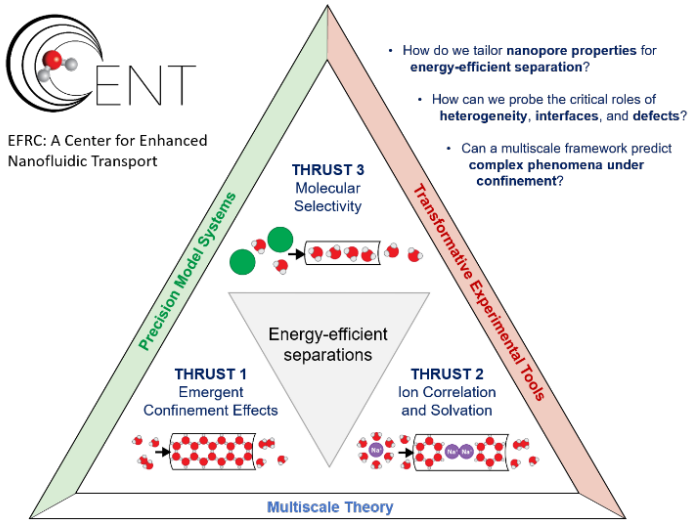
Center for Enhanced Nanofluidic Transport (CENT)
EFRC Director: Michael S. Strano
Lead Institution: Massachusetts Institute of Technology
Class: 2018 – 2022

Mission Statement*: To address emerging and compelling gaps in our knowledge of fluid flow and molecular transport in single digit nanopores and establish the scientific foundation for developing transformative molecular separation technologies impacting the Water-Energy Nexus.*

Not all nanopores are created equal. By definition, all have characteristic diameters or conduit widths between approximately 1 and 100 nm. However, experiments indicate that the narrowest of such pores, Single Digit Nanopores (SDNs), defined as those with less than 10 nm diameters, display surprising behaviors resulting in extraordinary transport efficiency and selectivity These studies expose critical gaps in our understanding of nanoscale hydrodynamics, molecular sieving, fluidic structure and thermodynamics. Examples of these gaps include the observation of slip flow enhancement - that the narrowest of nanopores counter-intuitively demonstrate higher mass transport rates; evidence of non-Gibbs-Thomson phase behavior – that fluid phase boundaries in SDNs are remarkably distorted from their bulk fluid counterparts; and highly non-linear, correlative effects in ion transport through SDNs not observed in even slightly larger nanopore dimensions. These and other 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 at the Energy-Water Nexus, from novel membranes for separations and water purification to new gas permeable materials and energy storage devices.

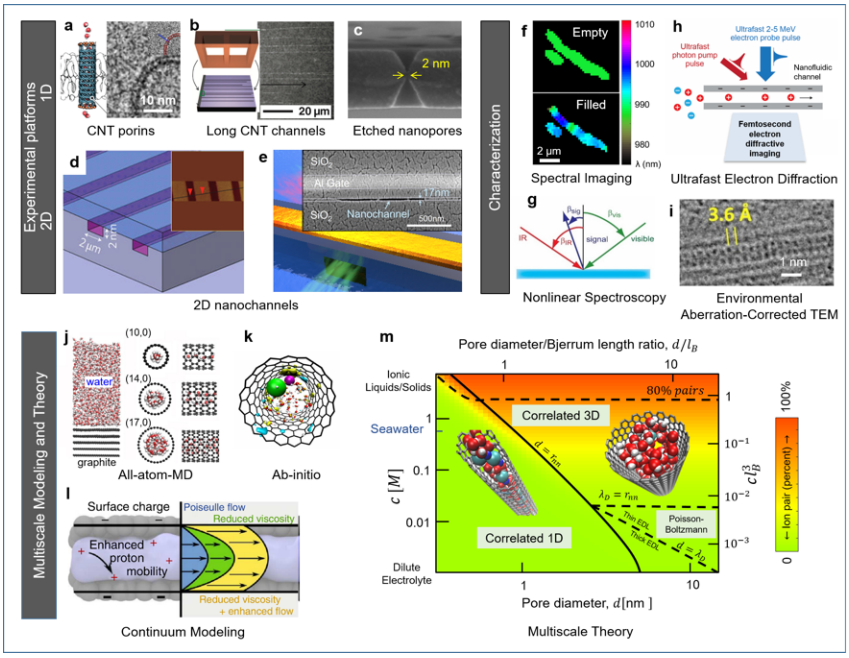


CENT is establishing the scientific foundation for transformative molecular separation technologies based on SDNs to impact the Water-Energy Nexus.

The Center for Enhanced Nanofluidic Transport (CENT) addresses 7 key nanofluidics knowledge gaps: (1) Slip Flow Enhancement in SDNs; (2) Fluid Phase Transitions in SDNs; (3) Phase-Separation under Confinement; (4) Defects and their Outsized Impact on SDN Transport; (5) Correlated Transport; (6) Nanoscale Solvation; and (7) Charge Exclusion to Significantly Enhance Selectivity. The CENT research program is organized into three distinct and interconnected Thrust Areas: Understanding Emergent Confinement Effects (Thrust 1), Quantifying Ion Correlation, Dissipation, and Solvation Phenomena (Thrust 2), and Engineering Selectivity for Chemical Separations (Thrust 3). Our approach is highly integrated and is augmented by the development of precision model systems, transformative experimental tools, and predictive, multiscale modeling and simulations.

CENT is focusing on experimental platforms and analytical tools to understand the physical effects of extreme confinement in SDNs. We are addressing solvation effects in aqueous media and in acetonitrile,

ethanol, and acetone solvents, which are important in energy-efficient separations, as well as propylene carbonate and representative ionic liquids used in energy storage devices. We also explore fundamentally new mechanisms of ionic and molecular selectivity that stem from extreme confinement. CENT is pioneering the development of high fidelity fabrication methods for as small as sub-1 nm SDNs with conduit lengths of angstroms to 1 mm, with specifically tailored surface and pore mouth chemistry. These model SDN systems set the scientific basis for developing next generation membrane materials. CENT also expands the ability to incorporate controlled, single defects into SDNs as a novel perturbation method and explores the impact of pore defects on nanofluidic transport. The CENT team pioneers the use of environmental aberration-corrected TEM, high resolution cryo-EM, ultrafast electron diffraction imaging, single ion traps, and single defect spectroscopy to transform our capability in probing water and ion structure in nanopores. CENT's work is producing a comprehensive, definitive theory, capable of predicting the thermodynamics and transport properties of fluids in SDNs. This knowledge in turn will motivate and enable new separation mechanisms for chemical purification and manipulation that would enhance the nation's competitiveness in the technologies at the Energy-Water Nexus.



CENT pursues an integrated, synergetic approach for probing emergent phenomena involving water and ions under confinement. CENT research combines experimental platforms that create 1D and 2D confinement with multi-scale simulation tools that model these effects using large scale, all-atom MD and *ab initio* simulations.

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