Center for Enhanced Nanofluidic Transport Phase 2
EFRC Director: Michael S. Strano
Lead Institution: Massachusetts Institute of Technology
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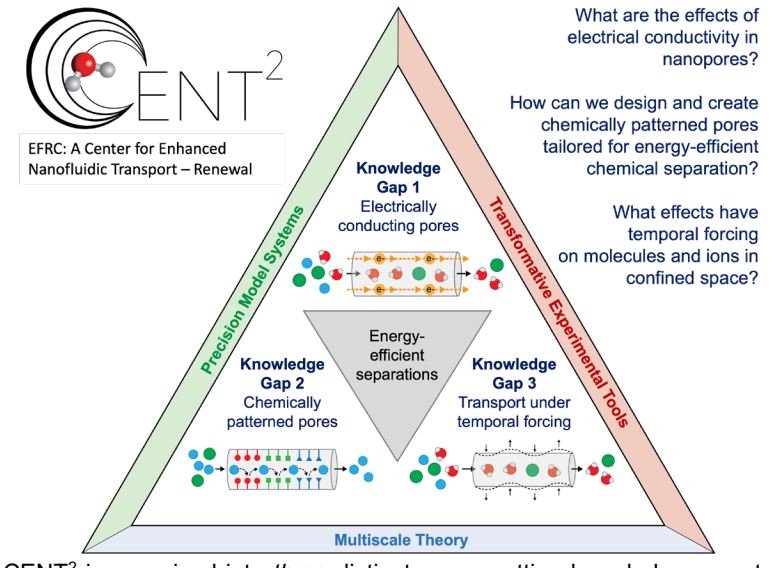
Mission Statement*: CENT2 is a pioneering Energy Frontier Research Center addressing critical knowledge gaps in our understanding of fluidic flow and molecular transport in extremely narrow pores. CENT2 will establish the scientific foundation for transformative molecular separation technologies impacting the water-energy nexus and Energy Earthshots.*

Not all nanopores are created equal. By definition, all have characteristic diameters or conduit widths of between approximately 1 and 100 nm. However, the narrowest of such pores, **S**ingle **D**igit **N**anopores (SDNs), are less than 10 nm in diameter and have only recently become accessible for precision transport measurements. What scientists within the Center for Enhanced Nanofluidic Transport (CENT) and the larger community have discovered about SDNs has been surprising, including demonstrations of extra-ordinary molecular flux and selectivities beyond theoretical predictions. These findings have in turn exposed critical gaps in our understanding of hydrodynamics, molecular sieving, fluidic structure, and thermodynamics under the confinement of SDNs that form the basis of CENT. Building on our groundbreaking work, the renewed CENT (**CENT^2**) will address fundamentally new questions of fluidic transport at the nanoscale that stand to impact a host of new technologies at the water-energy nexus, from new membranes for precise separations and water purification, to new permeable materials for water electrolyzers and energy storage devices, as well as enabling new emerging energy technologies such as hydrovoltaics. Our effort directly responds to the need for *Basic Research in Energy and Water* as outlined in the DOE-EFRC FOA. Furthermore, the fundamental knowledge gained on the selective transport of molecules and ions as part of CENT^2 will broadly support the *Energy Earthshot* cross-DOE initiatives.

CENT^2 will continue as a pioneering Energy Frontier Research Center, leveraging its newfound insights of fluidic flow and molecular transport in extremely narrow nanopores to inspire the next generation of water purification and membrane separation processes. This vision encompasses vastly more precise and energy efficient separations at the water-energy nexus as well as in many other sectors of the U.S. economy. In phase 2, our Center will focus on *three* distinct and interconnected Knowledge Gap (KG) activities to advance our four-year research goals: **Electrically Conducting Pores (KG1); Chemically Patterned Pores (KG2); and Transport under Temporal Forcing (KG3).** CENT^1 has developed fundamental understanding of **slip flow enhancement** (i.e., substantially



CENT^2 is organized into *three* distinct, cross-cutting knowledge gaps to establish the scientific foundation for transformative molecular separation technologies.

higher mass transport rates in *smaller* nanopores), which now enables us to devise new mechanisms of fluidic enhancement, such as electrically driven boundary flow, involving the coupled transport of fluid in the SDN and electrons in the confining material that forms the nanopore (**KG1**). Our thermodynamic measurements inside SDNs have uncovered fluid phase boundaries that are remarkably distorted from their bulk fluid counterparts, demonstrating the so-called **non-Gibbs-Thomson** behavior and leading to an inability of existing models to predict the existence of vapor, liquid or solid phases within the narrowest of pores. **KG2** then seeks to use chemically patterned SDNs that are only otherwise found in nature, to manipulate fluid phase boundaries as well as transport behavior at the extreme confinement for fundamentally new separation regimes. Finally, **KG3** will examine molecular transport and separations under forced modulation, either electrokinetic (**3A**) or mechanical (**3B**), with tunable frequency and amplitude to exert new types of control over transport at the molecular scale. **These fundamental studies hold the potential to uncover new insights for the development of next-generation water purification and membrane separation processes that could encompass self-pumping membranes, pores with strongly defined and tunable single-species selectivity, and feedback control schemes that directly modulate the transport medium itself.** We define these three new areas of investigation as **knowledge gaps** because existing theories, whether continuum, atomistic, or molecular simulations, fail to adequately quantify or even describe the basics of these exotic effects. Leveraging the knowledge gained from the previous performance period, CENT^2 will establish the foundation for transformative molecular separation technologies impacting basic energy research needs. We have assembled a new multidisciplinary team of the leading experts in SDN research from MIT, UMD, Yale, UCI, Stanford, Univ. Florida, and LLNL, including the addition of a Hispanic serving institution, UT Austin, and the addition of three faculty PIs that further expand our diversity. The basic science developed by CENT^2 will enable new energy-efficient separation processes. We address the DOE *Grand Challenge* of the atomic-level synthesis of new materials that exhibit precise control of molecular permeation. Additionally, the fundamental knowledge gained by CENT^2 on the selective transport of molecules and ions will be foundational to addressing the *Energy Earthshots*.

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