Probing, Charging and Discharging of Single Nanopores in a Supercapacitor

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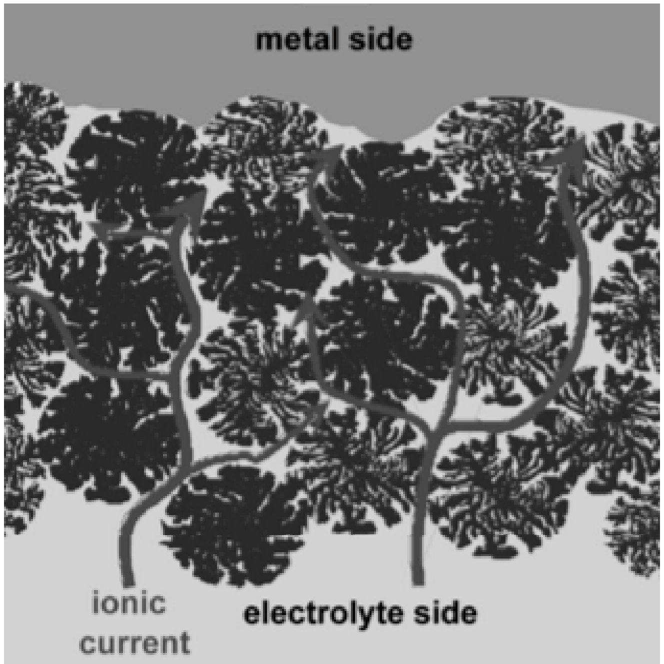
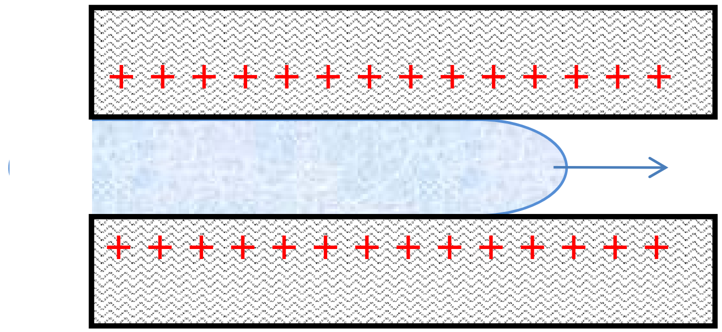
Contents

- Background
  - Probing the fundamental processes in electrochemical capacitors (EC)
  - On-chip dielectric spectroscopy with microfluidic and nanofluidic channels
- Dielectric spectroscopy with planar micro/nanofluidic channels for EC process probing
  - Nanofluidic channel fabrication
  - Dielectric spectroscopy methods
  - Molecular dynamics simulation

Background: Wetting and ion transport in ECs



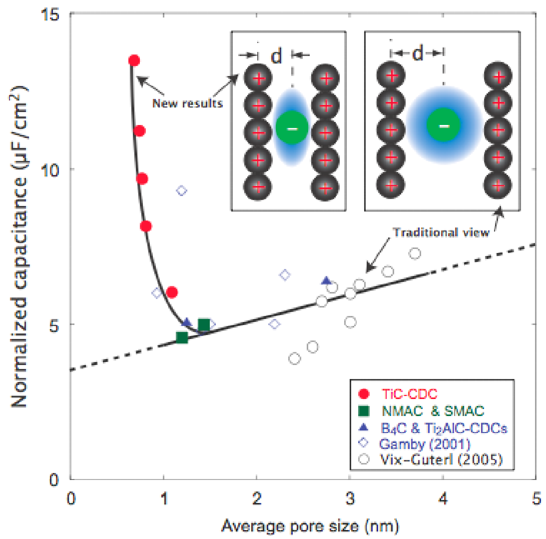
Nanoscale systems
Pores: 0.5–3 nm in size)

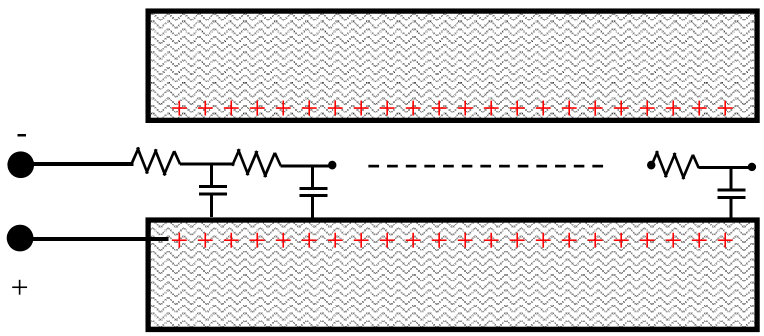


- Wetting characteristics in nanopores
- Ion transport: electrolytes for performance

* Modified from Fig. 16 on p. 55 of Basic Research Needs for Electrical Energy Storage

Background: Charging and discharging at atomic level



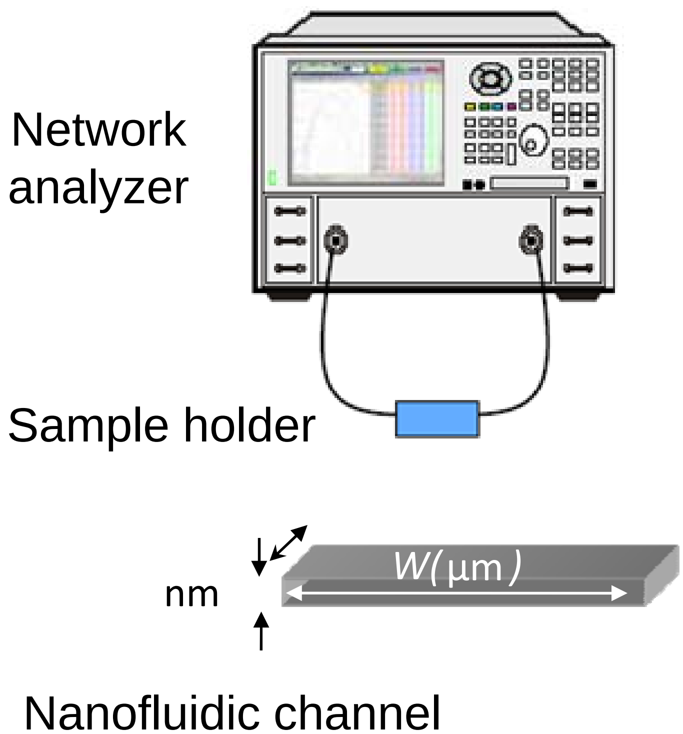


- Correlation between pore size, ion size, surface area, surface chemistry and EC performance
- Solvation dynamics, molecular interactions at the interfaces
- Electrolyte/electrode interface during charging/discharging at molecular and atomic levels
- Calibrated and valibrated predictive models for capacitive energy systems: nm to mm and picosecond to microsecond.

* Modified from Fig. 16 on p. 49 of Basic Research Needs for Electrical Energy Storage

Background: on-chip dielectric spectroscopy with micro/nanofluidic channels

- Dielectric spectroscopy (Impedance spectroscopy)



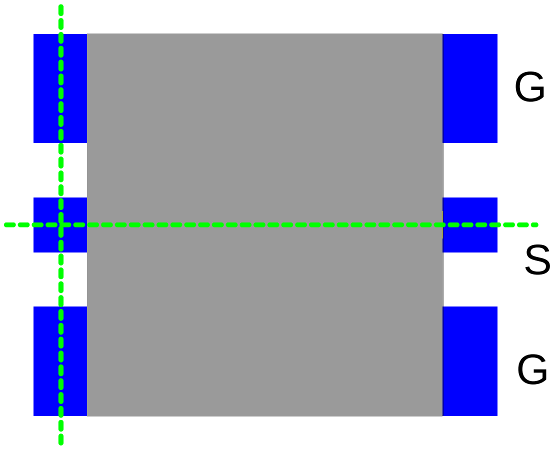
Dielectric spectroscopy is complementary to

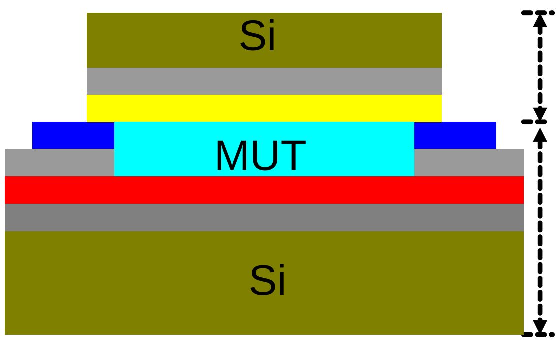
- Nuclear magnetic resonance (NMR)
- Neutron scattering
- Mechanical spectroscopy
- Debye relaxation

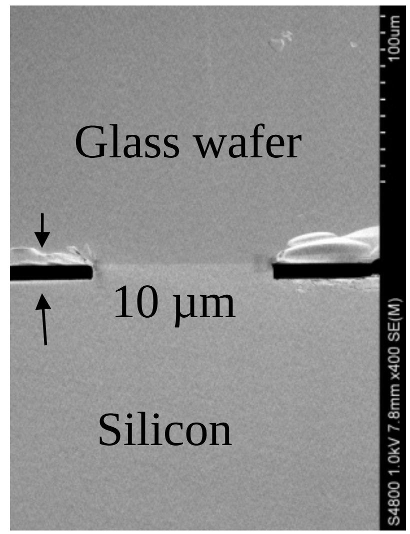
$$\hat{\varepsilon}(\omega) = \varepsilon_{\infty} + \frac{\Delta\varepsilon}{1 + i\omega\tau},$$

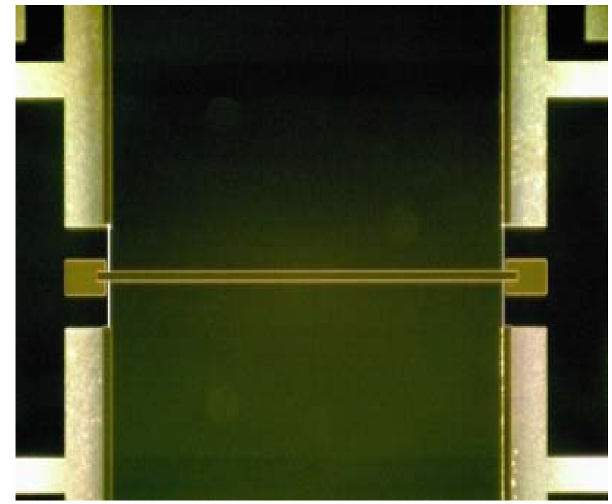
where ε_{∞} is the permittivity at the high frequency limit, $\Delta\varepsilon = \varepsilon_s - \varepsilon_{\infty}$,ε_s is the static, low frequency permittivity, and τ is the characteristic relaxation time of the medium.

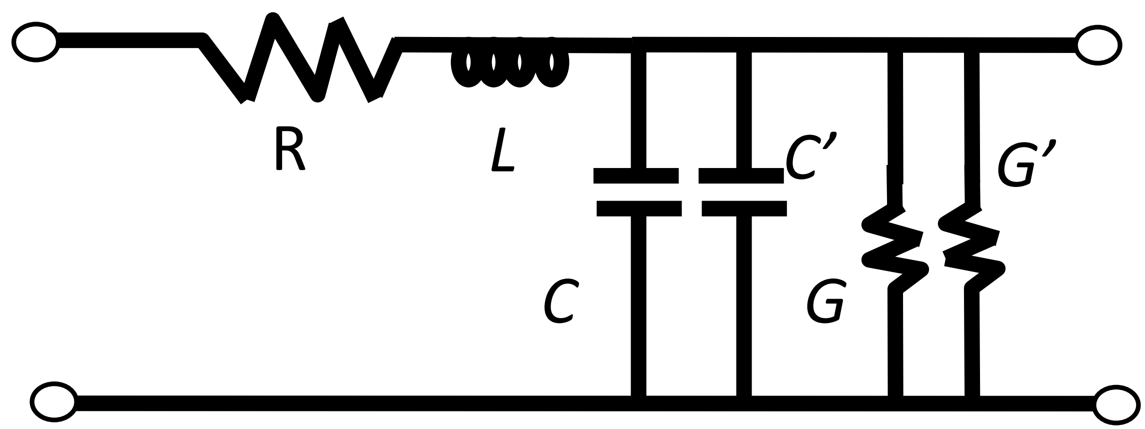
Background: micro/nano fluidic channels



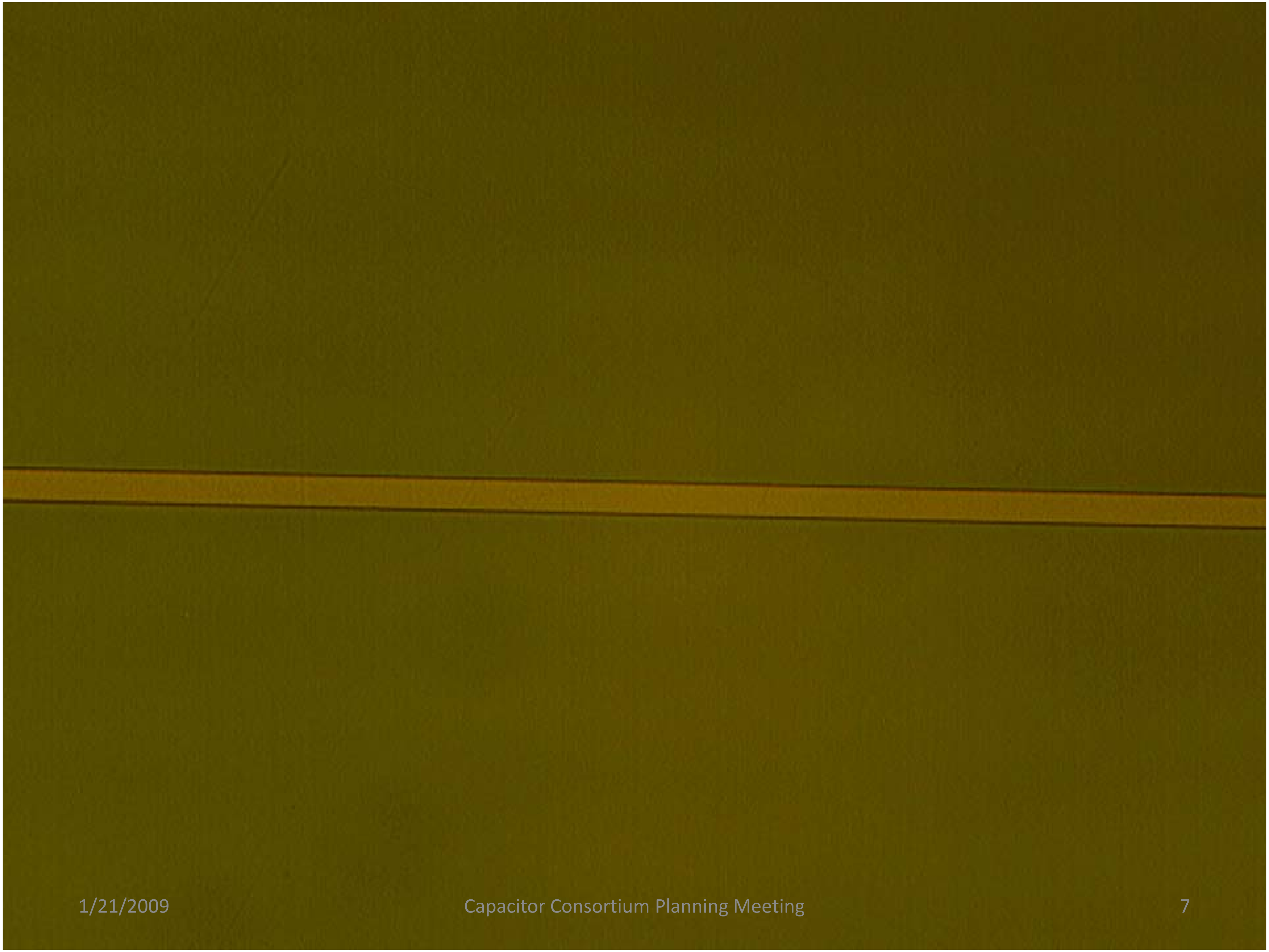






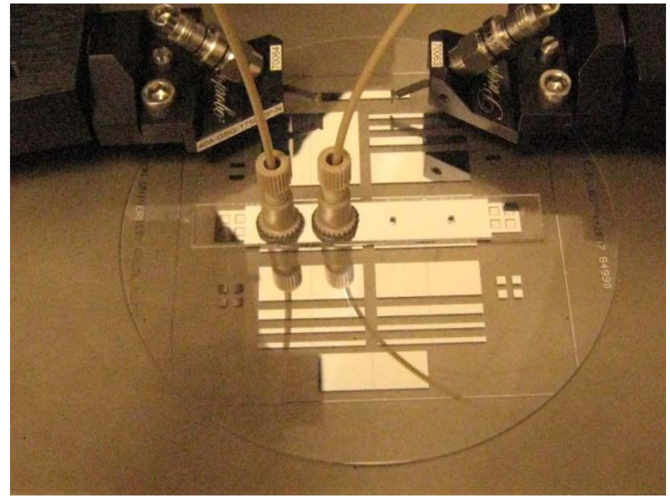


Water flow video

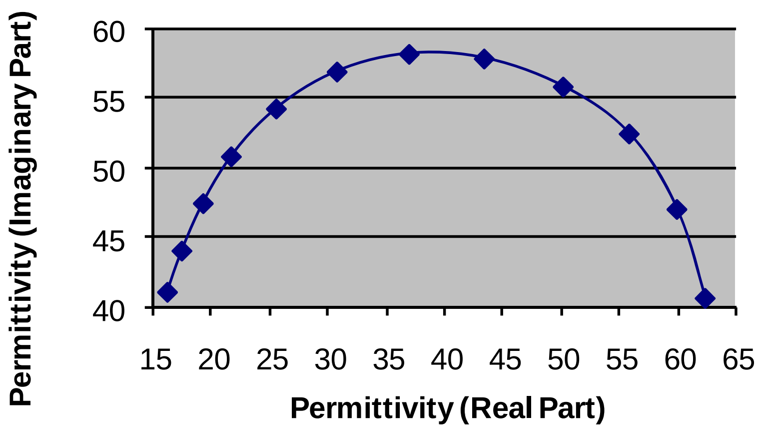


Background: microfluidic channels and results

Microfluidic channels



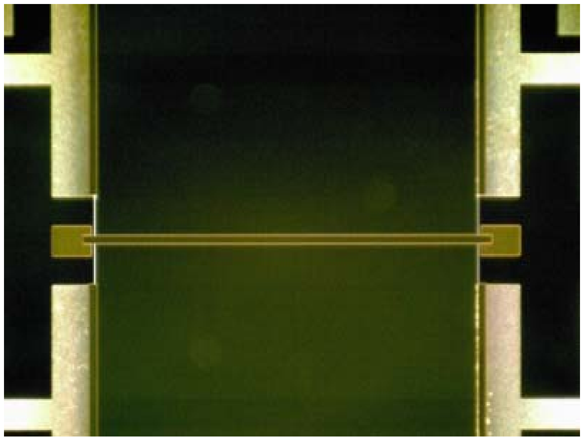
Measurement setup

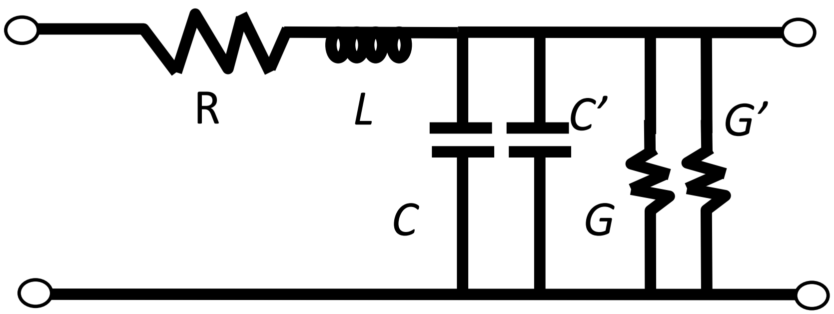


Water dielectric permittivity

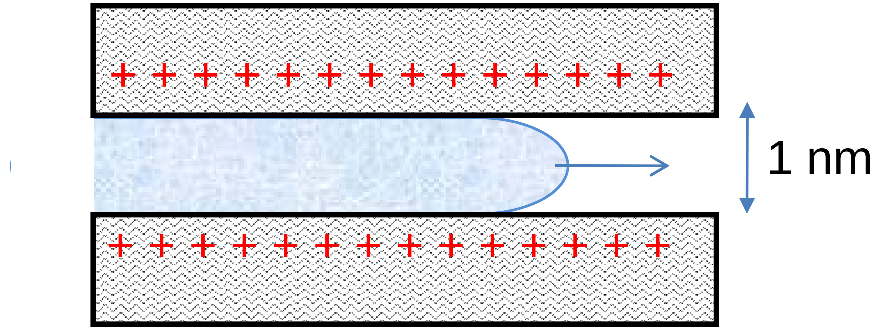
- ~ 50 kV/cm electric field
- Slightly different from ordinarily accepted 80

Proposal: probing fundamental process in ECs with 1-1000 nm planar micro/nanofluidic channels

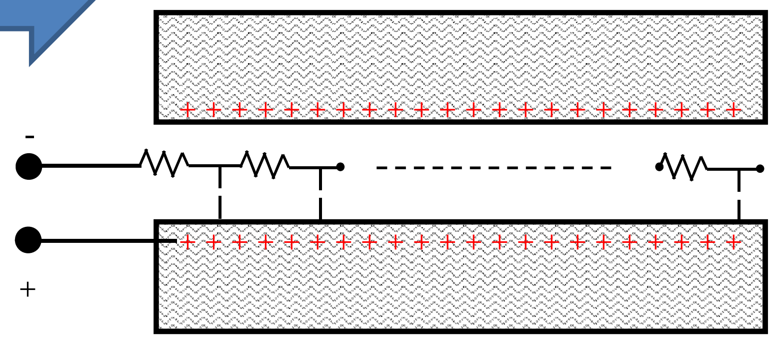




On-chip dielectric spectroscopy



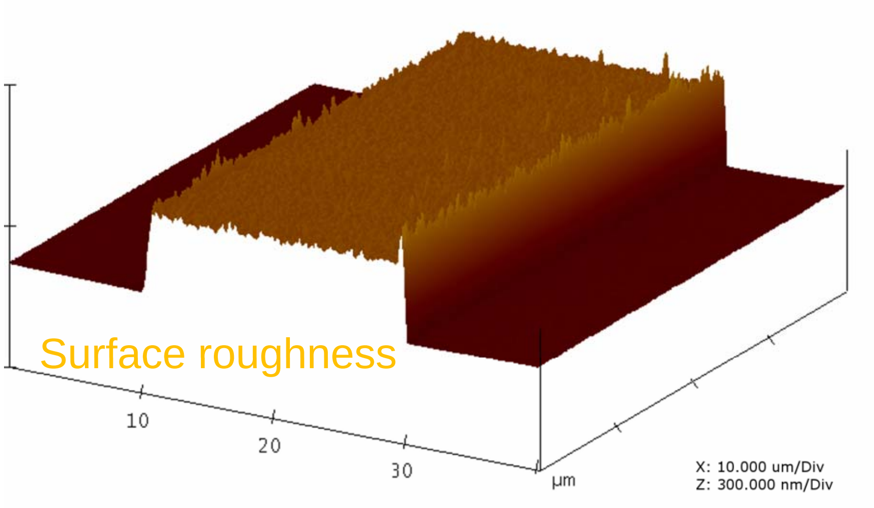
Wetting

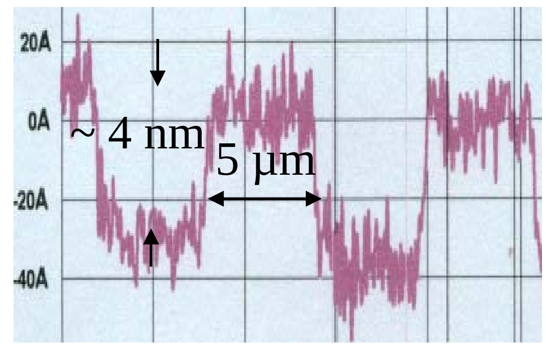


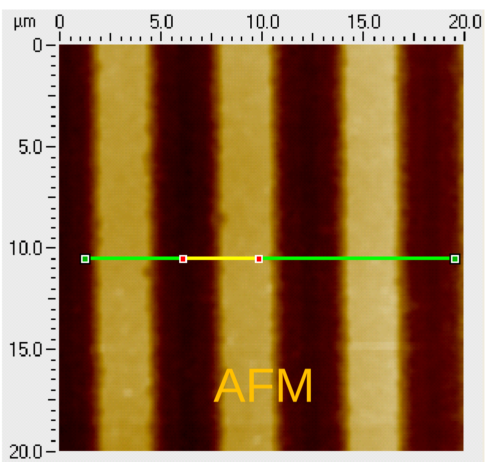
Charging and discharging

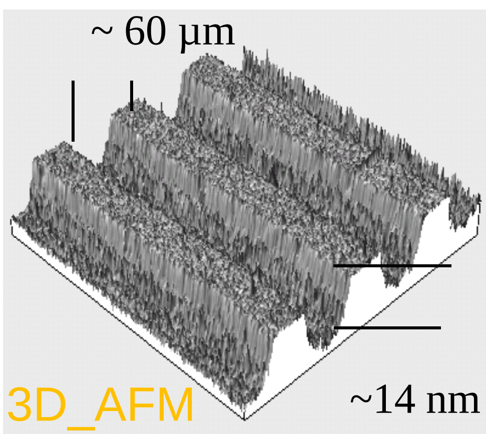
Different electrolytes
(bulk vs. confined)

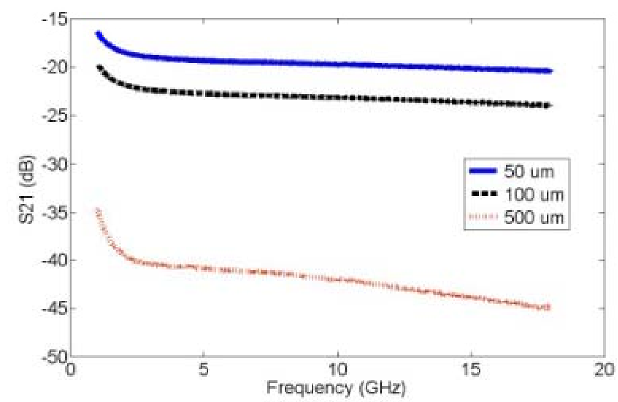
Microfluidic channels: fine.
Nanofluidic channels: is it possible?





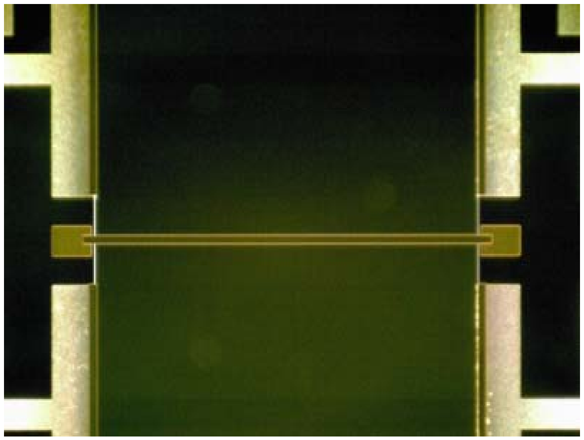


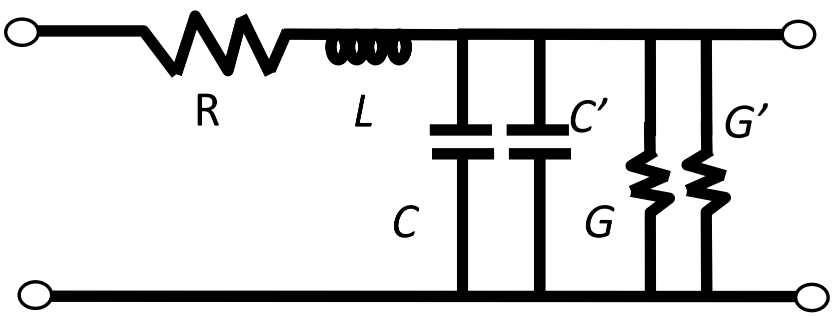


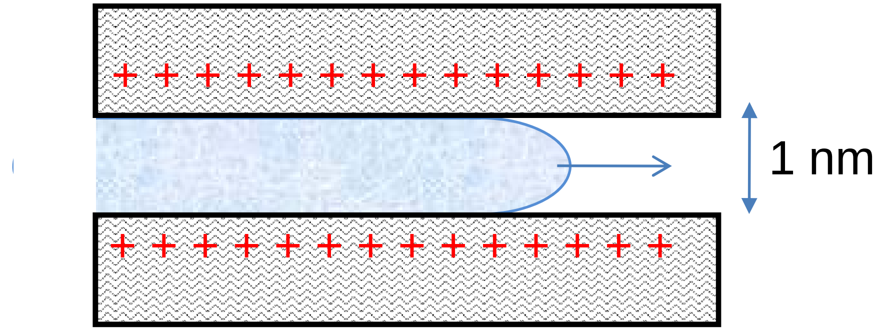


Silicon transmission lines

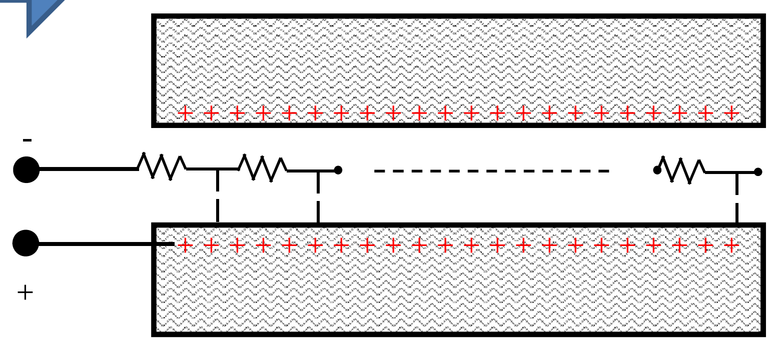
Proposal: probing fundamental process in ECs with 1-1000 nm planar micro/nanofluidic channels







Wetting



Charging and discharging

1 M quaternary ammonium bis(oxalato) borates (QABOBs)/propylene carbonate solutions
1 M Et4NBF4/propylene carbonate

Long term goals and 1-year deliverables

- Long term goals
  - Understand wetting, charging and discharging processes of ECs at the atomic level
  - Establish corresponding models
  - Understand the interactions charged electrodes and electrolytes
  - Help identify the properties of perfect electrolytes for ECs
- First year deliverables
  - Microfluidic channels and dielectric characterization of two electrolytes: 1 M quaternary ammonium bis(oxalato) borates (QABOBs)/ propylene carbonate solutions, and 1M Et_4NBF_4/propylene carbonate.
  - Planar nanofluidic channels with ~ 1 nm (silicon and SiO_2 surface)
  - Initial results on wetting and charging and discharging models