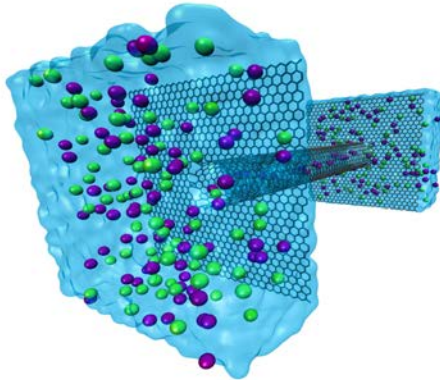


# Multiscale Simulations of Electronic and Fluidic Nanoscale Systems



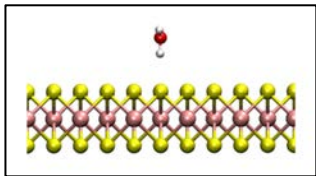
**Amir Taqieddin**, Mohammad Heiranian, and Narayana Aluru

Beckman Institute for Advance Science & Technology  
Mechanical Science & Engineering Department  
University of Illinois at Urbana-Champaign

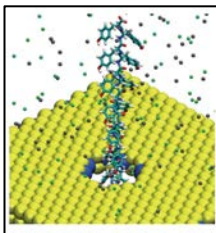


# Acknowledgment

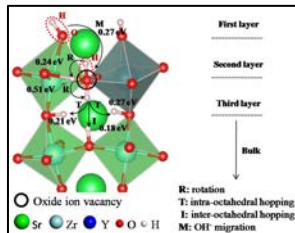
- We use Blue Waters in performing multiscale simulations and to study multi-physics systems.



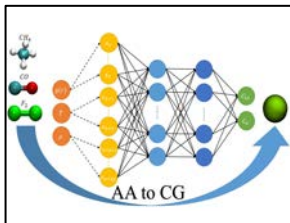
M. Heiranian et al., THE JOURNAL OF CHEMICAL PHYSICS 147, 104706 (2017)



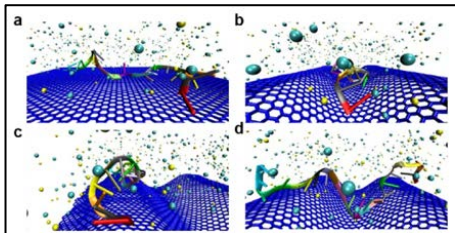
A. Farimani et al., Npj 2d Materials and Applications 2, 1-9 (2018)



Y. Jing et al., Chemistry of Materials 2018, 30 (138-144)



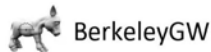
A. Moradzadeh & N.R. Aluru, The Journal of Physical Chemistry Letters 2019, 10 (6), pp 1242-1250



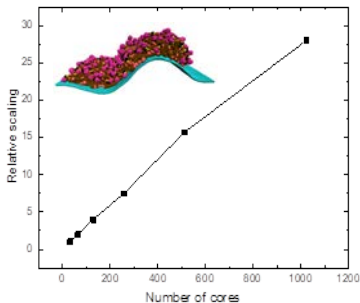
M.T. Hwang et al.,  
submitted to  
publication in April  
2019

# Acknowledgment

- Blue Waters allowed us to use different software with high computational performance.

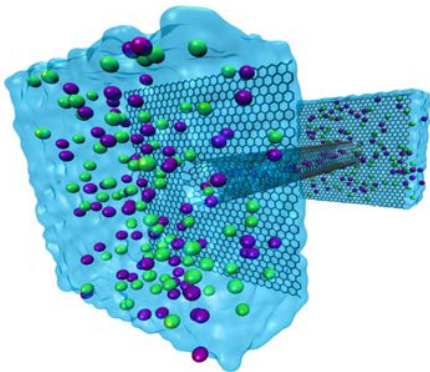


- We were able to obtain ~28 times scaling compared to 1 node (32 cores).
- The code performs up to 90% of the ideal performance.

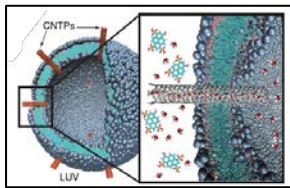


# Outline

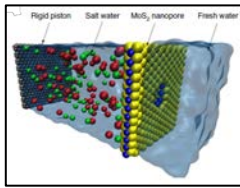
- New Power Scaling in the Concentration - Ionic Conductance Relation in CNT.
- Thickness Dependent Nanofluidic Transport in Nanopores and Nanochannels.



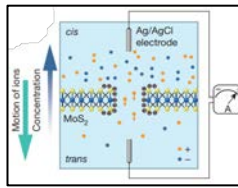
# Ionic Conductance



R.H. Tunuguntla et al. *Science* 357.6353 (2017): 792-796.



M. Heiranian et al. *Nature communications* 6 (2015): 8616.



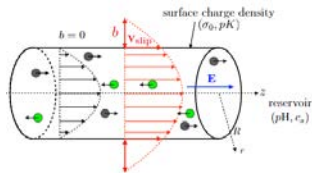
J. Feng et al. *Nature* 536.7615 (2016): 197.

- Ionic transport in nanofluidic systems is associated with multi-physics phenomena:

- 1) Diffusion and migration of ions.
- 2) Electro-osmotic flow.
- 3) Surface charge regulation.
- 4) Confinement.

- The ionic conductance in CNTs shows a power law relation.

$$G \propto c^\alpha; \alpha = 1, 0, 1/3, 1/2, \text{ and } 2/3$$



M. Manghi et al. *Physical Review E* 98.1 (2018): 012605.

# Ionic Conductance

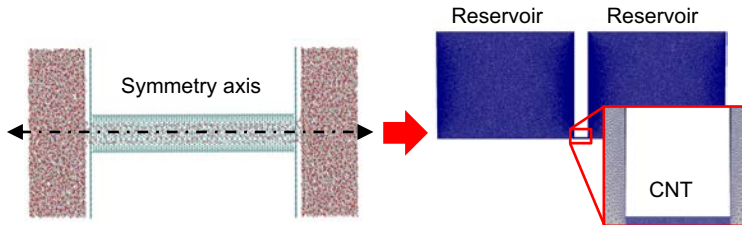
- Continuum simulations allow us to investigate the contribution of each component (diffusion, migration, and convection).
- We couple Poisson-Nernst-Planck (PNP) with Navier-Stokes (NS):

$$\text{Total ionic flux: } \Gamma_i = \underbrace{-D_i \nabla c_i}_{\text{Diffusion}} - \underbrace{\frac{z_i D_i F}{RT} c_i \nabla \phi}_{\text{Migration}} + \underbrace{c_i \mathbf{u}}_{\text{Convection}} \quad \text{Transport of species: } \frac{\partial c_i}{\partial t} = -\nabla \cdot \Gamma_i$$

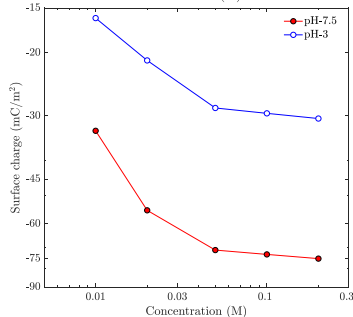
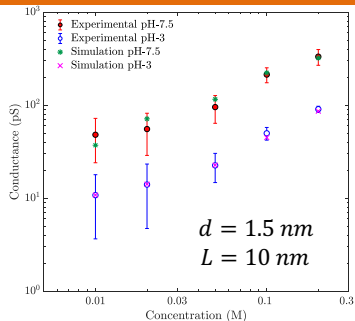
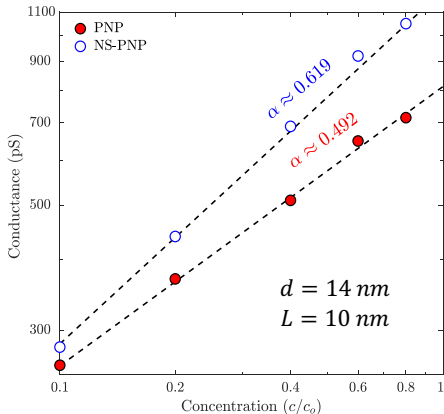
$$\text{Electric potential: } \nabla \cdot (\epsilon_r \nabla \phi) = -\frac{F \sum_i z_i c_i}{\epsilon_0}$$

$$\text{Momentum: } \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} - (F \sum_i z_i c_i) \nabla \phi$$

$$\text{Continuity: } \nabla \cdot \mathbf{u} = 0$$



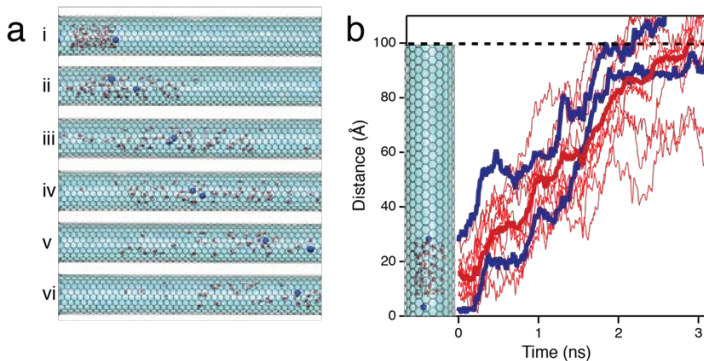
# Ionic Conductance



- Observed 2/3 power scaling.
- Used molecular dynamics to correct the continuum model and estimate the experimental surface charge.
- Selectivity coefficient ( $I_{\text{cation}}/I_{\text{anion}}$ ) of  $\sim 3.7$ .

# Ionic Conductance

- Studied the effect of surface charge on the molecular transport.



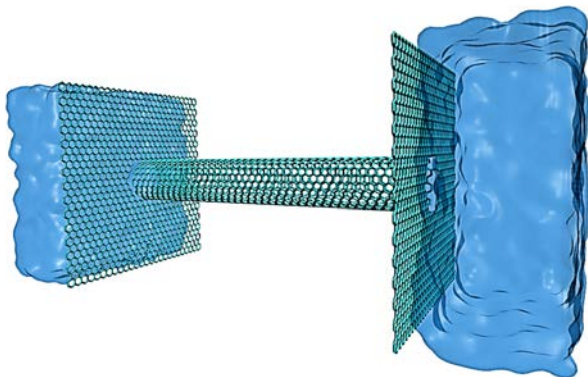
- Computed average velocity of water and potassium ions in (11,11) CNT with  $L = 10$  nm at a concentration of 1 M using molecular dynamics simulations.

Surface charge ( $\text{mC}/\text{m}^2$ )	$u_{\text{water}}$ (m/s)	$u_{\text{K}^+}$ (m/s)
-27	$2.9 \pm 0.29$	2.31
-54	$3.01 \pm 0.28$	2.45
-114	$1.98 \pm 0.42$	2.15





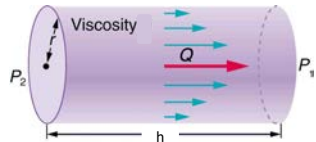
- ✓ New Power Scaling in the Concentration - Ionic Conductance Relation in CNT.
- Thickness Dependent Nanofluidic Transport in Nanopores and Nanochannels.



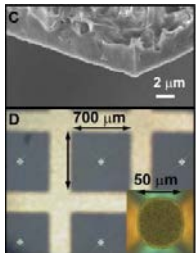
# Thickness Dependent Nanofluidic Transport

- In fluid dynamics, the flow rate of pressure driven fluid is generally described by Hagen-Poiseuille equation, in a circular pipe:

$$Q = \frac{\pi \Delta P r^4}{8 \mu h}$$

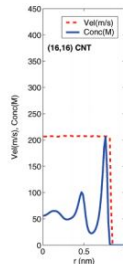


- Carbon nanotubes are shown to have several orders of magnitude higher permeation rate than that of existing membranes.



Experimentally, CNT is shown to very high flow rates (enhancement over no slip classical theory of  $\sim 1000$ ).

Holt et al. Science (2006).



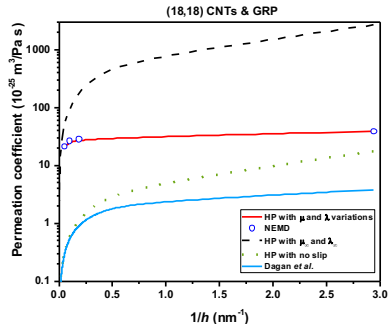
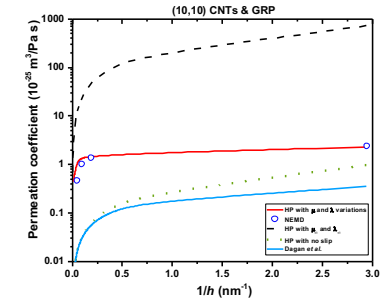
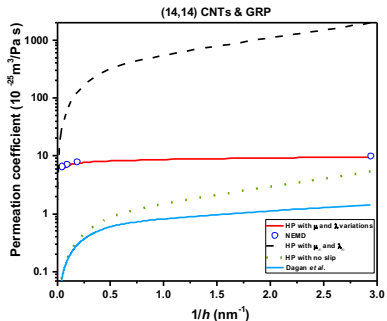
Fast water transport is also observed computationally due to highly frictionless walls of CNTs.

Joseph et al. Nano Lett. (2008).



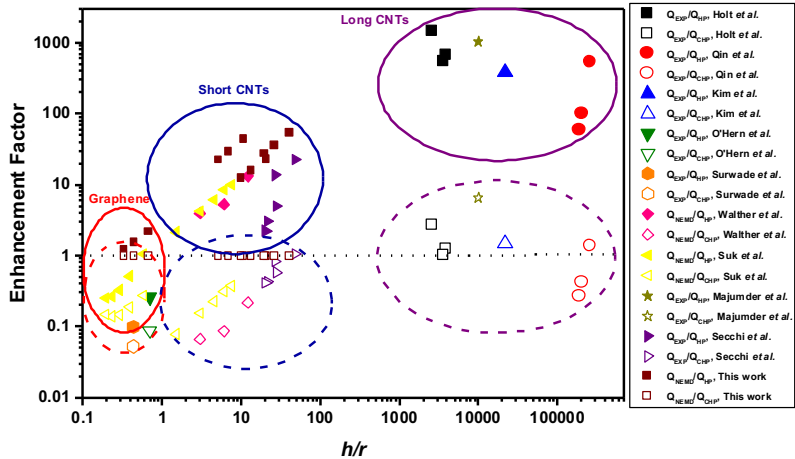
# Thickness Dependent Nanofluidic Transport

- We compared our corrected HP with:
  - HP with no slip
  - Dagan model for finite-length tubes
  - HP with bulk properties
  - HP with MD simulations



# Thickness Dependent Nanofluidic Transport

- In experiments, transport rates have been shown to be enhanced by several orders of magnitudes over the rates predicted by the no-slip HP theory.
- When the enhancement factors were reassessed using the corrected HP theory, they approach unity.



# Conclusion

- We performed continuum and molecular dynamics simulations to obtain a new power-law scaling relation between the concentration and the conductance of ionic transport.
- The continuum model was corrected using molecular dynamics inputs to predict quantities for length scales less than 10 nm.
- We studied the effect of surface charge density in CNT on the electroosmotic velocity and selectivity of ions.
- We corrected the classical Hagen-Poiseuille equation to describe fluid flow rates in nanoscale systems.
- The enhancement factor of flow rates approaches unity with the corrected Hagen-Poiseuille theory.



# Acknowledgment



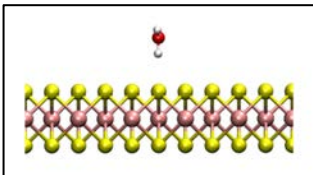
Professor Aleksandr Noy



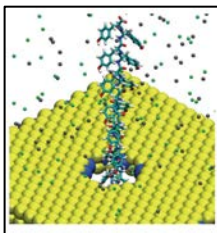
# Acknowledgment



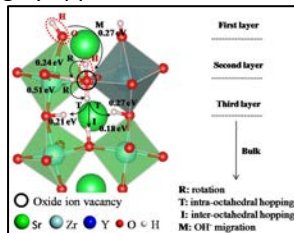
- This year we have used till now almost 70 K in two different allocations.
- Blue Waters support is highly appreciated.



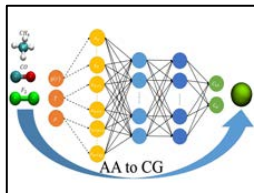
M. Heiranian et al., THE JOURNAL OF CHEMICAL PHYSICS 147, 104706 (2017)



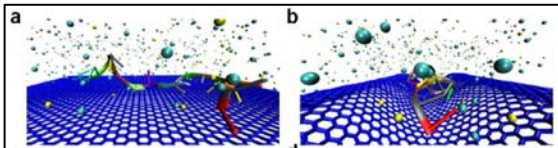
A. Farimani et al., Npj 2d Materials and Applications 2, 1-9 (2018)



Y. Jing et al., Chemistry of Materials 2018, 30 (138-144)



A. Moradzadeh & N.R. Aluru, The Journal of Physical Chemistry Letters 2019, 10 (6), pp 1242-1250



M.T. Hwang et al., submitted to publication in April 2019



Thank you!

