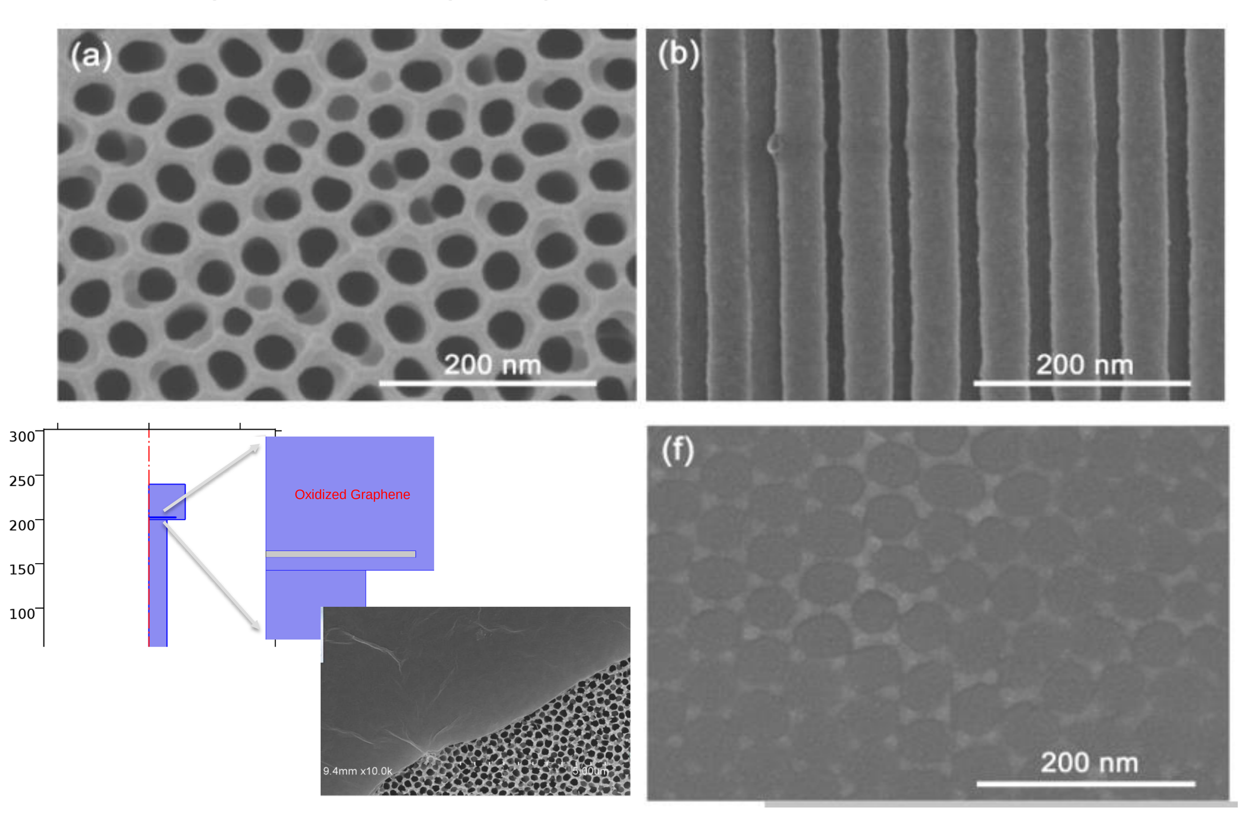
Elucidating The Mechanisms Of Charge (pH-induced) And Temperature (plasmon-induced) Modulated Ionic Transport In Nanochannels

Yu Zhao[1], Guigen Zhang[1]

1. Department of Biomedical Engineering, University of Kentucky, Lexington, KY, USA

INTRODUCTION: The transport of fluid through nanochannels is of importance in a variety of technological applications, including biological sensing, chemical separation and many others. Synthetic nanofluidic architectures that mimic the gating functions of biological ion channels have attracted broad interest in both fundamental research and applications because of the outstanding performance on the modulation of molecule and ion transport. In this work we propose two types of nanodevices that make use of surface charge density and temperature, respectively, to modulate and control the ion/molecule transport process.

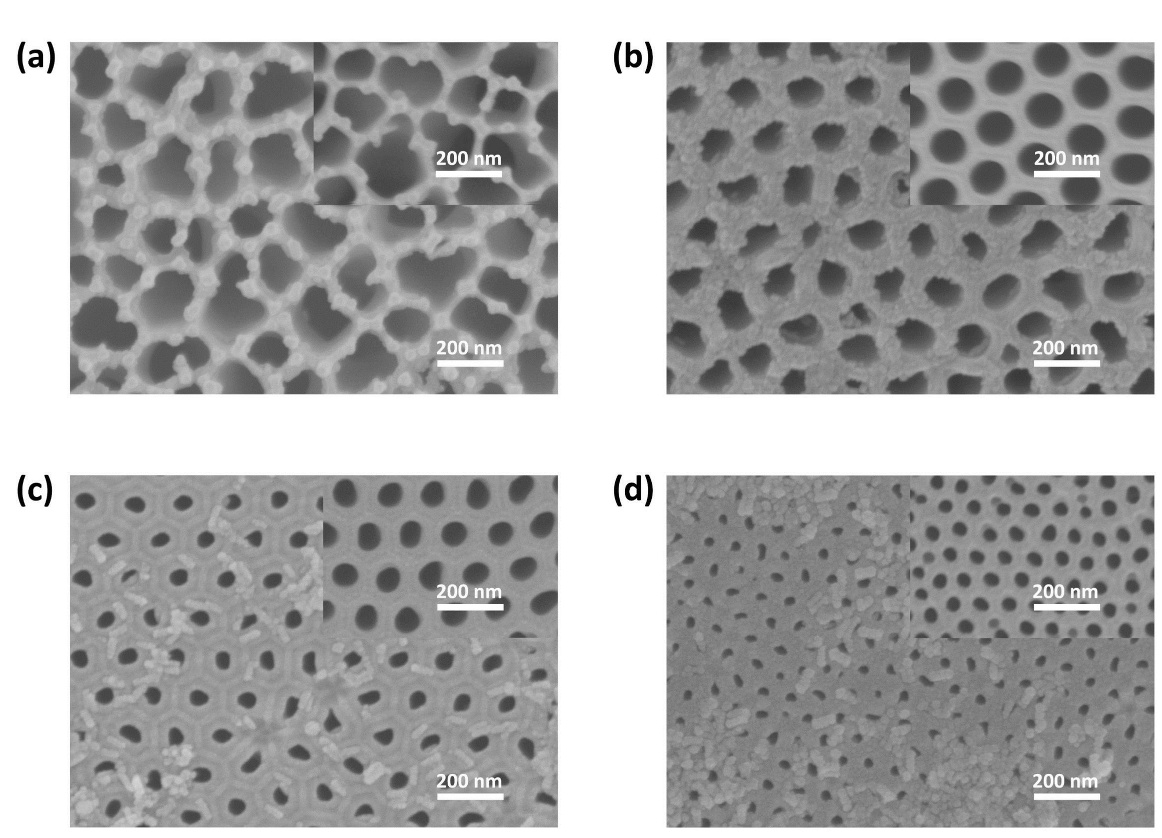
EXPERIMENTAL SETUP AND COMPUTATIONAL METHODS: The charge modulated ionic rectification device is fabricated using PAA (porous anodic alumina) and GO (graphene oxide) via dopamine polymerization.



(a) Top SEM image of as prepared PAA membrane. (b) Cross-section SEM image of as prepared PAA membrane.

(f) SEM image of PAA/GO composite membrane

The temperature modulated nanochannel is fabricated by coating gold nanorods on the surface of PAA membrane.



SEM top views of the PAA membranes before and after modification with AuNRs. The pore diameters of PAA membranes are (a) 200 nm, (b) 90 nm, (c) 50 nm, (d) 20 nm, respectively.

The creep flow physics is governed by Navier-Stokes equation

$$\rho\frac{\partial \mathbf{u}}{\partial t} = \nabla\cdot\left[-p\mathbf{I}+\eta\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^{T}\right)\right]+\mathbf{f} \qquad \mathbf{f}=\mathrm{F}(c_K-c_{Cl})\mathbf{E}$$

The electric field is determined by solving Poisson Equation

$$-\nabla^2\phi = \frac{\mathrm{F}(c_K-c_{Cl})}{\varepsilon} \qquad \mathbf{E}=-\nabla\phi$$

The transport of ions is controlled by diffusion, convection and migration as governed by the following Nernst-Planck Equation

$$\frac{\partial c_i}{\partial t}+\nabla\cdot(-D_i\nabla c_i - z_i\mu_i \mathrm{F} c_i\nabla\phi)+\mathbf{u}\cdot\nabla c_i = 0$$

RESULTS: Present your results from the simulation work. You may want to present your results as simulation images, tables or graphs.

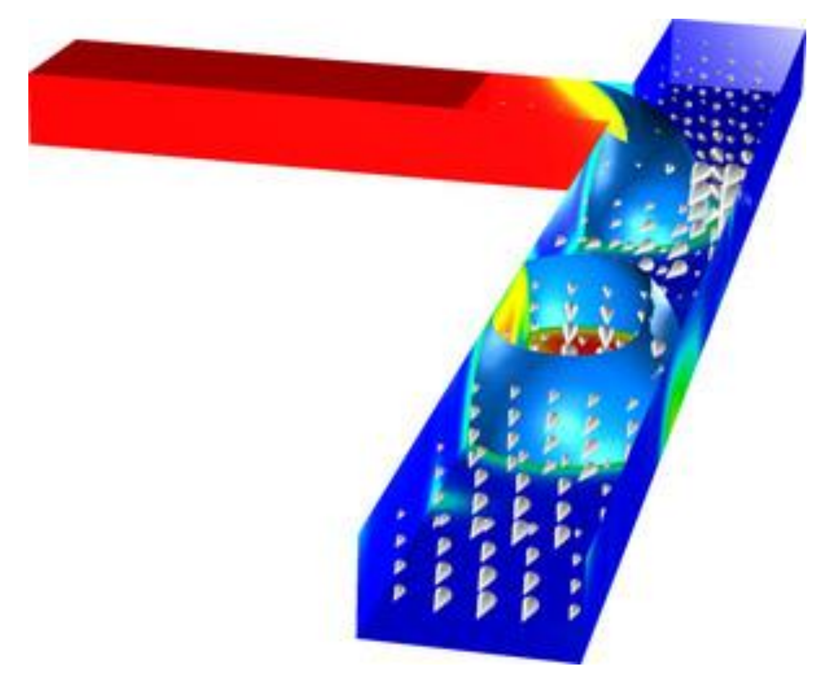


Figure 3. Title of the figure

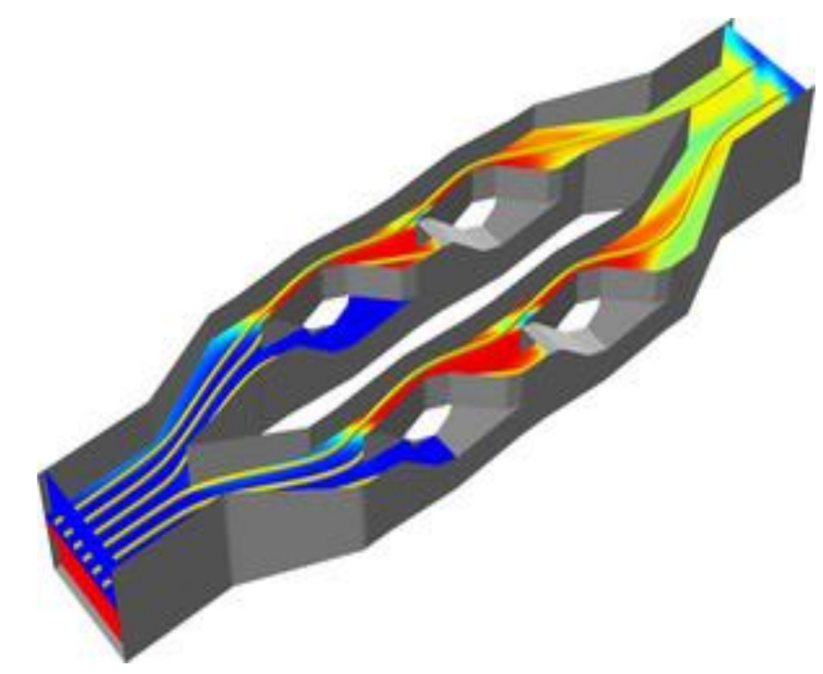


Figure 4. Title of the figure

Variable	Value	Units
Density	1000	Kg/m3
Dynamic Viscosity	1	Pa.s
Diffusion Coefficient	0.5	m2/s
Shear Modulus	200	Pa

Table 1. Title of the table

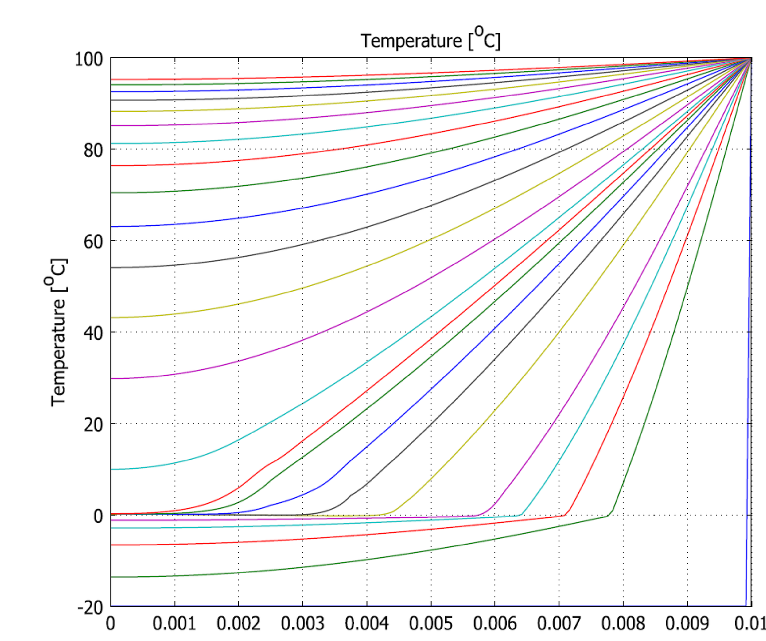


Figure 5. Title of the figure

CONCLUSIONS: State the findings or outcome of the simulation work. You may want to mention the relevance or impact of your findings to real world applications. You may want to mention the future direction of your work.

REFERENCES:

1. Author, Article Title, Journal, Volume, Page numbers (year)
2. Author, Article Title, Journal, Volume, Page numbers, (year)
3. Author, Article Title, Journal, Volume, Page numbers (year)

Excerpt from the Proceedings of the 2018 COMSOL Conference in Boston