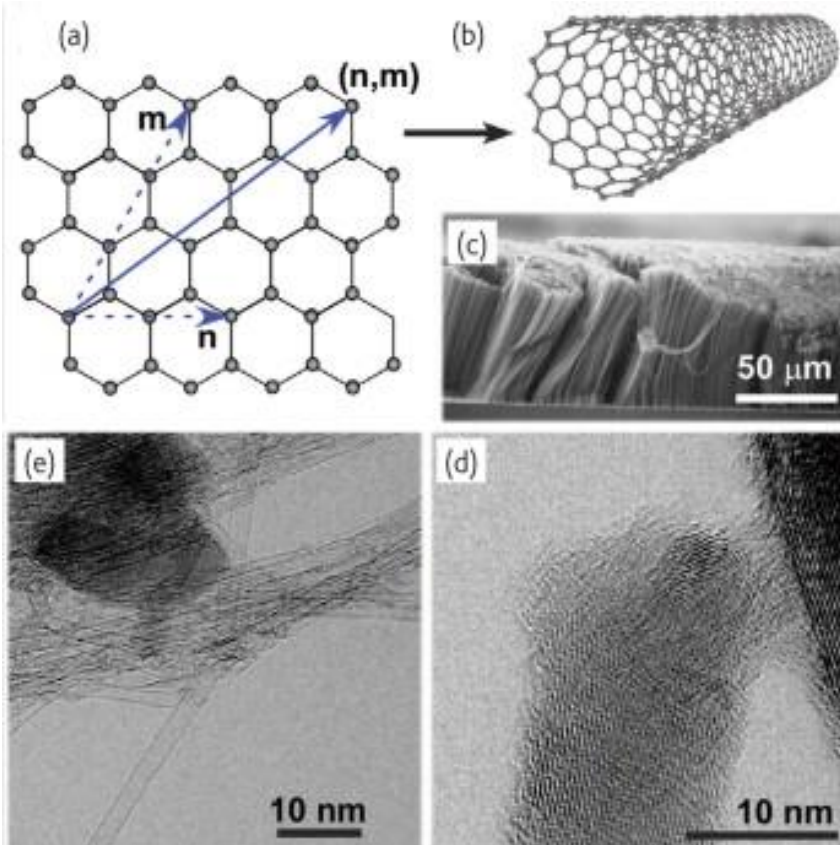
*E-mail: \*noy1@llnl.gov, †bakajin1@llnl.gov*

# Basic structure and Properties of CNTs

- Rolled-up graphene

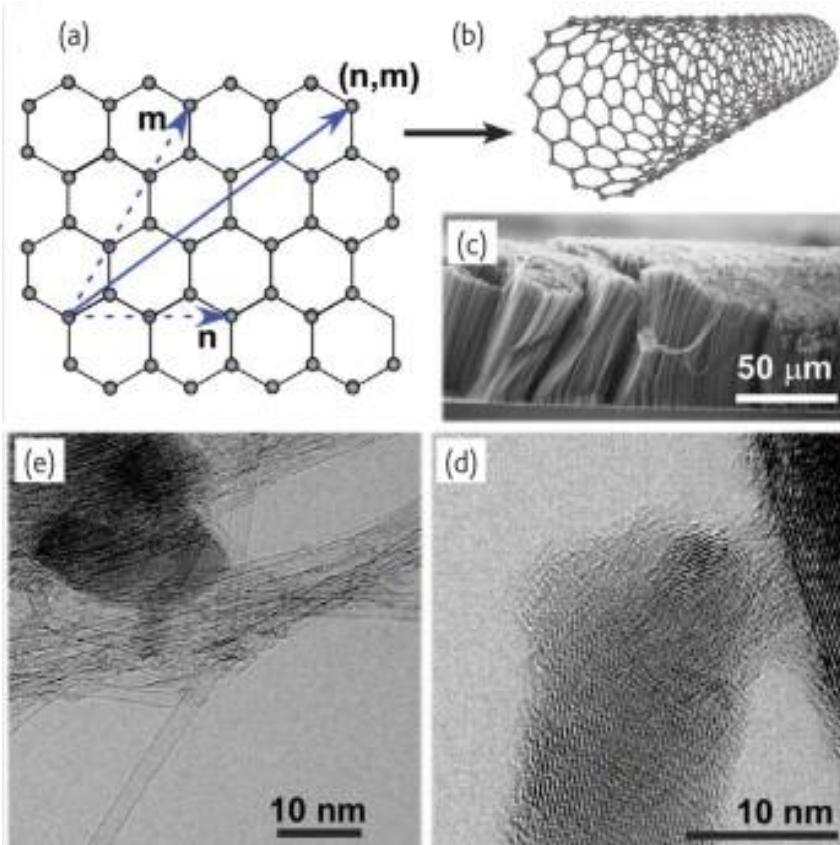


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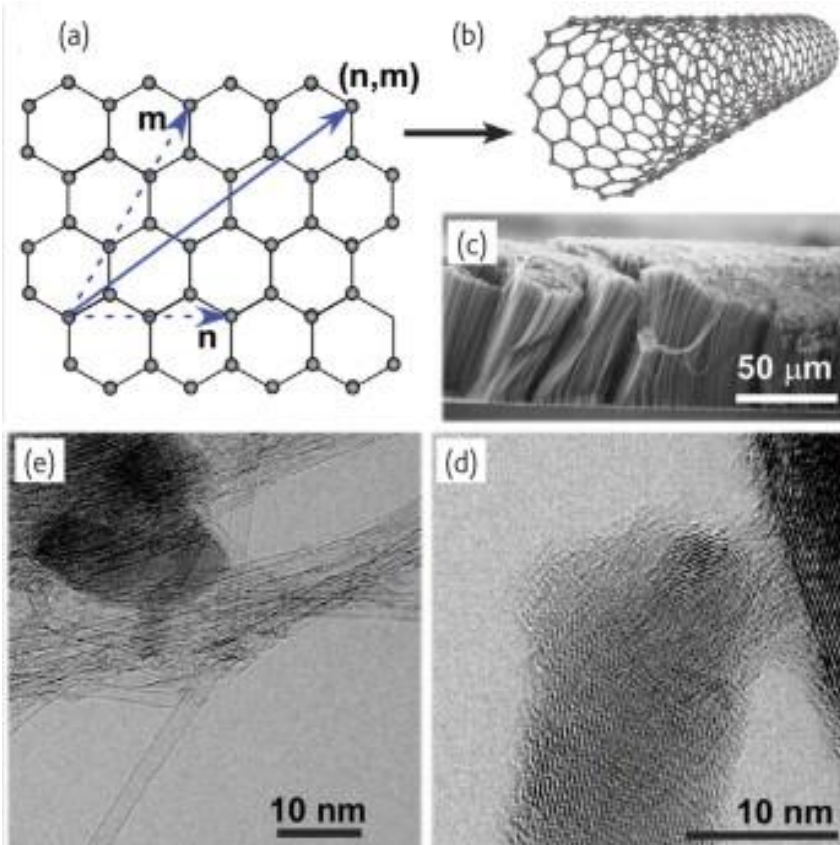
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- Characterized by its roll-up vectors  $(n,m)$
- Atomic scale smoothness
- Chemical vapor deposition (CVD) is preferred production method

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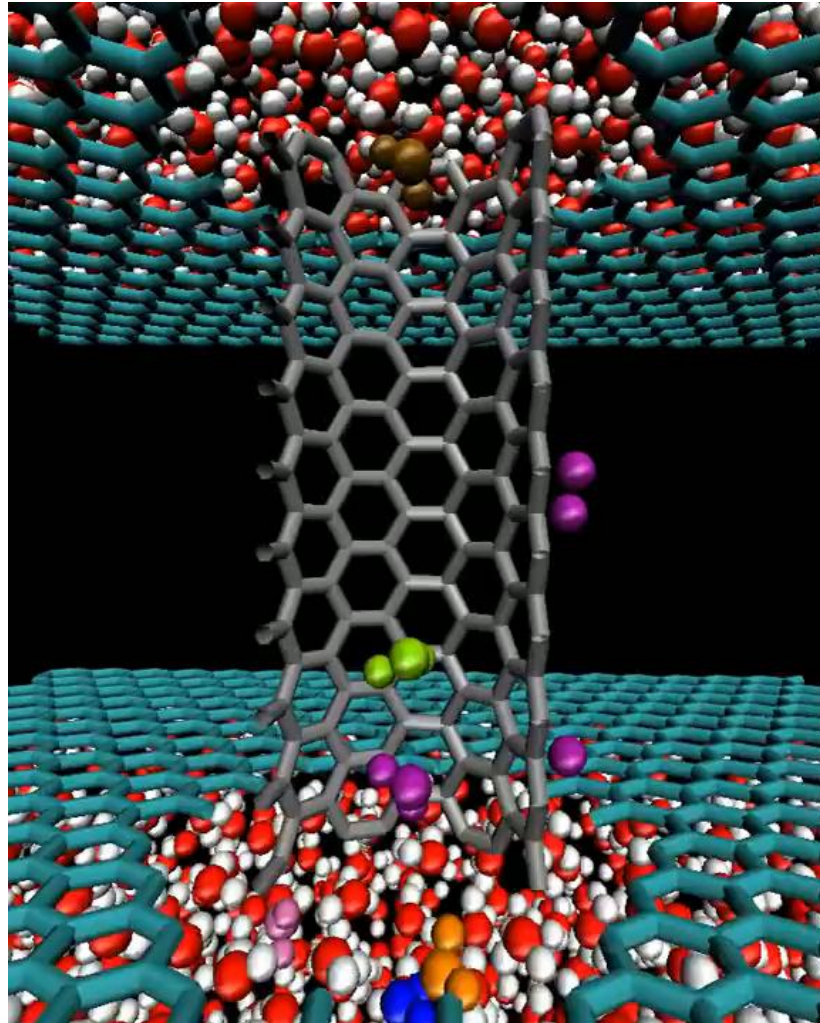
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**Answer**

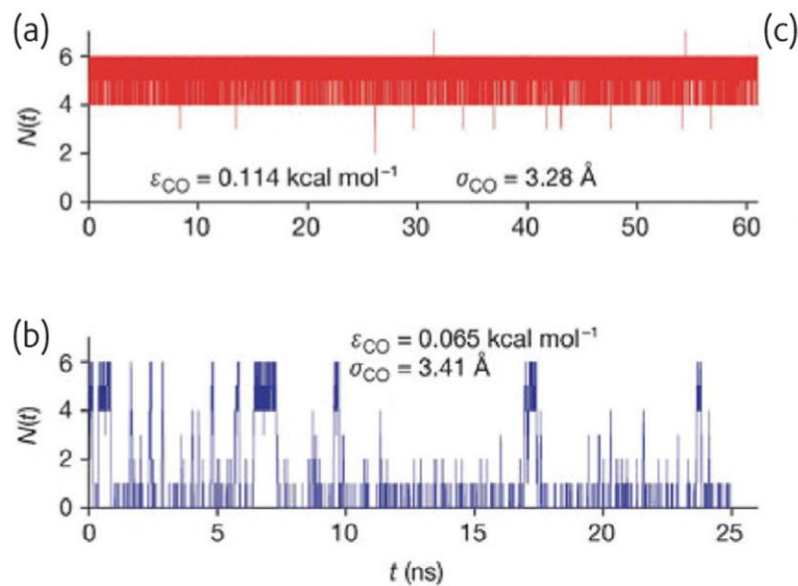
**Molecular Dynamic Simulations !!!**

# Simulation of water and gas in CNTs



<https://www.youtube.com/watch?v=9L-SfLwBbto>

# Simulation of water and gas in CNTs



- Water enters the CNTs (increased degree of freedom)
- High rate of water transport (5.8 molecules/ns)

# Analogy to aquaporins

**THEORETICAL AND COMPUTATIONAL  
BIOPHYSICS GROUP**

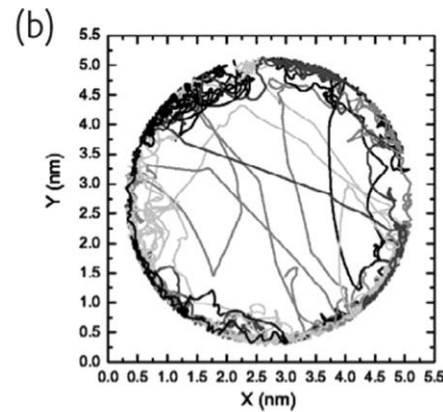
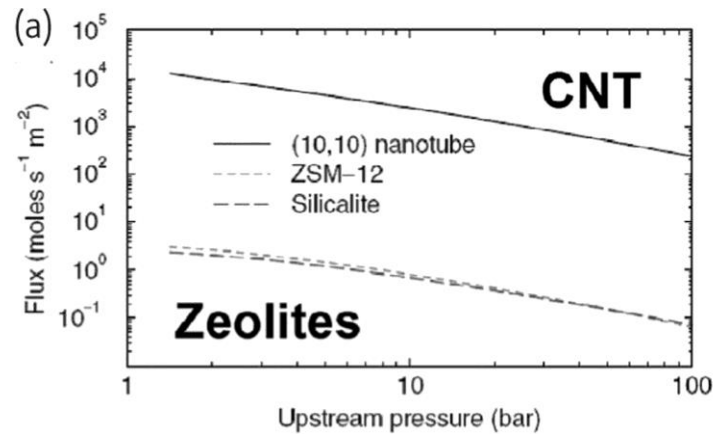
NIH Center for Macromolecular Modeling and Bioinformatics  
[www.ks.uiuc.edu](http://www.ks.uiuc.edu)

*presents*

**Water Channels in Cell Membranes**

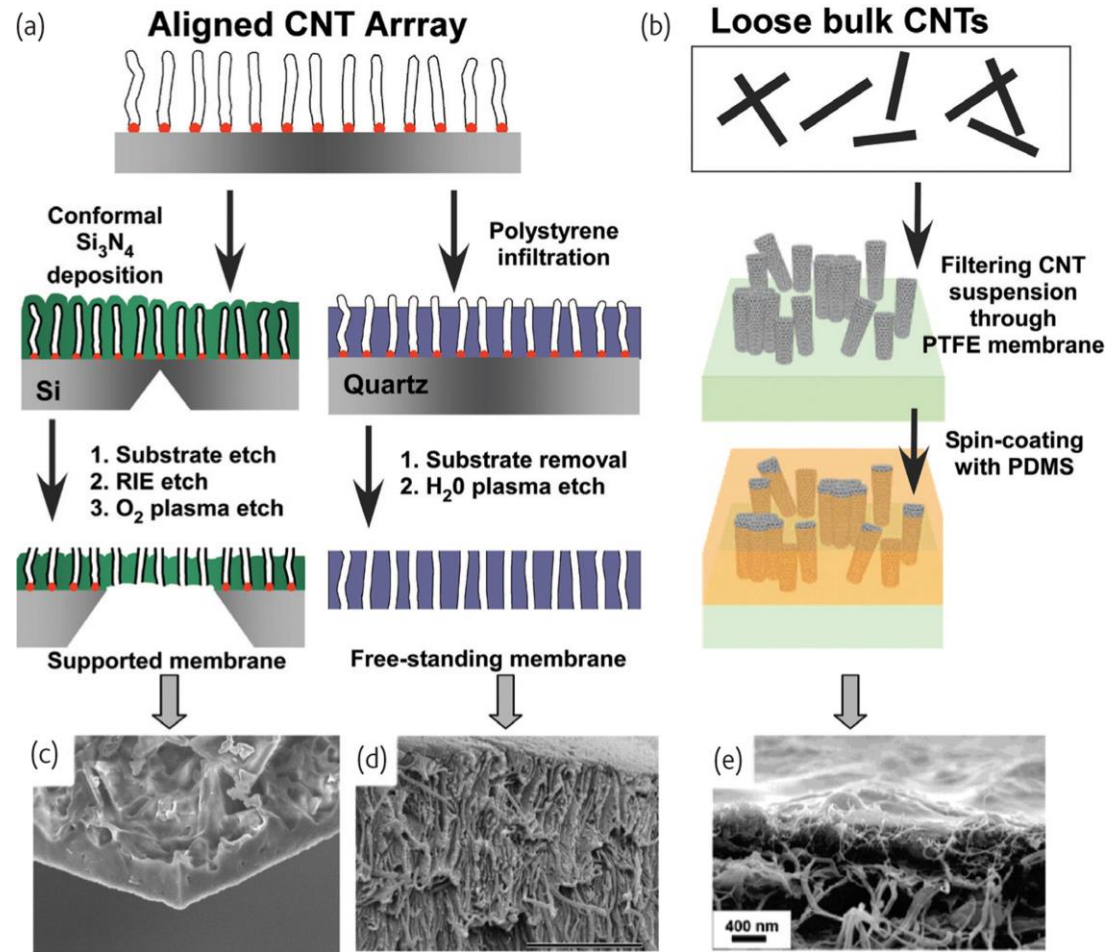
<https://www.youtube.com/watch?v=GSi5-y6NHjY>

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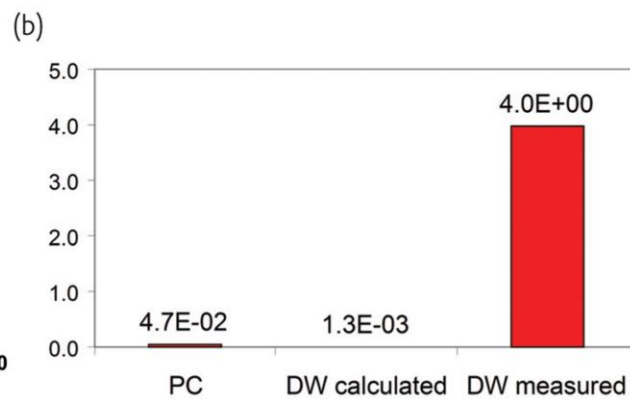
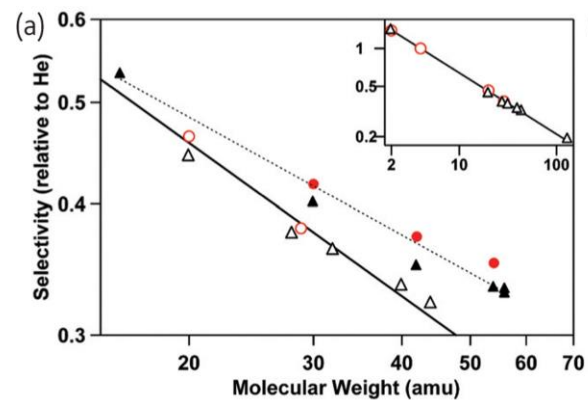
- Ballard-ball like propagation
- Gas transport is three orders of magnitude higher compared to similar porous membranes

# Fabrication of CNT membranes

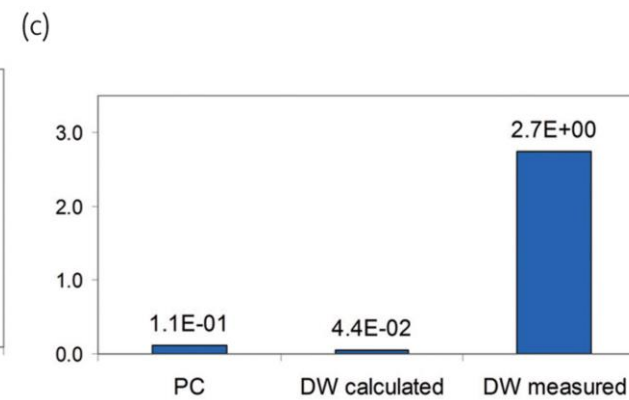




# Gas and water transport measurements

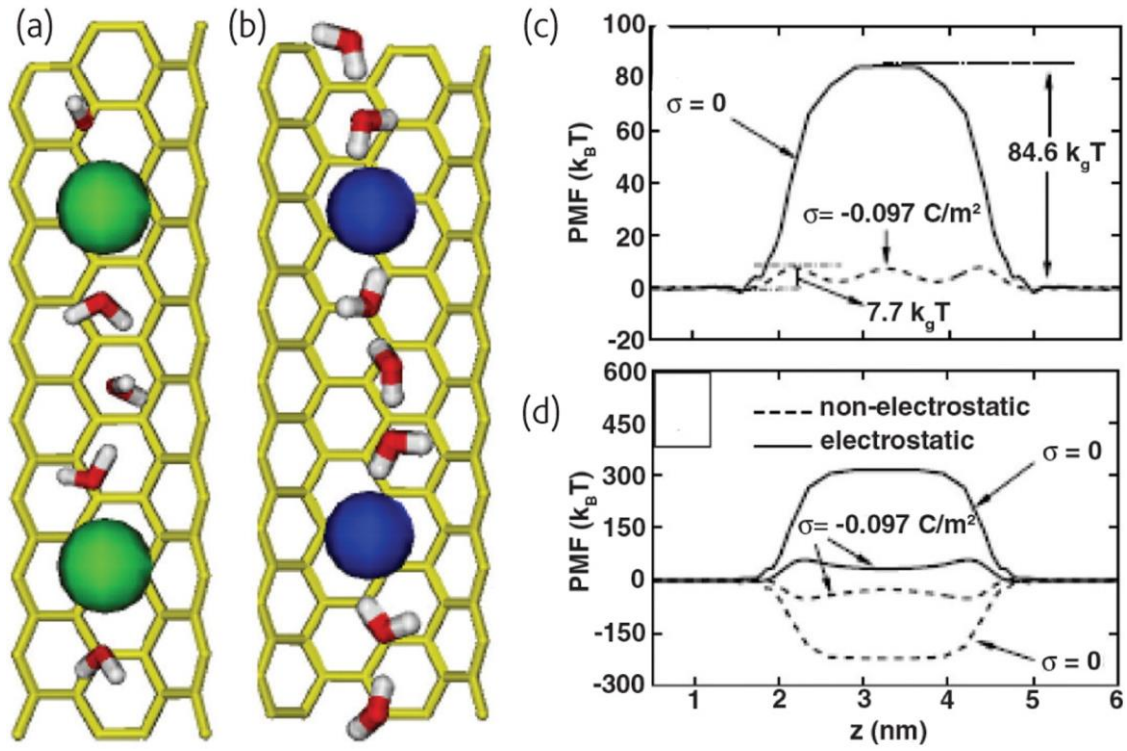


Water flux



Air flux

# Nanofiltration and ion exclusion



- Fast filters due to high water transport
- Charging of the CNTs leads to ion exclusion
- Modification of the CNTs ends



Thanks to your  
attention

▶ Questions???