## Center for Materials for Water and Energy Systems (M-WET) EFRC Director: Benny D. Freeman

Lead Institution: The University of Texas at Austin Class: 2018 – 2022

**Mission Statement**: To discover and understand fundamental science to design new membrane materials, develop tools and knowledge to predict new materials' interactions with targeted solutes from recalcitrant water sources, provide fit for purpose water, and recover valuable solutes with less energy.

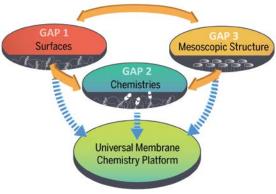
Contaminated water from energy-related activities is an enormous burden (wastewater management) and an exciting untapped opportunity (resource recovery). Synthetic membranes are widely used for purifying relatively clean water due, in part, to low energy requirements of membranes relative to alternatives (e.g., thermally based separations). However, today's membranes were not designed to treat highly impaired water, such as produced water, due to extensive fouling and poor separation properties. Existing membranes: (1) are poor at discriminating between ions of the same valence (e.g., Na<sup>+</sup> v. Li<sup>+</sup>), (2) have low selectivity for many neutral contaminants (e.g., boron, arsenic), (3) are always subject to fouling, (4) exhibit a pernicious tradeoff between permeability and selectivity, and (5) are produced in poorly understood, highly non-equilibrium processes that limit deliberate control of their properties. Fundamental knowledge gaps contributing to these shortcomings and frustrating membrane design include: (1) structure/dynamics of hydration water and solutes (e.g., ions, dissolved organics, etc.) near membrane/fluid interfaces, in membrane separation layers, and in pores, (2) thermodynamic and kinetic properties of solutes in aqueous mixtures, near membrane/fluid interfaces and in membranes that depend, in part, on solute and surface hydration properties, and (3) rational design of selectivity-enhancing interactions between water, solutes and membranes.

The Center for Materials for Water and Energy Systems (M-WET) will bridge the chemistry, materials and process separation communities to: (1) design new interfaces to achieve optimal affinity and reactivity for water/energy systems (e.g., ion-specific separation); (2) precisely control mesoscopic materials architecture to achieve exquisite control of pore size and pore size distribution in membranes; (3) develop novel materials imaging and spectroscopic tools that operate in-situ/in operando in complex, aqueous fluid environments to probe water, solute and material interactions; and (4) model interfaces, separation membranes, fluid mixtures, and mesoporous architecture to radically transform water and energy

demands, resiliency, and efficiency of membrane/materials systems.

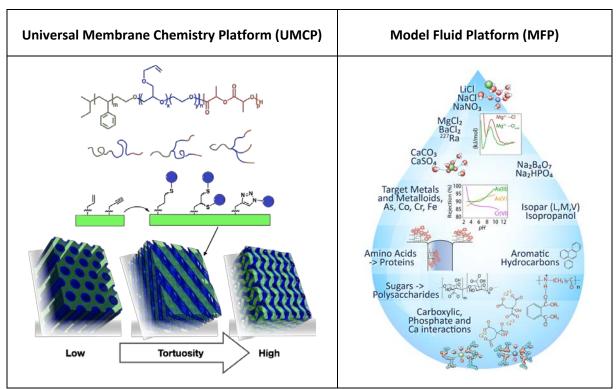
M-WET comprises three Gap Attack Platforms (GAPs) focused on: (1) molecular design of surfaces to control and tune water properties at interfaces; (2) designing specific interactions to improve membrane separation properties; and (3) mesoscale structures to tailor fluid flow through porous and isoporous membranes. A cross-cutting Integrating Framework leverages these materials design insights to provide directions for breakthrough improvements in real separation processes. Achieving these goals requires deep, sustained, and interdisciplinary efforts in synthesis, characterization, and modeling.

Integrating Framework



M-WET scientific framework, illustrating the Gap Attack Platforms (GAPs) and Integrating Framework.

A single, modular model materials platform, the Universal Membrane Chemistry Platform (UMCP), is used and functionalized in GAPs 1–3, so breakthroughs are seamlessly transferred among GAPs and across length scales. The GAPs also share a Model Fluid Platform (MFP) to provide continuity, coherence, and relevance among research projects. The MFP comprises a hierarchy of increasingly complex fluids for use across all GAPs, beginning with water, water + simple salts, water + organics (e.g., dissolved organics or emulsified oil or both), water + salt + organics, and ultimately, model produced water containing organic and inorganic components.



M-WET's Universal Membrane Chemistry Platform and Model Fluid Platform.

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