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 Nanofluidic Transport

[EFRC – CENT] Michael Strano[1], YuHuang Wang[2], Aleksand Noy[3], Zuzanna Siwy[4], Mark Reed[5], Narayana Aluru[6], Martin Bazant[1], Daniel Blankschtein[1], John Cumings[2], Menachem Elimelech[5], John T. Fourkas[2], Heather Kulik[1], Arun Majumdar[7], Charles Martin[8], Tuan Anh Pham[3], Eric Schwegler[3].

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

CENT: The Center for Enhanced

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 Noy[1], Yun-Chiao Yao[1], Amir Taqieddin[3], Narayana R. Aluru[3]

[1]Lawrence Livermore National Laboratory; [2]University 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 vary 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

[EFRC – CENT] Narayana R Aluru[1], Mohammad Heiranian[1], Archith Rayabharam[1], Samuel Faucher[2], Michael Strano[2], Alex Noy[3], John Fourkas[4], Zuzanna Siwy[5], Haoran Qu[4], YuHuang Wang[4], Tuan Anh Pham[3]

[1]University of Illinois at Urbana-Champaign; [2]Massachusetts Institute of Technology; [3]Lawrence Livermore National Laboratory; [4]University of Maryland; [5]University 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.

Posters:

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 Qu[1], James Xiaojian Wu[1], Yunfeng Li[1], YuHuang Wang[1], Jeff Fagan[2], Archith Rayabharam[3], Narayana R. Aluru[3]

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

P3 - THE ELECTRICAL DOUBLE LAYER REVISITED

[EFRC – CENT] *Amanda Souna[1], Jake Polster[2], Jason Tran[1], Rachel Lucas[2], Narayan Aluru[3], John Fourkas[1], Zuzanna Siwy[2]*

[1]*University of Maryland*; [2]*University of California Irvine;* [3]*University of Illinois at Urbana-Champaign*

P4 - ELECTROCHEMICAL STUDIES OF SOLUTIONS CONFINED WITHIN NANOPORES

[EFRC – CENT] Stevie Walters[1], Charles R. Martin[1], *Jake Polster[2], Zuzanna Siwy[2]*

[1]*University of Florida*; [2]*University of California Irvine*

P5 - ADVANCED IMAGING TO ENABLE STUDIES OF CONFINED FLUIDS

[EFRC – CENT], Ze Zhang[1], Joel Martis[1], Kyle Sendgikoski[2], Joy Chao[2], Zoey Warecki[2], Arun Majumdar[1], John Cumings[2]

[1]*Stanford University;* [2]*University of Maryland*