Nanofluidics and graphene

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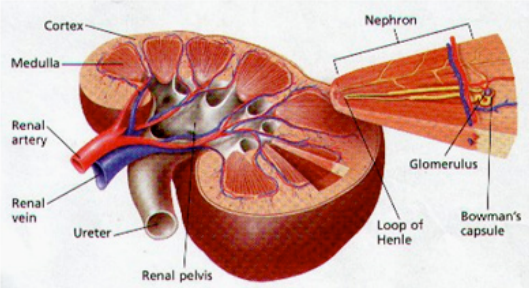
L. Joly (ILM), M.-L. Bocquet (ENS-Lyon) - simulations

Nanofluidics: fluid transport *at nanoscales*

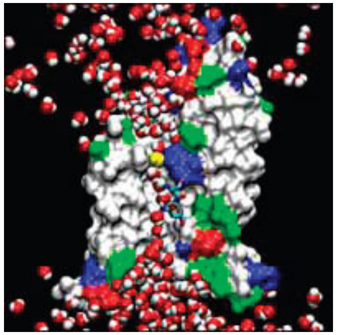
Applications:

biological analysis, energy harvesting, filtration, desalination…

- Get inspiration from efficient natural systems
- Explore new materials / create new functionalities
- Fundamentals of fluid transport: change of paradigm ?

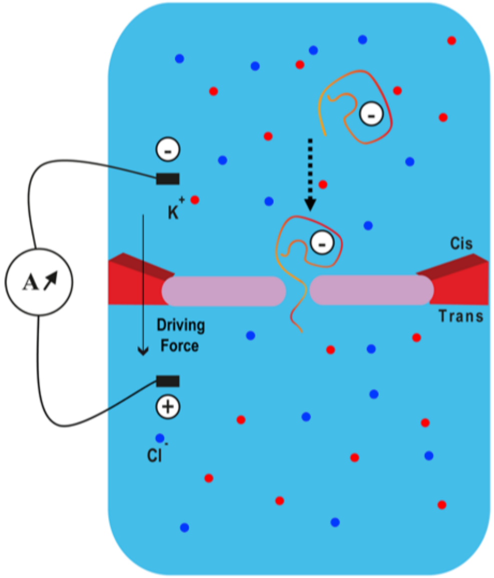


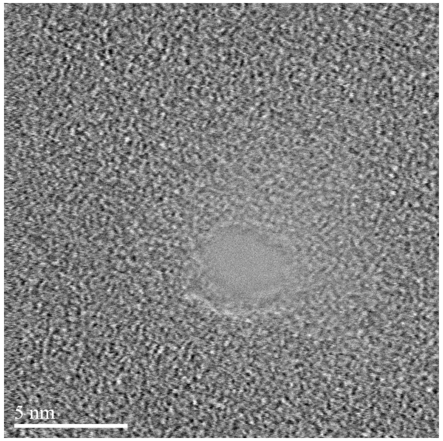
Greger and Windhorst,
Comprehensive human physiology (Springer)

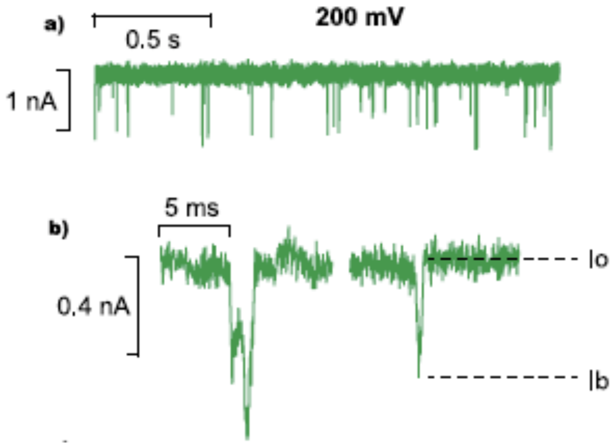


AQP-1: water filter- High permeation/high selectivity

Biomolecular analysis







Oukhaled et al., PRL 2007
Cressiot et al., ACS Nano (2012)

Solid state nanopores as bio-sensors

Loïc Auvray et al.

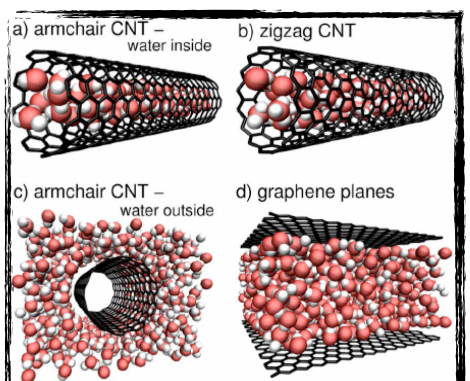
New materials, new behaviors

Fast Mass Transport Through Sub–2-Nanometer Carbon Nanotubes

Jason K. Holt,[1*] Hyung Gyu Park,[1,2*] Yinmin Wang,[1] Michael Stadermann,[1] Alexander B. Artyukhin,[1] Costas P. Grigoropoulos,[2] Aleksandr Noy,[1] Olgica Bakajin[1]†

Holt et al. Science (2006)

Enhancement over no-slip, hydrodynamic flow† (minimum)
1500 to 8400
680 to 3800
560 to 3100



Falk et al. Nanoletters (2010)

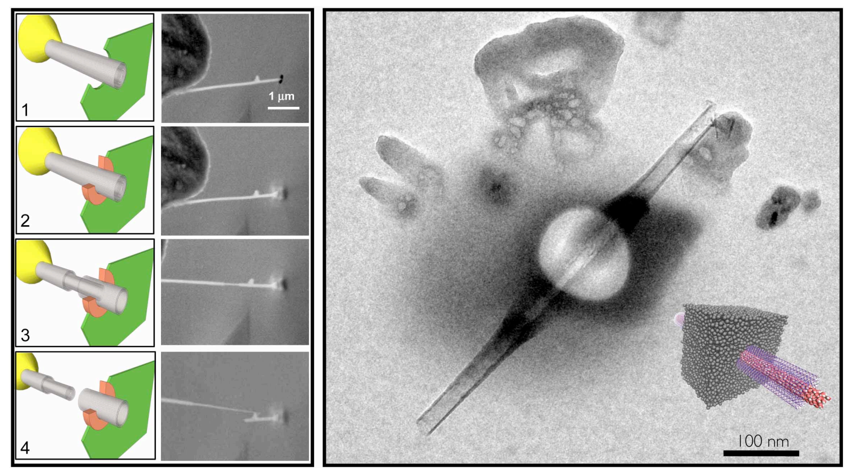
LETTER

Siria et al. Nature (2013)

doi:10.1038/nature1187

Giant osmotic energy conversion measured in a single transmembrane boron nitride nanotube

Alessandro Siria[1], Philippe Poncharal[1], Anne-Laure Biance[1], Rémy Fulcrand[1], Xavier Blase[2], Stephen T. Purcell[1] & Lydéric Bocque



- New tools for fundamental understanding
- Huge produced osmotic power in BN tube
  4kW/m² (versus ~5 W/m²)

Why graphene?

Graphene for fluidic applications

Ultimate membrane: atomic thickness (down to Angstroms)

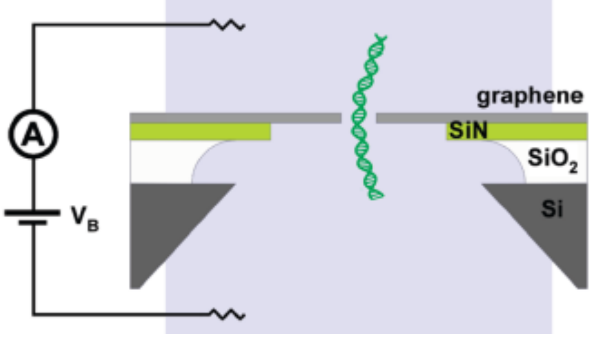
✓ Sculpting smaller nanopores (limited by aspect ratio)

✓ Huge increase in flow permeability

✓ Fine tuning of chemical sensitivity: selectivity, functionalization

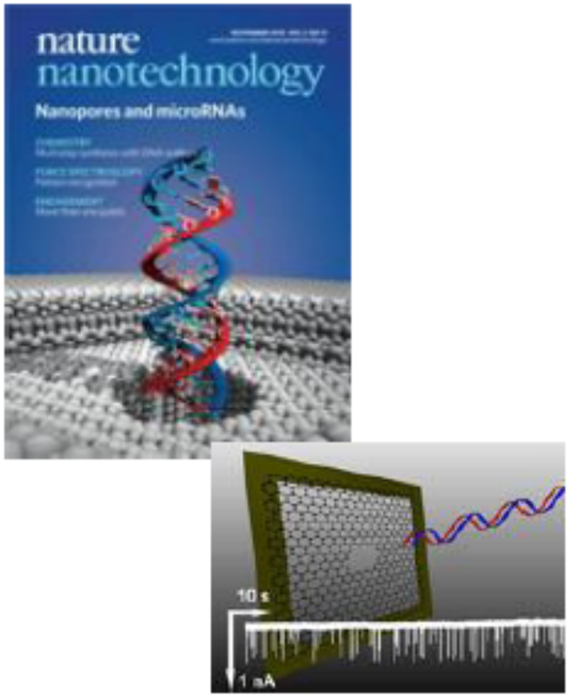
✓ A new fundamental tool: water and ion transport at the molecular scales

« Reading » molecules



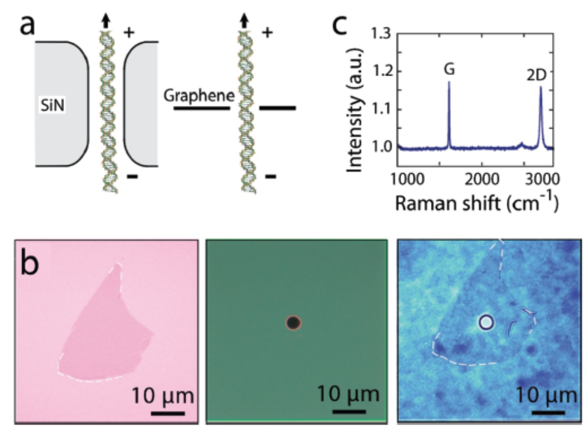
Merchant et al. Nanoletters (2010)

Ultimate biological sensor



C.A. Merchant et al.
DNA translocation through graphene Nanopores
NanoLetters (2010)

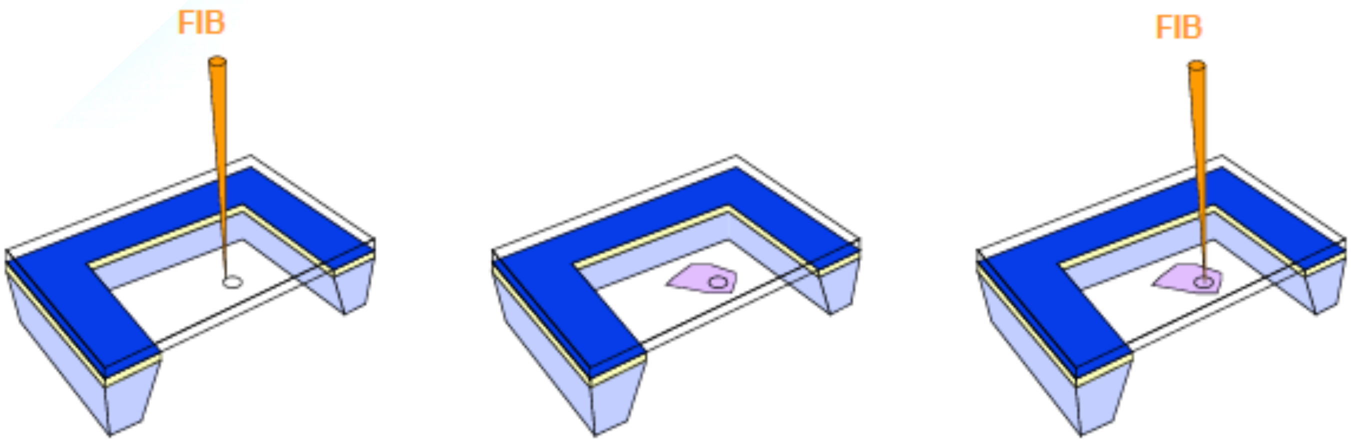
S. Garaj et al.
Graphene as a sub-nanometer transelectrode membrane
Nature (2010)



Dekker et al., Nanoletters (2013)

Nanopores in graphene sheets

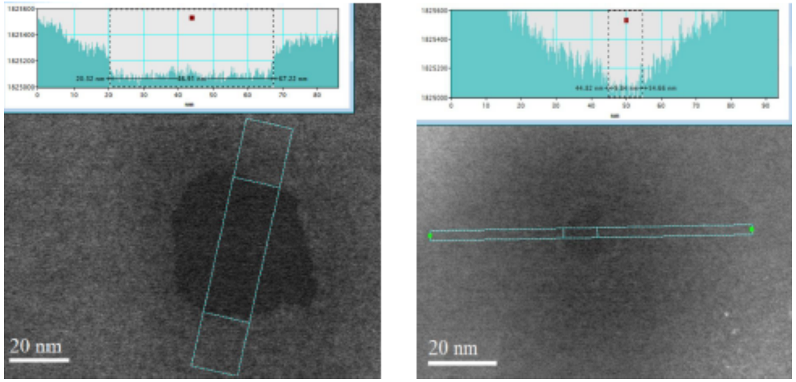
3 step process: FIB drilling



(a) **Template**
SiNx (50 nm thick) membrane
patterned µm-sized hole (FIB)

(b) **Graphene** Flake deposition

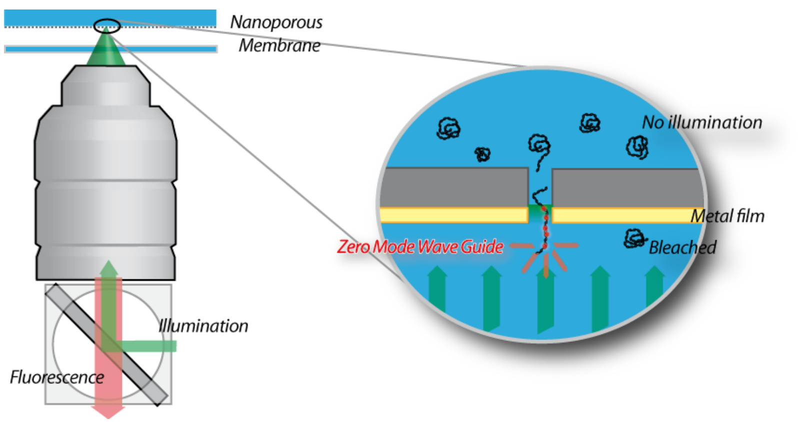
(c) **Nanopore** carved
into the in high-
resolution mode



J. Gierak et al. (LPN)

To probe biomolecule structure

- Goals:
  - DNA sequencing
  - Protein folding and/or molecular structure probes



- Advantages:
  - very high sensitivity due to atomic thickness
  - fine tuning of molecular interactions

- Challenges:
  - Chemical functionalization
  - Optical characterization (more sensitivity and selectivity)

L. Auvray, F. Montel (MSC)

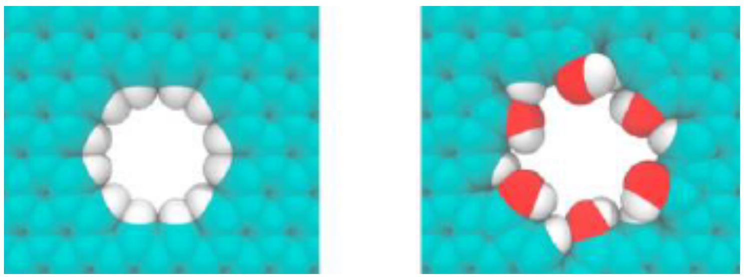
Ultrafiltration and desalination

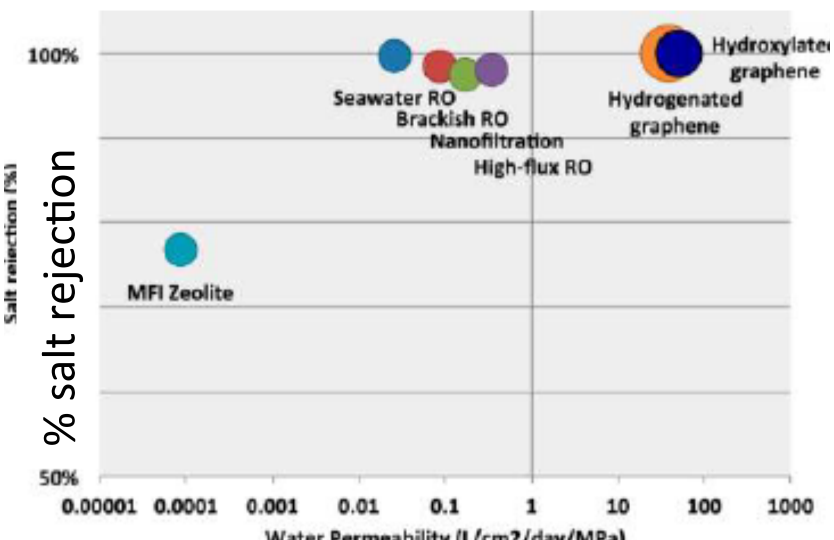
NANO LETTERS
Letter
pubs.acs.org/NanoLett

Water Desalination across Nanoporous Graphene

David Cohen-Tanugi and Jeffrey C. Grossman*

Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, United States





Predictions of (classical) MD simulations

Allows:

- Best selectivity
- Huge permeability

Challenges:

- Need for experiments
- Scale up

Aims:

- Desalination
- New osmotic membranes

A. Siria, A.-L. Biance, L. Bocquet (ILM)

Blue energy harvesting

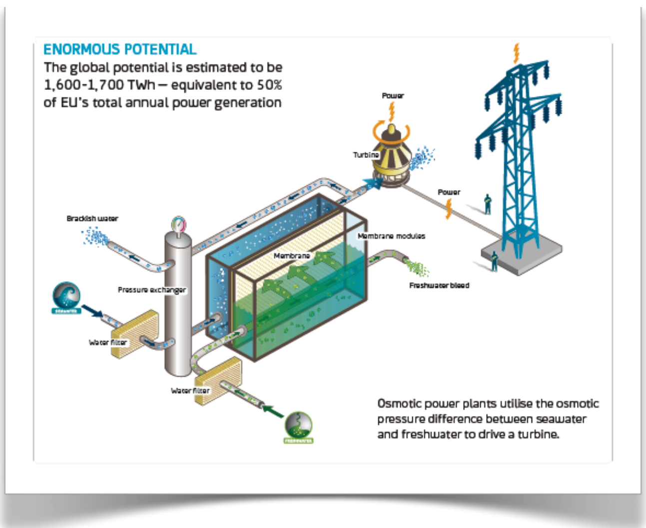
Harvest free energy available from difference in salinity (sea-river)

REVIEW Logan & Elimelech, Nature (2012)

doi:10.1038/nature11477

Membrane-based processes for sustainable power generation using water

Bruce E. Logan[1] & Menachem Elimelech[2]



- Dedicated membranes:

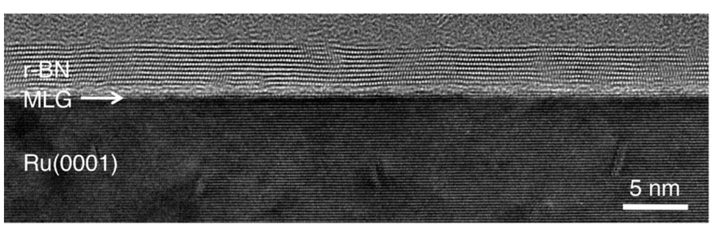
Selective (semi-permeable) or ion-selective, chemically coated…

- Efficiency:

State of the art (Majumdar, 2010): ~ 7W/m^2

BN nanotubes (Siria et al., 2013): 4000 W/m^2

Graphene or BN membrane: 10$^{??}$ W/m^2



BN few layers membranes
Sutter et al. Nanoletters (2013)

A. Siria, A.-L. Biance, L. Bocquet (ILM)

Models

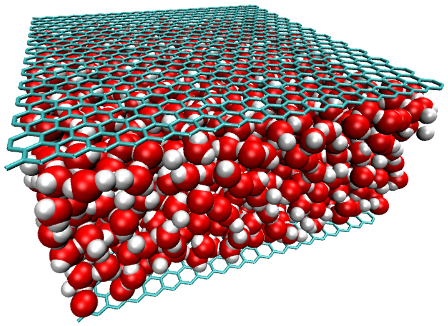
Aim:

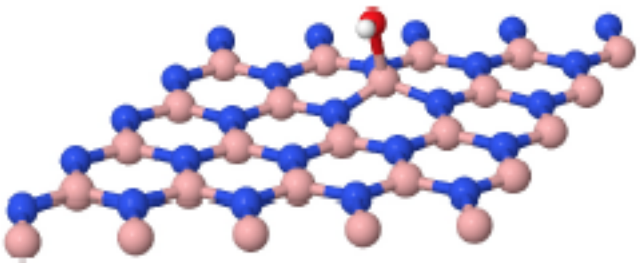
- modeling of fluid transport through/close to graphene
- fundamental understanding to develop new functionalities

Two levels of modeling:

- semi-empirical: collective dynamics of water and ions
- Ab initio: molecular interactions and electronic properties

Mesoscale bridge required at quantum/classical interface





Water-BN interaction
with X. Blase
(Siria et al. 2013)

L. Joly, L. Bocquet (ILM), M.-L. Bocquet (ENS Lyon)

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LABORATOIRE
DE PHOTONIQUE
ET DE NANOSTRUCTURES

Nanofluidics and graphene

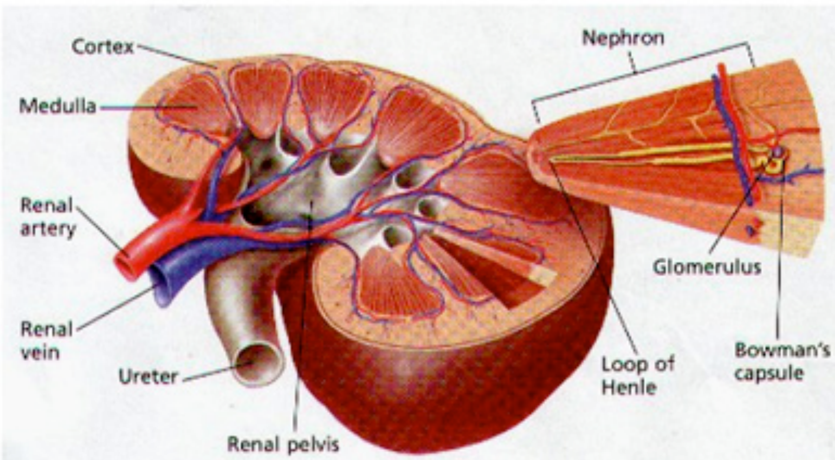
- ✓ Nanofabrication
- ✓ Bio-diagnosis
- ✓ Energy harvesting and desalination
- ✓ Linking classical and quantum properties

MSC

LABORATOIRE DE CHIMIE

ENS DE LYON

Kidney: a very advantageous nano-filter



Greger and Windhorst,
Comprehensive human physiology (Springer)

AQP-1: water filter
High permeation/high selectivity

Artificial systems can be improved!