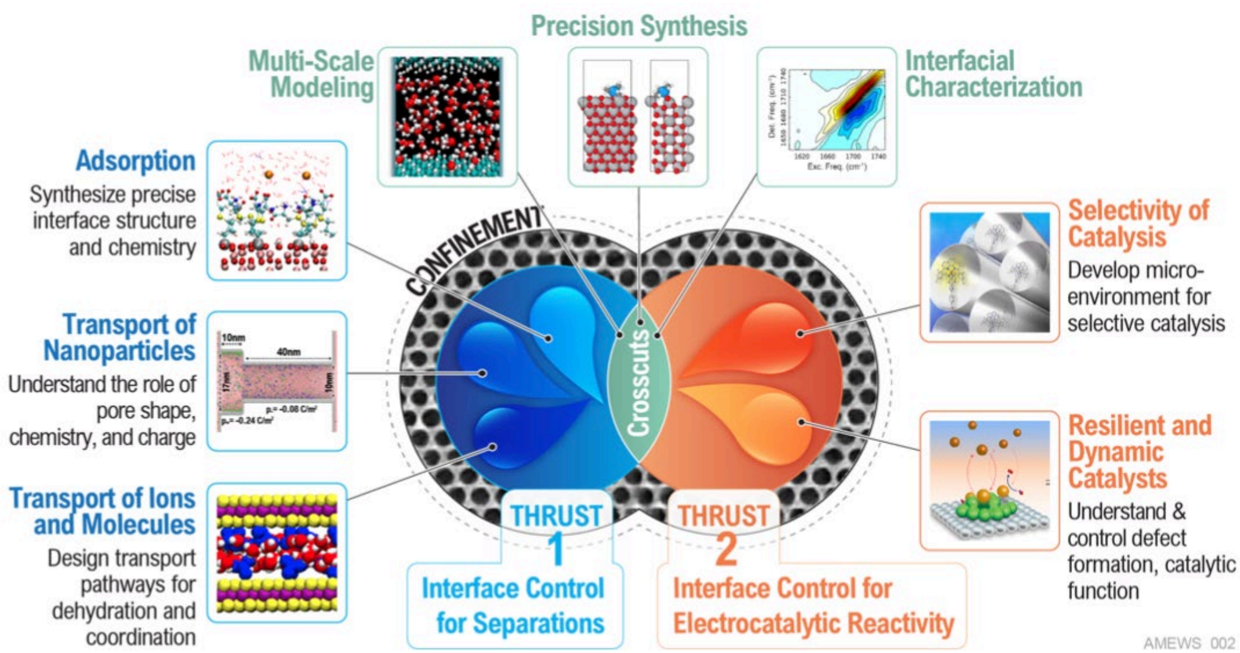
Advanced Materials for Energy-Water Systems (AMEWS)
EFRC Director: Seth Darling
Lead Institution: Argonne National Laboratory
Class: 2018 – 2026

Mission Statement: *To revolutionize our understanding of aqueous solutes in confined and electrified environments at interfaces.*

Deeper insights into water-solid interfaces are essential for development of innovative and efficient technologies to extract valuable resources from wastewater and to deliver clean water to all people. However, numerous fundamental questions about what happens at water-solid interfaces and why it happens remain unanswered despite decades of study. At the heart of these issues are questions involving the molecular-scale nuances of water's hydrogen bonding at interfaces with electrolyte solutions, interfacial transfer of energy in the form of electrons, and adsorption, transport, and chemical reactivity of solutes at structured, confined, and electrified interfaces. With the emergence of newfound capabilities to experimentally probe and computationally model these complex systems, the chemistry and physics of aqueous solution/solid interfaces is poised for new breakthroughs in understanding.

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

- Design and control transport properties of ions, molecules, and nanoparticles under confinement
- Discover pathways to capture and control release of trace solutes from complex aqueous solutions
- Identify new mechanisms to drive selective electrocatalysis in complex aqueous mixtures
- Predict and synthesize catalysts that are resilient under electro-active aqueous environments



These goals target the two legs of fundamental bases of water-solid chemistry: Interface control for separations and electrocatalytic reactivity.

Water-solid interfaces can result in intriguing properties and activities for both the solution and the solid material in contact with the solution. The organization and dynamics of water, ions, and solutes at the water-solid interface differ significantly from those in bulk solution because of the complex effects of solute-solid interactions, the electrical properties of the interface and solution, and the organization of the water's hydrogen-bond network. It is even more intriguing to describe confining water-solid interfaces that can arise in channels, where there can be two interfaces at distances comparable to the size of a few water molecules. We aim to uncover the principles governing selective adsorption and transport of different target solutes through integrated synthesis, characterization, and theory and modeling.

The research program is further focused on understanding the materials design principles required for effective and selective chemical transformations relevant to water remediation by 1) predicting and synthesizing catalysts that are resilient under electro-active aqueous environments, and 2) identifying new mechanisms to drive selective electrocatalysis in complex aqueous mixtures. To accomplish these scientific goals and address critical knowledge gaps, our team will develop a fundamental atomic- and molecular-level understanding of *dynamic* interfacial structure and concentrate most of our studies on electrocatalysts composed of earth-abundant elements.

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