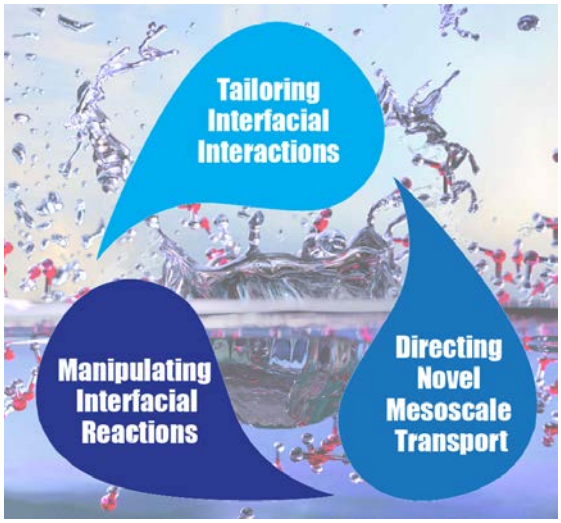
Advanced Materials for Energy-Water Systems (AMEWS)
EFRC Director: Seth Darling
Lead Institution: Argonne National Laboratory
Class: 2018 – 2022

Mission Statement*: To understand and design water-solid interfaces to enable future advances in materials for efficient water treatment.*

The direct connection between water and energy takes its most tangible scientific form at water/solid interfaces that mediate energy conversion and transduction processes, or are designed to influence water chemistry. Water/solid interfaces are central to a broad array of scientific and technological processes including heterogeneous catalysis and electrochemistry, life sciences and biomedical applications, and environmental and geosciences. The importance of such systems cannot be overstated. Yet, numerous fundamental questions in these areas remain unanswered despite decades of study. At the heart of these issues are molecular-scale questions involving the nuances of water's hydrogen bonding at interfaces with electrolyte solutions, the interfacial transfer of energy in the form of protons and electrons, the adsorption and chemical reactivity of solutes at structured and confined interfaces, and many other particulars connected to water. With the emergence of newfound capabilities to experimentally probe and computationally model these deceptively complex systems, the chemistry and physics of aqueous solution/solid interfaces has become one of the most exciting fields in science.



The AMEWS team brings together a confluence of capabilities to tackle the knowledge gaps outlined above. We have identified three integrated 4-year goals toward which we will work collectively as a center:

- Design and synthesize responsive interfaces to selectively and reversibly adsorb specific components from a complex aqueous fluid.
- Decipher and harness the interplay between confinement and charge on catalytic reactivity at water/solid interfaces.
- Predictively describe the transport of water, aqueous solutions, and charged species across multiple time and length scales, especially under extreme confinement and in the presence of charged interfaces.

These goals target the three legs of water/solid interfaces: adsorption, reactivity, and transport. Our first goal aims to understand interactions between constituents of a multi-component aqueous fluid and a solid interface sufficiently well to enable selective adsorption of particular species in the solution while rejecting others. Further, we aim to design these affinity and repulsive interactions with precision such that they can be switched or tuned for reversible adsorption. We will explore how electrostatics, hydrogen bonding, surface chemistry, and microstructure influence interfacial affinity and the organization of the solution's boundary layers.

Confinement and charge have long been investigated in the context of reactivity and catalysis in aqueous systems, but emerging computational and experimental capabilities enable unprecedented potential for progress in understanding these essential phenomena. AMEWS will explore the explicit role of water in reactive processes on the surfaces and near-surface of solid/liquid interfaces, particularly (electro)catalytic processes. We will study the effect that precise spatial confinement (including electric fields) may have on catalytic function in complex aqueous media, relying on unprecedented control of hierarchical architectures over length scales from Ångstroms to microns and using advanced in situ and time-resolved spectroscopic methods. We will also utilize our ability to design and synthesize atom-precise catalysts to investigate the reactions in complex aqueous media on designer reactive interfaces.

Macroscopic aspects of aqueous solution transport are reasonably well understood, but as the dimensions of the channel through which the fluid flows approach the molecular scale and interface effects increase in prominence relative to the bulk, current models fail to predictively capture transport behavior. This is particularly true when the interfaces are charged and interact electrostatically with ions and polar (or polarizable) species in the solution—including water itself. Building predictive models will only be possible if the various interactions are well understood at each of the relevant length scales at play. Experimentally, AMEWS will work toward this goal by applying new methodologies such as directed self-assembly—coupled with our expertise in atomic layer deposition—to generate extremely well-defined nanoporous media in which the pore diameters are nearly monodisperse and the pore wall chemistry and charge can be tuned at will.

Advanced Materials for Energy-Water Systems (AMEWS)	
Argonne National Laboratory	Wei Chen, Seth Darling (Director), Juan de Pablo*, Jeffrey Elam, Giulia Galli* (Deputy Director), Alex Martinson, Karen Mulfort, Paul Nealey*, David Tiede, Matthew Tirrell*, Nestor Zaluzec
University of Chicago	Chong Liu, Steven Sibener, Dmitri Talapin, Andrei Tokmakoff, Gregory Voth (* - joint appointee)
Northwestern University	Harold Kung, George Schatz

Contact: Seth Darling, Director, darling@anl.gov
630-252-4580, https://www.anl.gov/amews