The Center for Materials for Water and Energy Systems (M-WET)
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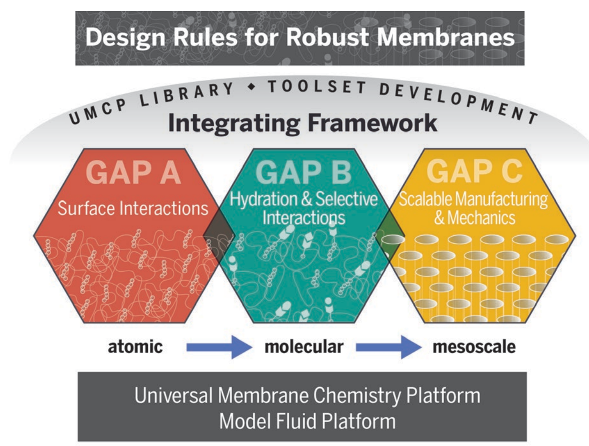
Mission Statement*: To discover and understand the fundamental science necessary to design new membrane materials and develop tools and knowledge to predict new materials' interactions with targeted solutes to provide fit for purpose water from low quality water sources and recover valuable solutes with less energy.*

Synthetic polymer membranes are widely used to purify water, mainly because they can be more energy efficient than competing (e.g., thermally based) technologies. However, water in energy applications is often heavily contaminated with a plethora of diverse organic and inorganic components. Current membranes were not designed (and are unsuitable) for such applications. Basic science knowledge gaps in thermodynamic and kinetic behavior of complex aqueous mixtures at interfaces, and the effect of such mixtures on the interfacial properties, limit our ability to translate fundamental understanding to transformative membrane materials design and manufacturing for energy/water applications. Moreover, current methods for synthesis and precision assembly of novel materials far from equilibrium do not allow for the scalable manufacturing of membranes with mesoscopic control over morphology for highly selective decontamination or resource recovery from such complex aqueous mixtures. The *Center for Materials for Water and Energy Systems* (M-WET) will fill these gaps in the understanding of fluids, materials, and non-equilibrium processing to catalyze the design of novel materials, highly selective solute/fluid interactions, mesoscopic structures, and transformative manufacturing strategies to prepare robust, high-performance membranes for energy applications.

Our central goal is to discover and design specific interactions with solutes of interest to create highly manufacturable, scalable, robust, selective, permeable membranes. Therefore, M-WET deploys **3 Gap Attack Platforms (GAPs)** to address fundamental knowledge gaps in water purification: *(A) Structure and Dynamics of Water and Solutes Near Interfaces*, *(B) Role of Hydration in Ion Transport and Separations*, and *(C) Fundamental Science of Membrane Manufacturing*. These **GAPs** work with an overarching ***Integrating Framework*** (**IF**) on *Bridging Between Systems/Developing the Bridging Toolset* to provide: (1) a common universal membrane chemistry platform (**UMCP**), (2) a model fluid platform (**MFP**), (3) high-throughput characterization methodologies to rapidly screen large regions of phase space, and (4) novel spectroscopic tools to provide unprecedented insight into water-solute-membrane interactions. A scalable, evolving library of **UMCP** materials will catalyze translation of discoveries between **GAPs** while the **MFP** provides continuity, coherence, and relevance



M-WET scientific framework, illustrating the proposed Gap Attack Platforms (GAPs) and Integrating Framework (IF) designed to uncover impacts of molecular/mesoscale water, solute, and polymer interactions on membrane properties. These GAPs are built on a foundation of a shared universal membrane chemistry platform (UMCP) and model fluid platform (MFP).

among research projects. Furthermore, we will develop/curate a highly functional, flexible database to organize M-WET's experimental data and provide a valuable information resource across M-WET and, ultimately, the scientific community. Via the **GAPs** and **IF**, M-WET will: (1) discover the key science drivers that link polymer structure and interfacial interactions to hydration, solute interactions, and fouling, (2) leverage fundamental understanding of ion solubility and transport in dry polymer systems to understand the role of hydration on water, ion, and solute transport in hydrated membrane materials relevant to water purification, (3) utilize high-throughput methods to rapidly identify selective interactants for incorporation into mechanically robust membranes, and (4) uncover the missing basic science that currently frustrates the facile manufacturing of high performance, robust, isoporous membranes via highly scalable non-equilibrium processes.

Today, specific interactions (and non-interactions) facilitate solute selectivity and fouling resistance, yet they cannot currently be "designed" *a priori* into membranes. To do so requires fundamental insights into the impact of functional groups on water dynamics near interfaces, an understanding of the impact of hydration on solute transport and membrane properties, and new routes to manufacture robust porous and nonporous membranes at scale. M-WET focuses on discovering and designing specific interactions with solutes of interest into highly manufacturable, scalable, robust, selective, permeable membranes. Motivated by the Basic Research Needs Report on Energy and Water, our specific goals are to: (1) design new interfaces with controlled topology and functionalities to achieve, for example, fouling-resistant surfaces and highly selective membranes; (2) precisely control mesoscopic material architecture to build novel, highly permeable, and selective membranes with rapid, component-resolved transport at multiple scales for resource recovery and producing fit-for-purpose water, while introducing design principles from (1); (3) develop novel imaging characterization tools for these systems; and (4) model multicomponent materials, fluid mixtures, and mesoporous architectures from atomistic to macroscale to radically transform membrane/materials systems' energy demands, resiliency, and efficiency.

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