2019 PI Meeting was held in Washington, DC during July 29 and 30.

CENT was represented by a delegation of 14 people that presented two talks and six posters.

**OVERVIEW POSTER – CENTER FOR ENHANCED NANOFUIDIC TRANSPORT**

[EFRC – CENT] Michael Strano¹, YuHuang Wang², Aleksand Noy³, Zuzanna Siwy⁴, Mark Reed⁵, Narayana Aluru⁶, Martin Bazant¹, Daniel Blankschtein¹, John Cumings², Menachem Elimelech⁵, John T. Fourkas², Heather Kulik¹, Arun Majumdar⁷, Charles Martin⁸, Tuan Anh Pham³, Eric Schwegler³.

¹Massachusetts Institute of Technology (lead institution); ²University of Maryland; ³Lawrence Livermore National Laboratory; ⁴University of California Irvine; ⁵Yale University; ⁶University of Illinois at Urbana-Champaign; ⁷Stanford University; ⁸University of Florida

Not all nanopores are created equal. By definition, all have characteristic diameters or conduit widths between approximately 1 and 100 nm. However, the narrowest of such pores, perhaps best called Single Digit Nanopores (SDNs), defined as those with less than 10 nm diameters, have only recently been accessible experimentally for precision transport measurements. What scientists are finding for pores in this size range has been surprising, with many experiments indicating extraordinary transport rates and selectivities. These studies expose critical gaps in our understanding of nanoscale hydrodynamics, molecular sieving, fluidic structure and thermodynamics. These gaps are, in turn, an opportunity to discover and understand fundamentally new mechanisms of molecular transport at the nanometer scale that may inspire a host of new technologies, from novel membranes for separations and water purification to new gas-permeable materials and energy storage devices.

**TALK 1 - HIGH ELECTROOSMOTIC COUPLING IN ION CONDUCTANCE OF 1.5 NM DIAMETER CARBON NANOTUBE PORINS**

[EFRC – CENT] Aleksandr Noy¹, Yun-Chiao Yao¹, Amir Taqieddin³, Narayana R. Aluru³

¹Lawrence Livermore National Laboratory; ²University of Illinois at Urbana-Champaign

Center for Enhanced Nanofluidic Transport (CENT) is dedicated to studying seven critical knowledge gaps (KGs) that exist in our understanding of fluid transport phenomena on the nanoscale. One such KG involves significant water flow enhancement and unusual ion correlation effects that occur when water and ions undergo extreme confinement in nanometer sized channels. These effects are especially
pronounced in very narrow lumen channels of carbon nanotube porins (CNTPs) that exhibit high slip flow enhancement due to smooth hydrophobic pore walls. We have studied ion transport and ion selectivity in 1.5 nm diameter CNTPs embedded in lipid membranes using single nanopore measurement setup. Our data show that CNTPs are weakly cation-selective at pH=7.5 and become non-selective at pH=3.0 when the negatively charged COO- groups at the CNTP ends become protonated. Remarkably, ion conductance of CNTPs exhibits an unusual 2/3 power law scaling with the ion concentration at both neutral and acidic pH values. This scaling is qualitatively different from the conductance-concentration scaling behaviors reported for most nanopores, including those of larger diameter carbon nanotubes. Coupled Navier-Stokes and Poisson-Nernst-Planck (NS-PNP) simulations and atomistic MD simulations reveal that this experimentally-observed scaling originates from strong coupling between water and ion transport in these channels. These effects could result in development of a new generation of new biomimetic membranes and carbon nanotube-based electroosmotic pumps.

**TALK 2 - MULTISCALE MODELING OF FLUIDS IN SINGLE DIGIT NANOPORES**

[Narayana R Aluru1, Mohammad Heiranian1, Archith Rayabharam1, Samuel Faucher2, Michael Strano2, Alex Noy3, John Fourkas4, Zuzanna Siwy5, Haoran Qu4, YuHuang Wang4, Tuan Anh Pham3]

1University of Illinois at Urbana-Champaign; 2Massachusetts Institute of Technology; 3Lawrence Livermore National Laboratory; 4University of Maryland; 5University of California, Irvine

Structure, dynamics and transport of fluids in single digit nanopores (SDNs) can be vastly different from their macroscopic counterparts. For example, water transport through carbon nanotubes has been shown to exhibit flow rates which are many orders of magnitude larger compared to those obtained from classical theories. While classical theories are fast, they do not account for the microscopic mechanisms that are important in single digit nanopores. Quantum and atomistic simulations can provide good accuracy, but they are limited in the length and time scales that can be dealt with. In this talk, we will present multiscale theories to describe fluidic behavior in SDNs. First, we will discuss multiscale approaches to calculate fluidic properties such as structure, interfacial friction, viscosity, permittivity, slip, etc. in SDNs. We will show that these properties can be vastly different when compared to their bulk counterparts. Second, we will discuss the development of nanofluidic theories incorporating microscopic physics and show that these theories can predict water flow rates which are consistent with experimental measurements. Third, we will discuss the physics of electrical double layers (EDLs) and show that the structure and dynamical properties of ions and water in EDLs of SDNs can be different from those in larger pores/channels. Finally, we will present evidence of molecular sieving of simple organic molecules using SDNs.
**P1 - Combined Experimental, Computational and Theoretical Investigation of Pure Fluids and Electrolytes Under Confinement**

[EFRC – CENT] Samuel Faucher, Rahul Prasanna Misra, Pedro de Souza, Strano, Daniel Blankschtein, Martin Bazant, Michael Strano

*Massachusetts Institute of Technology*

**P2 - Evidence of Molecular Sieving of Hexane and Cyclohexane in Carbon Nanotube Single-Digit Nanopores**

[EFRC – CENT] Haoran Qu¹, James Xiaojian Wu¹, Yunfeng Li¹, YuHuang Wang¹, Jeff Fagan², Archith Rayabham⁳, Narayana R. Aluru³

¹University of Maryland; ²NIST; ³University of Illinois at Urbana-Champaign

**P3 - The Electrical Double Layer Revisited**

[EFRC – CENT] Amanda Souna¹, Jake Polster², Jason Tran¹, Rachel Lucas², Narayan Aluru³, John Fourkas¹, Zuzanna Siwy²

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**P4 - Electrochemical Studies of Solutions Confined Within Nanopores**

[EFRC – CENT] Stevie Walters¹, Charles R. Martin¹, Jake Polster², Zuzanna Siwy²

¹University of Florida; ²University of California Irvine

**P5 - Advanced Imaging to Enable Studies of Confined Fluids**

[EFRC – CENT], Ze Zhang¹, Joel Martis¹, Kyle Sendgikoski², Joy Chao², Zoey Warecki², Arun Majumdar¹, John Cumings²

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