COMSOL CONFERENCE BOSTON 2013

Numerical Modeling of the Bistability of Electrolyte Transport in Conical Nanopores

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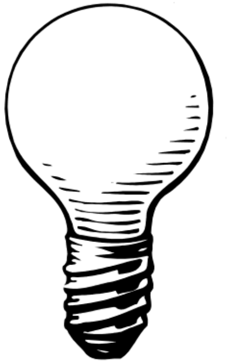
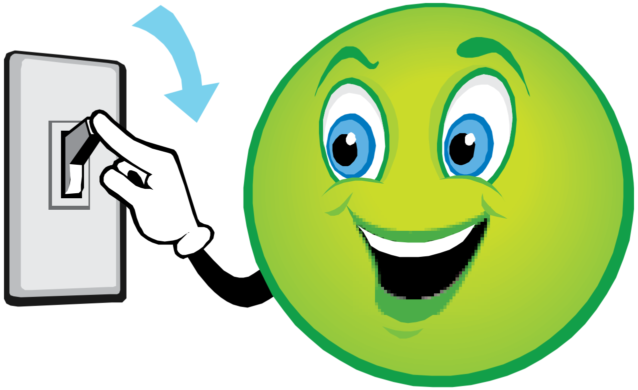
Bistability



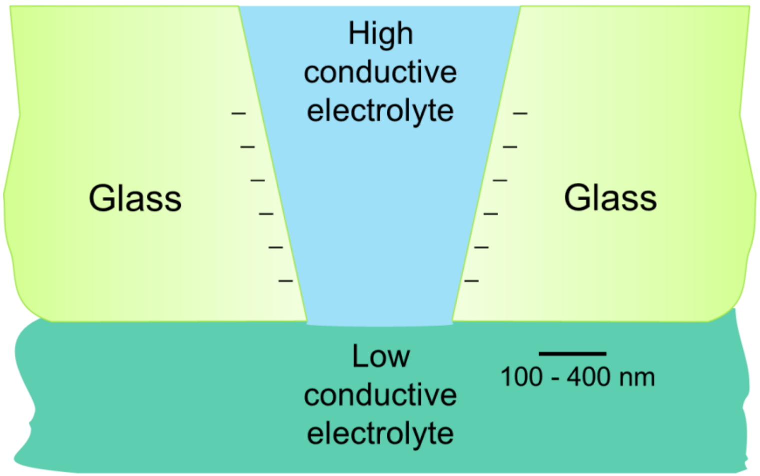
Off

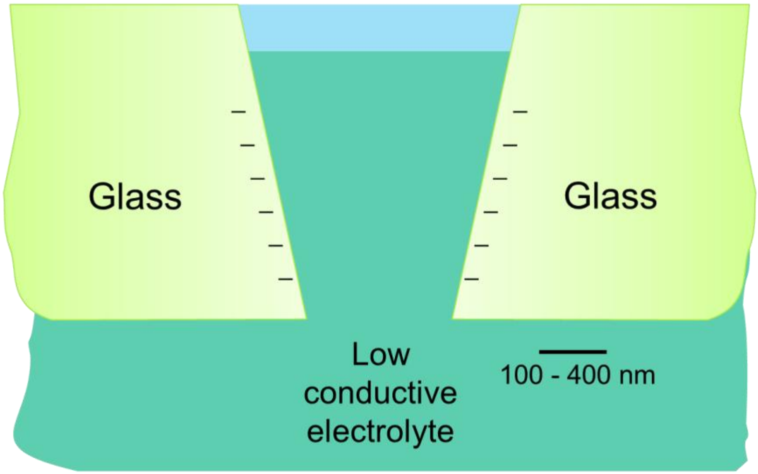
On



Critical condition

Electrolyte Transport Bistability

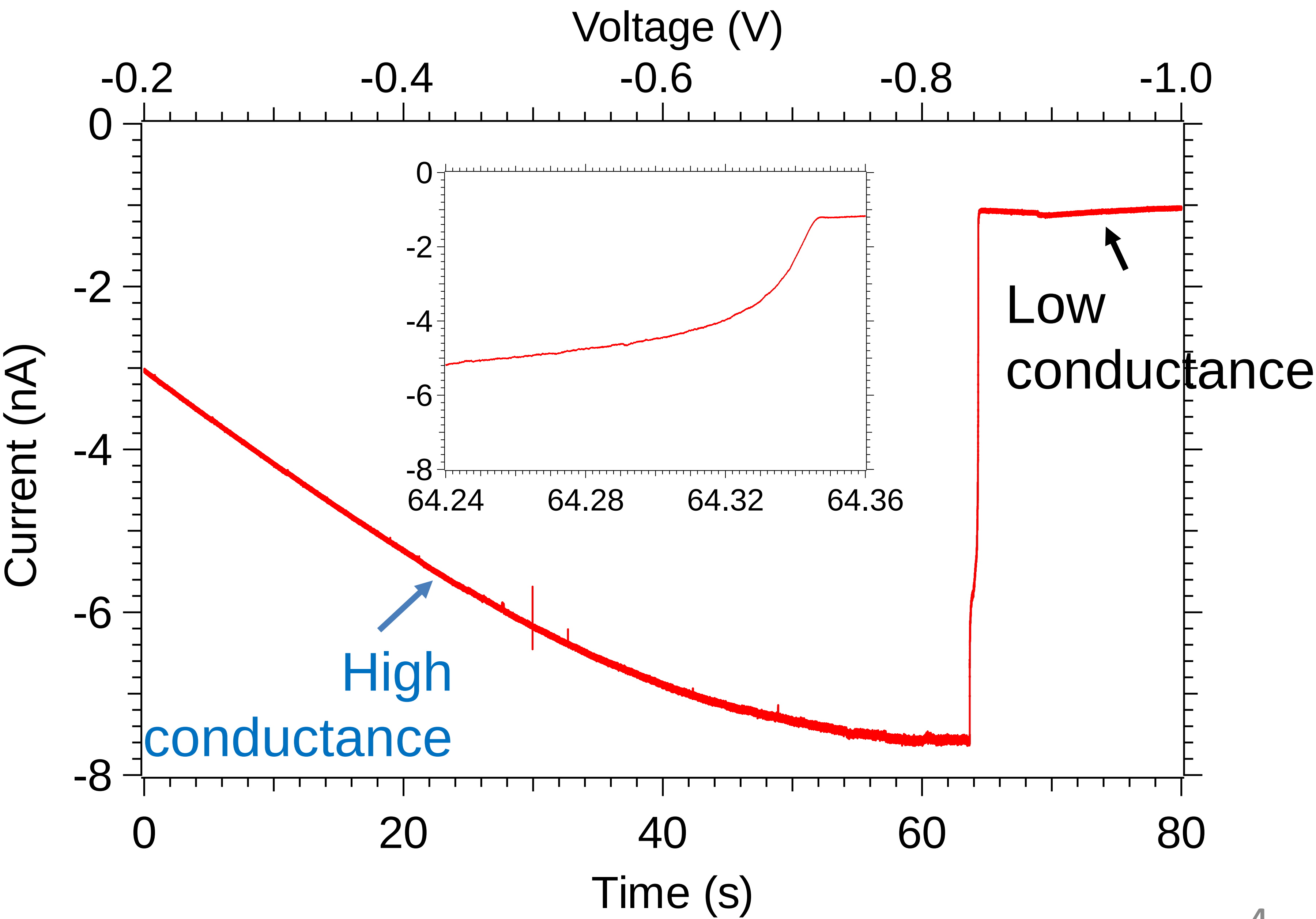




High conductance state (HCS)

Low conductance state (LCS)

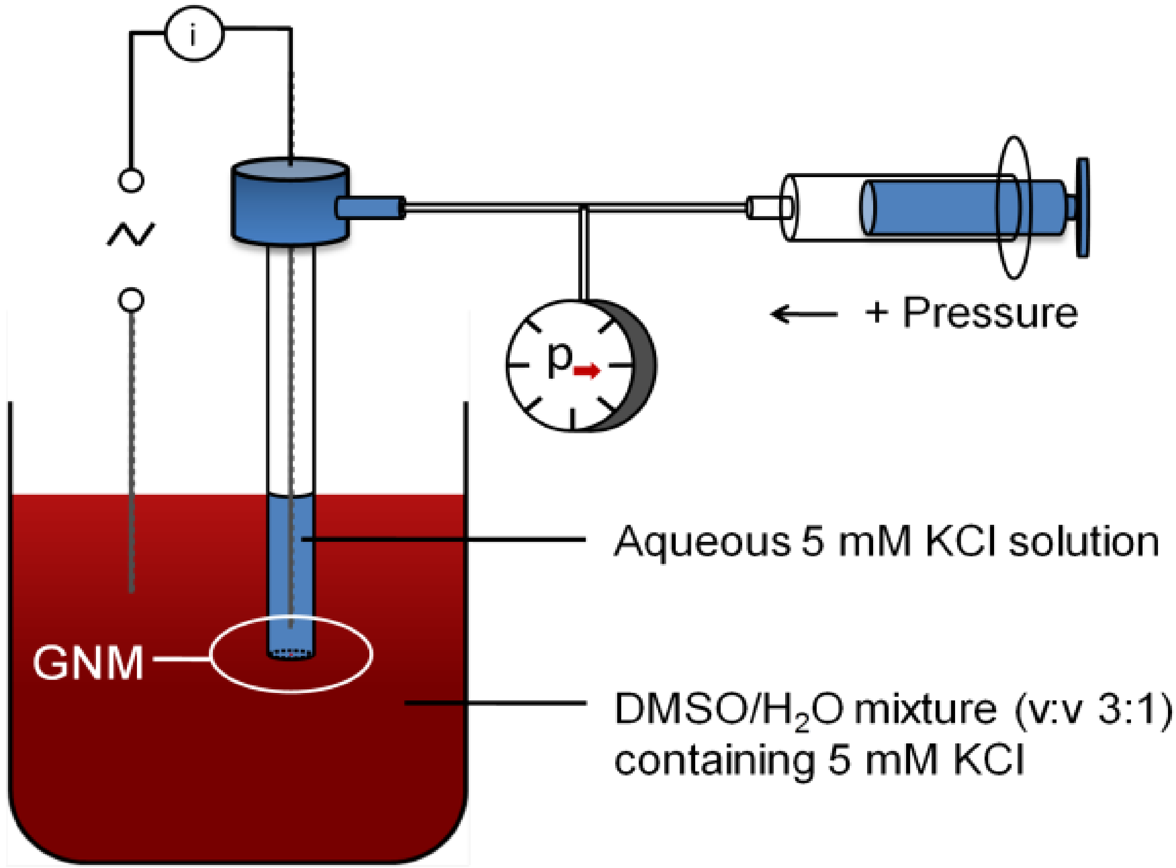
Critical voltage



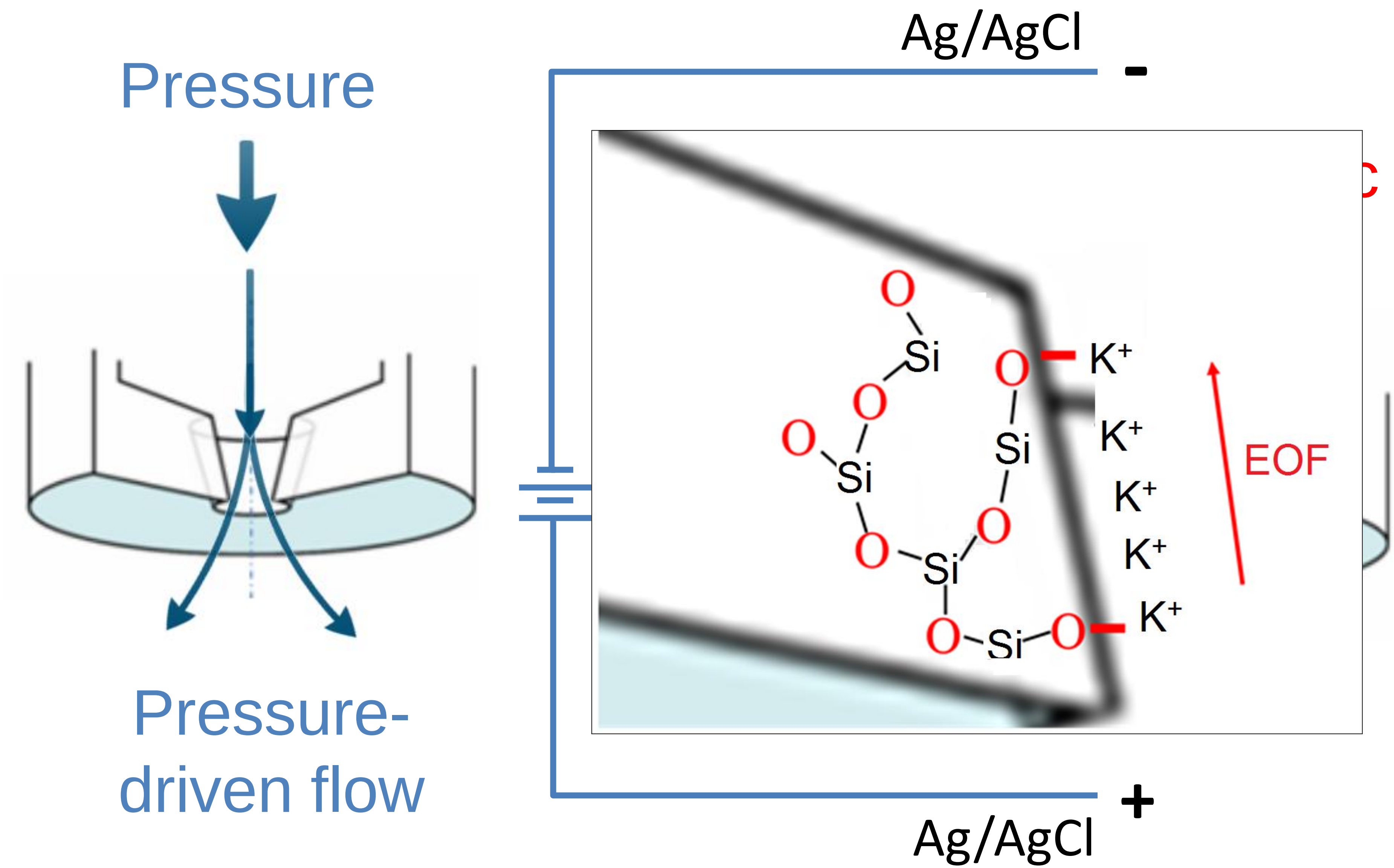
Voltage (V)
-0.2
-0.4
-0.6
-0.8
-1.0
Current (nA)
0
-2
-4
-6
-8
Time (s)
0
20
40
60
80
High conductance
Low conductance
64.24
64.28
64.32
64.36

Experimental Design

Glass Nanopore Membrane (GNM)
Orifice radius: 200-500 nm

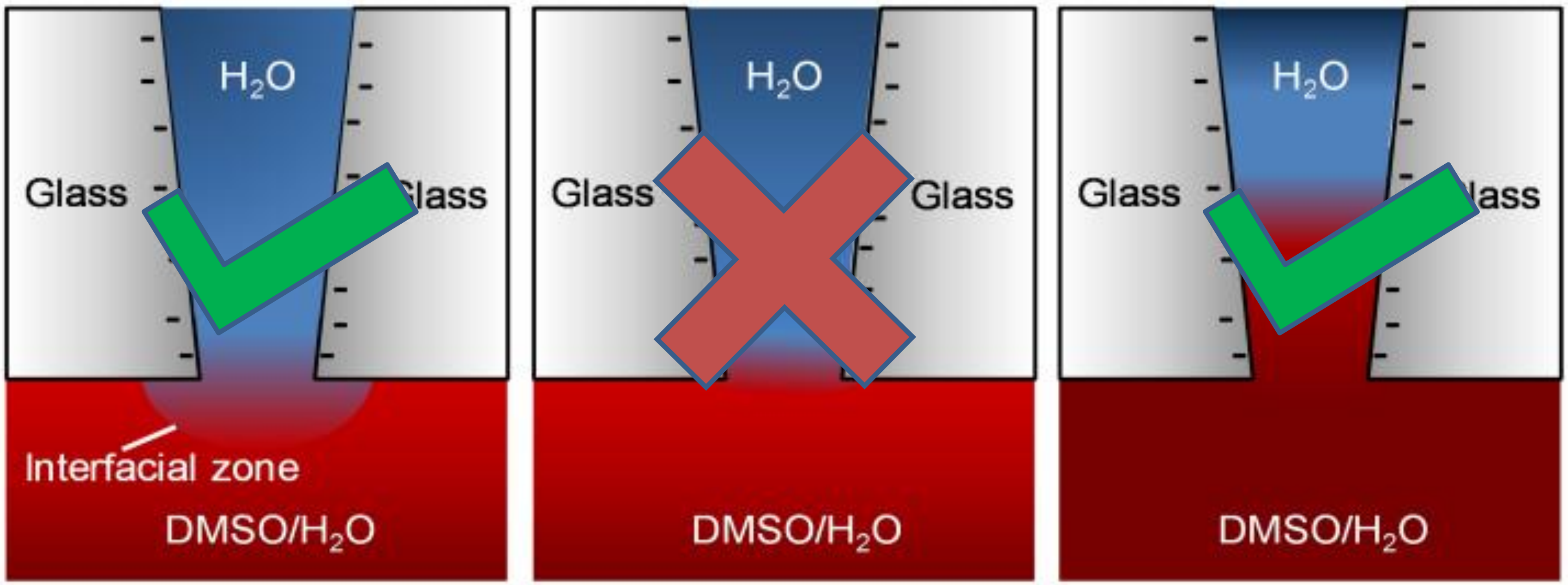


Experimental Design

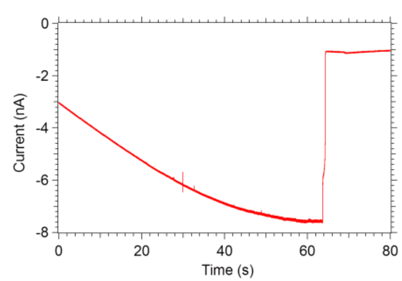


Electrolyte Transport Bistability

(a) (b) (c)

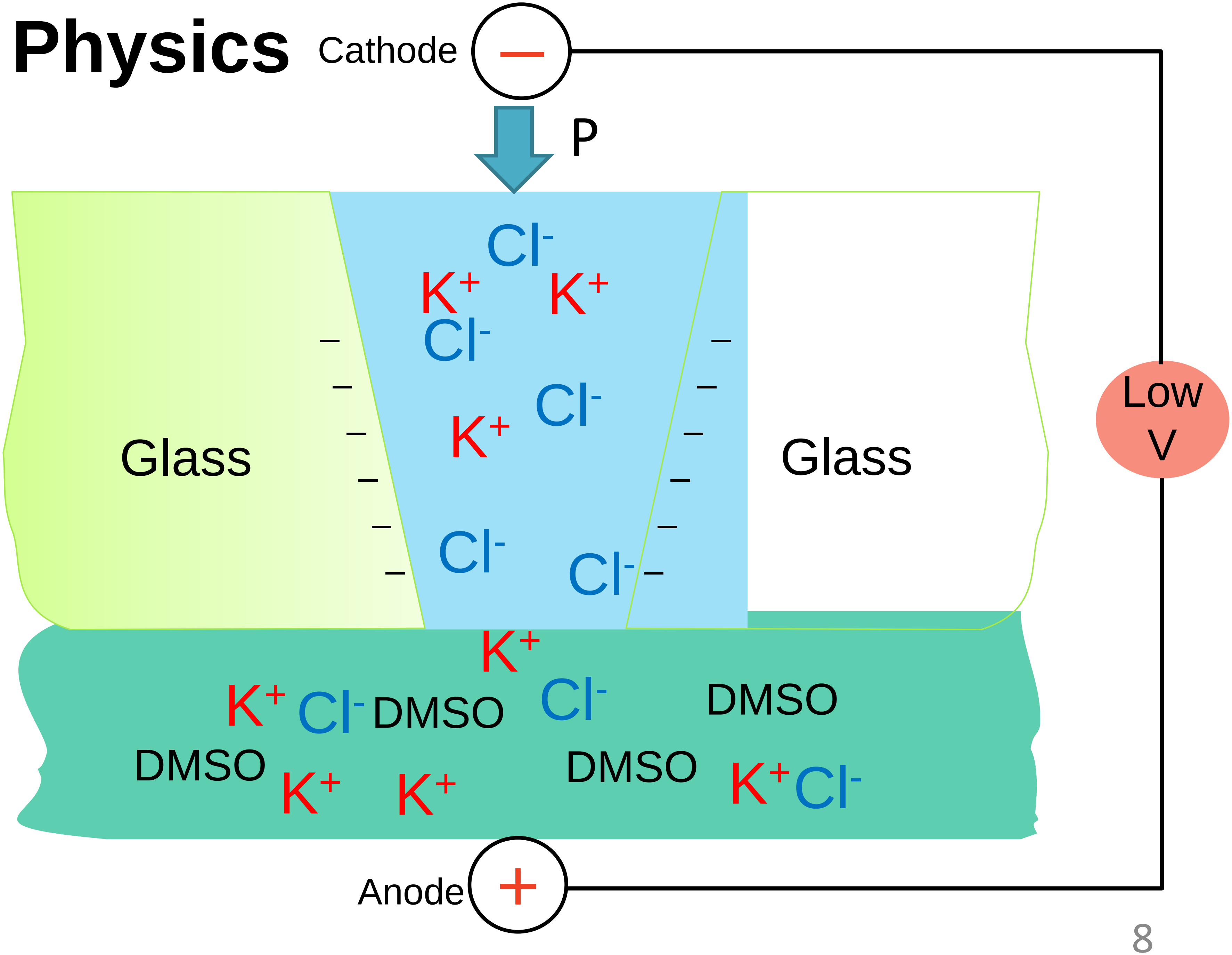


Stable
High conductance state
(HCS)

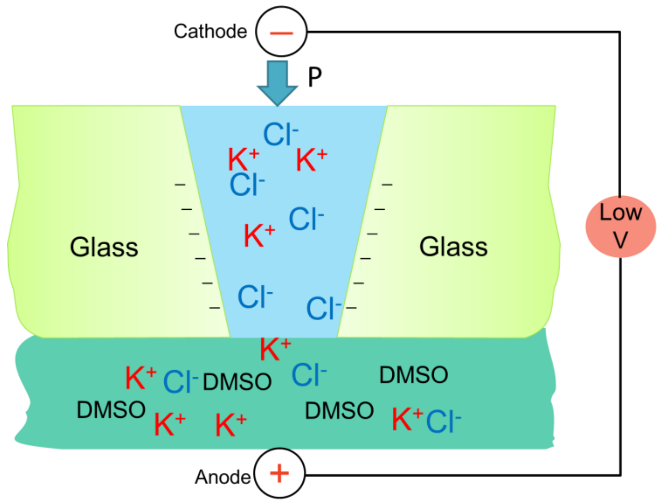


Stable
Low conductance state
(LCS)

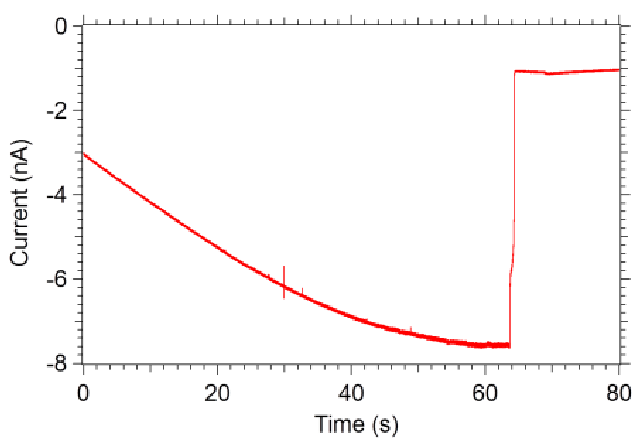
Physics


Cathode
–
P
Cl-
K+
K+
Cl-
Cl-
K+
Glass
Glass
Low V
Cl-
Cl-
K+
K+
Cl-
DMSO
Cl-
DMSO
DMSO
DMSO
K+
K+
K+
Cl-
Anode
+

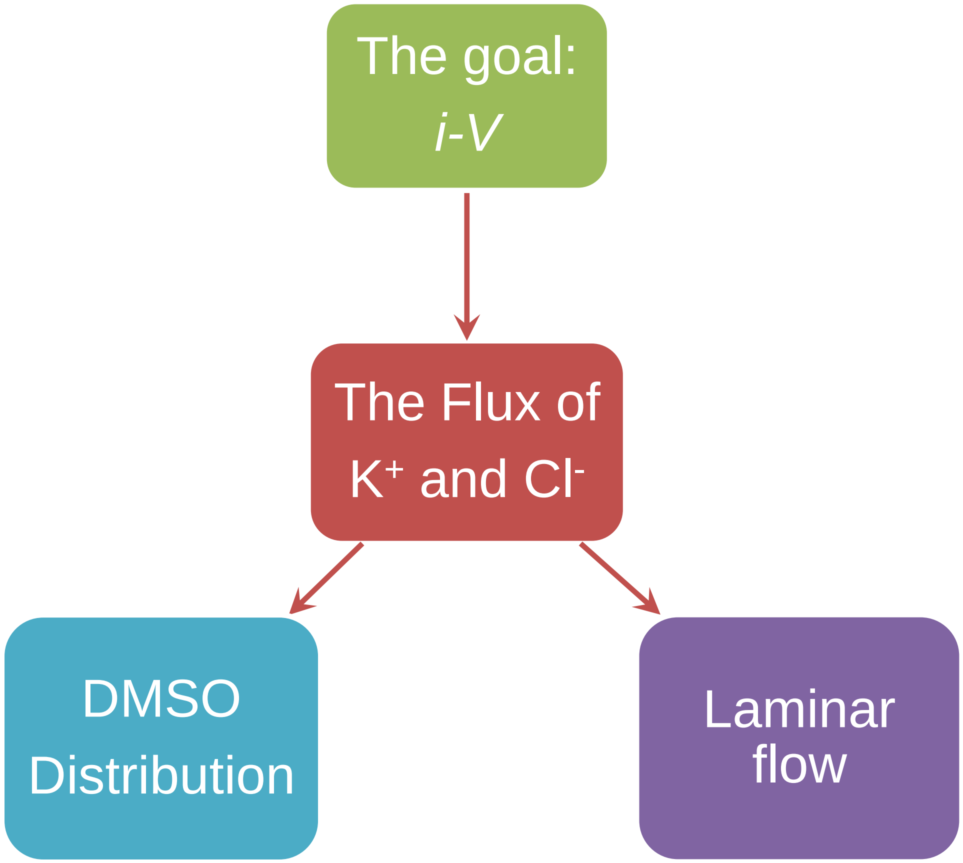
Physics



Cathode
P
Glass
Glass
Low V
DMSO
Anode



Current (nA)
Time (s)



The goal: *i-V*
The Flux of K^+ and Cl^-
DMSO Distribution
Laminar flow

COMSOL Model

1) Laminar flow

$$\mathbf{u}\nabla\mathbf{u} = \frac{1}{\rho}(-\nabla p + \eta\nabla^2\mathbf{u} - F(\sum_i z_i c_i)\nabla\Phi$$

2) Mass transfer

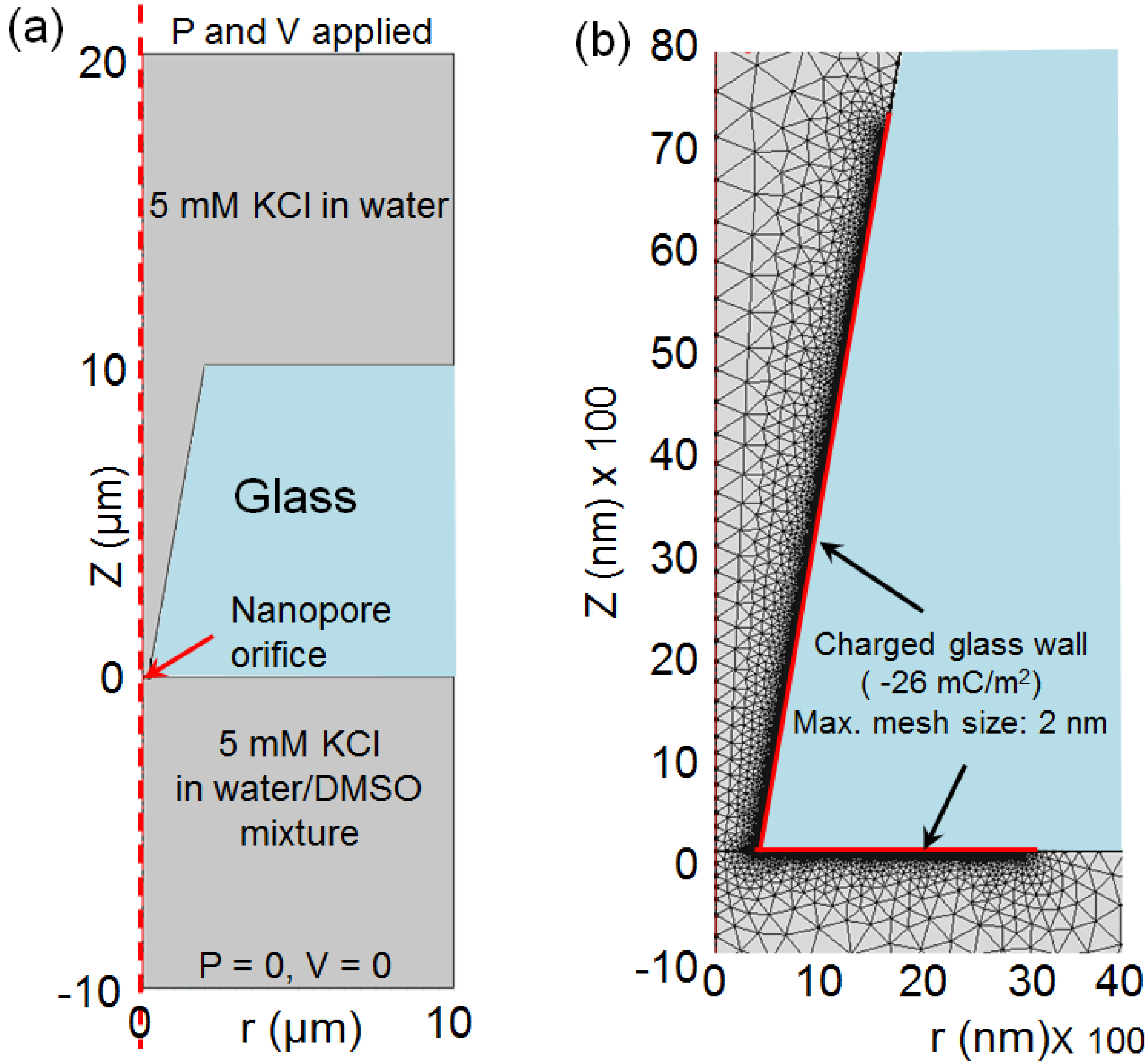
$$\mathbf{J}_i = -D_i\nabla c_i - \frac{Fz_i}{RT}D_i c_i\nabla\Phi + c_i\mathbf{u}$$

$$\mathbf{J}_{DMSO} = -D_{DMSO}\nabla c_{DMSO} + c_{DMSO}\mathbf{u}$$

3) Electrostatics

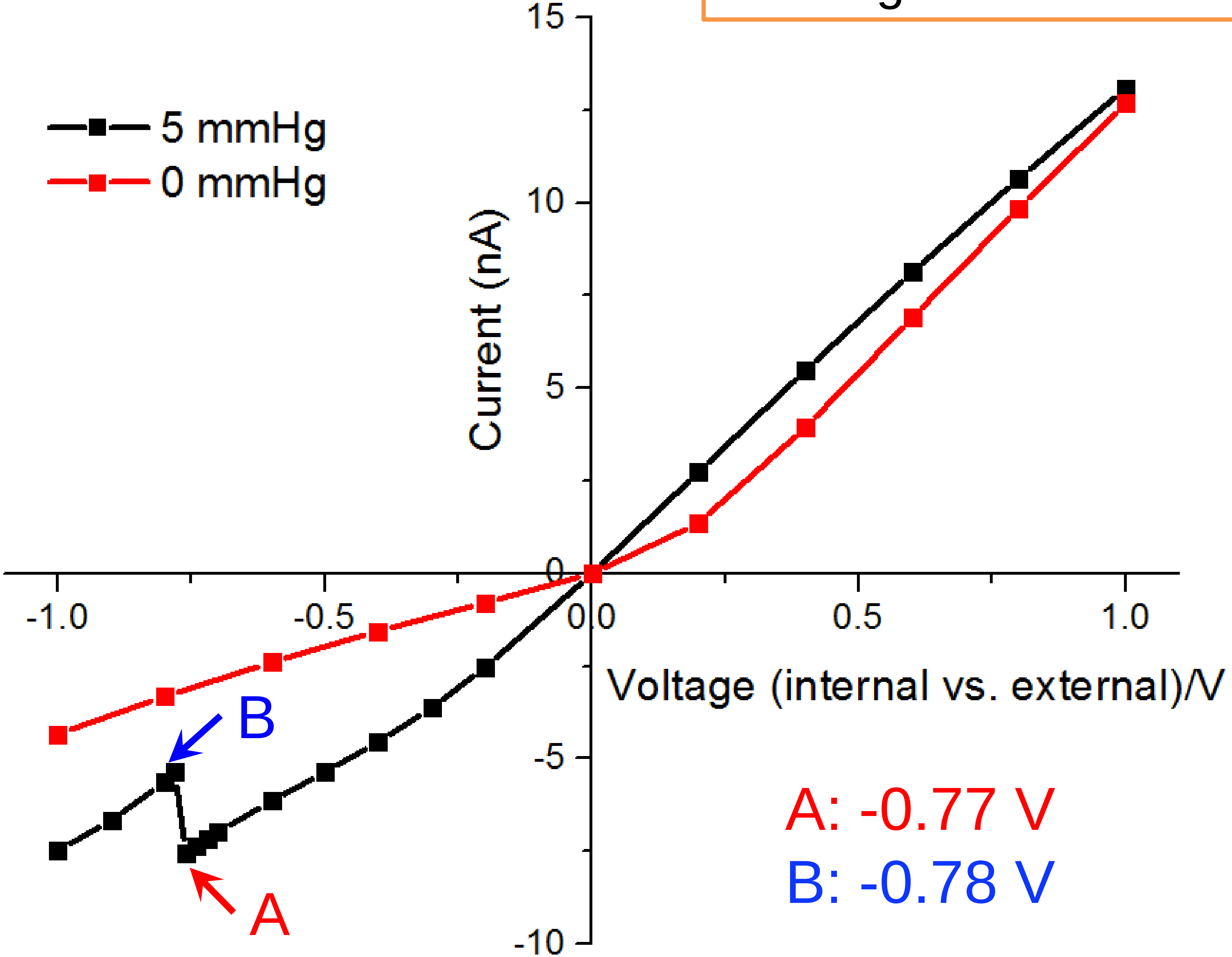
$$\nabla^2\Phi = -\frac{F}{\varepsilon}\sum_i z_i c_i$$

Geometry and Mesh



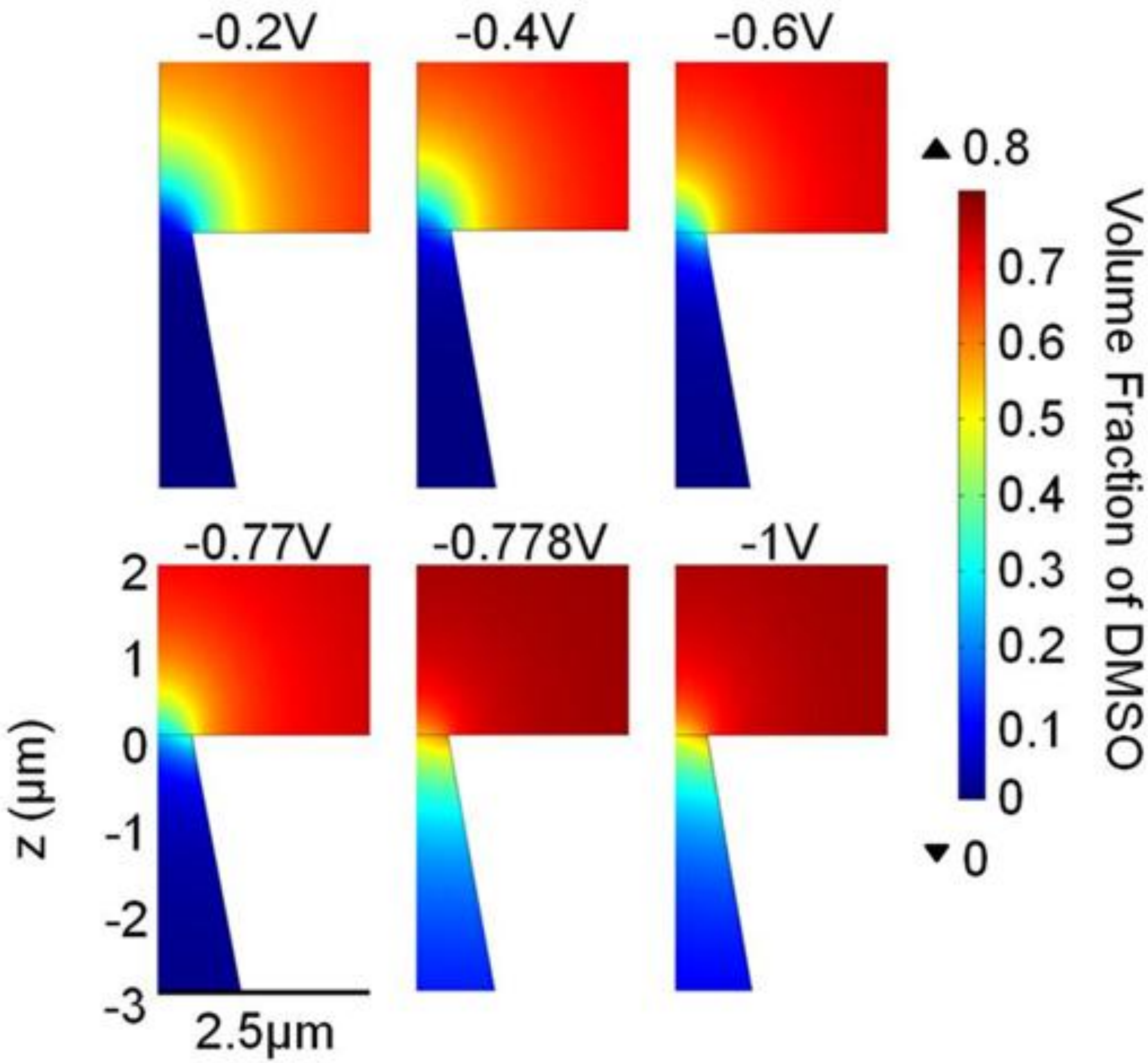
Simulation Results

The model doesn't converge between A and B!



A: -0.77 V
B: -0.78 V

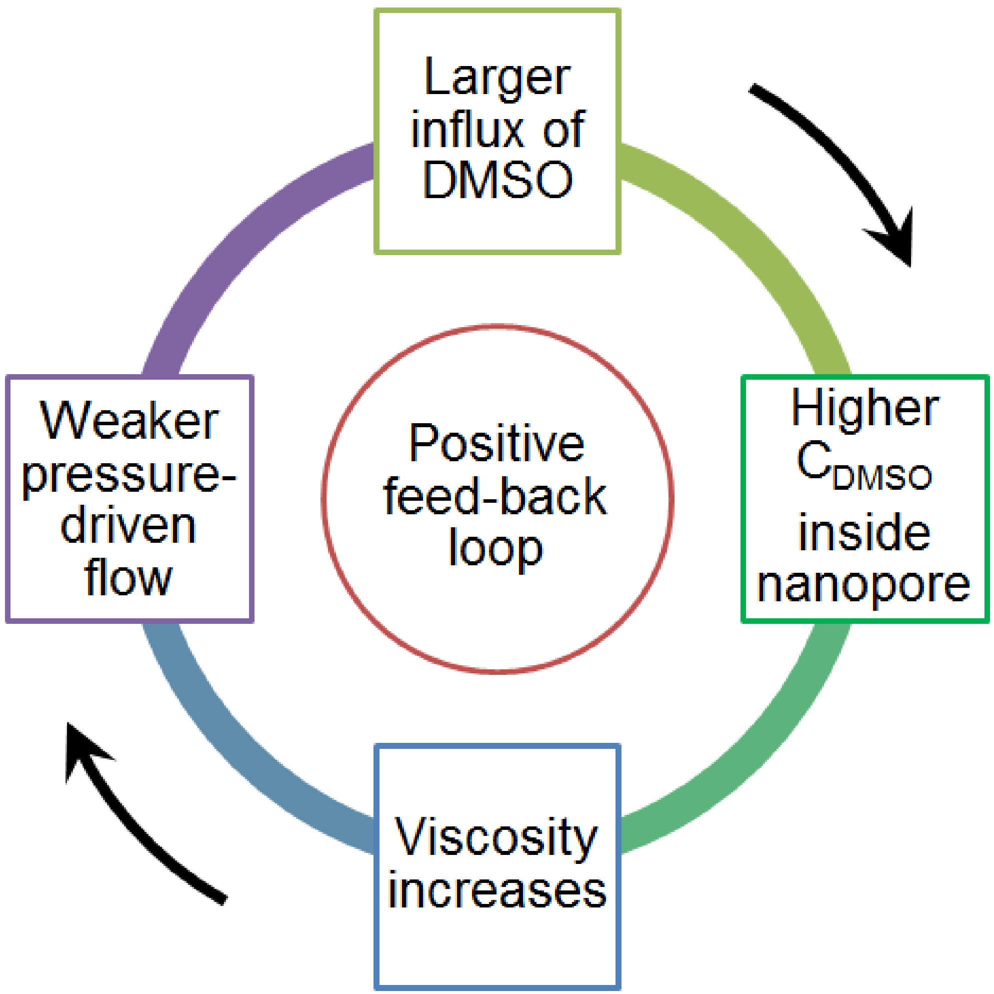
DMSO Distribution

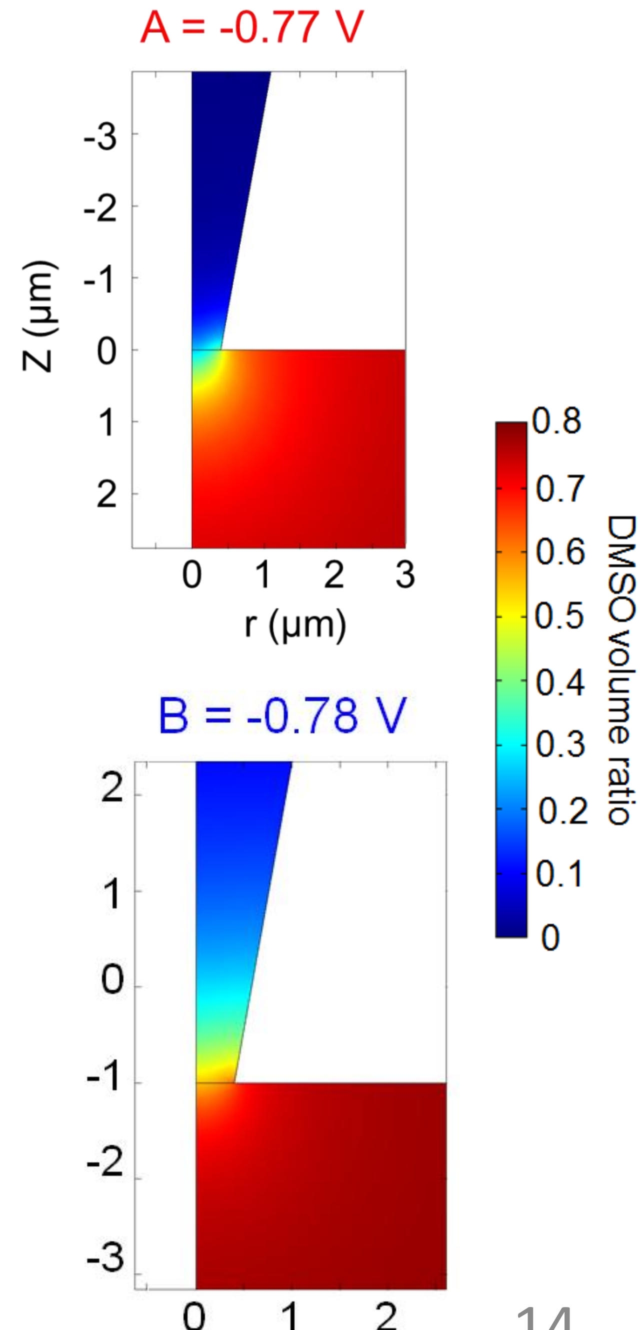


A **B**

Mechanism

Positive feedback loop





The key point

Bistability

Steady State Solver

Off On

Thanks for your attentions!