

Basic Research Needs for

Energy and Water



*Energy and Water—Science to Enable Energy-Efficient
Clean Water and Water-Efficient Energy*

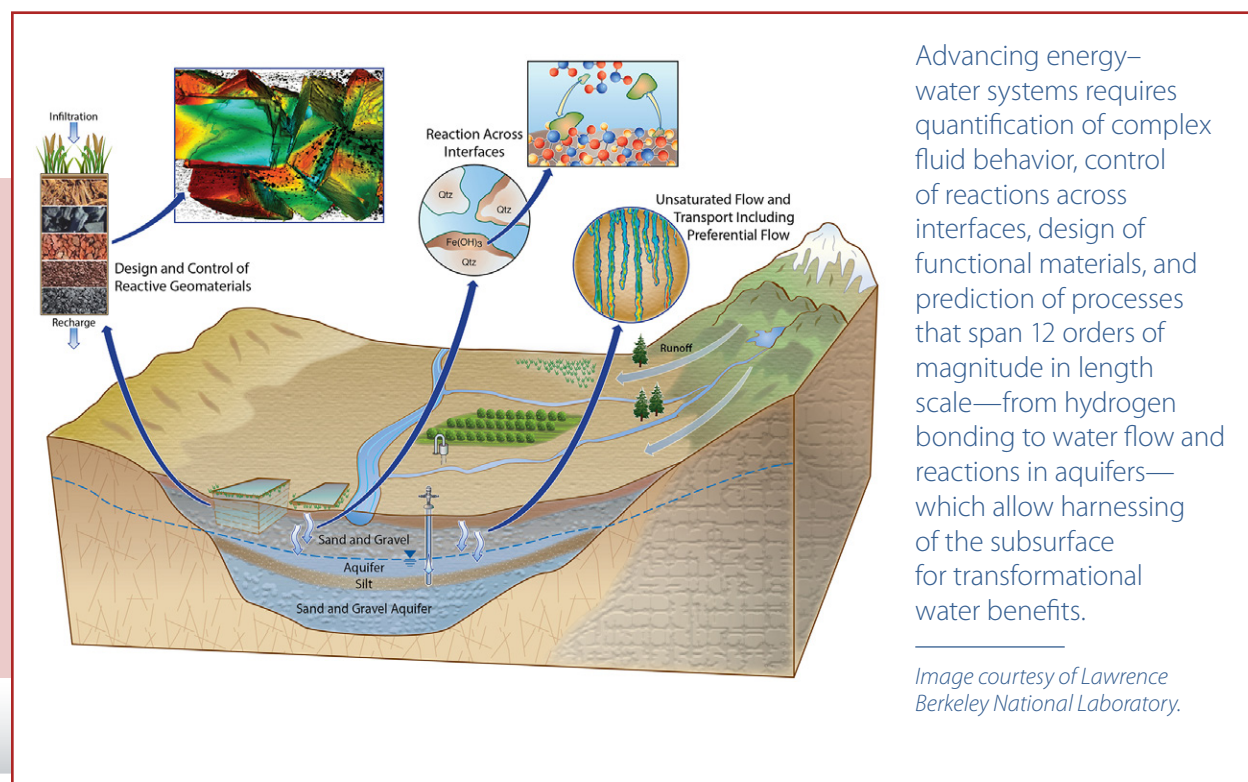
Energy and Water—Understanding fundamental phenomena and translating that knowledge into innovation

Water is precious. This unique, indispensable resource is essential not only for life, but also for practically all forms of economic activity. The food we eat, the clothes we wear, the goods we use, and the electricity we consume all require water. Cooling in power plants, refining petroleum, producing fuel, and extracting energy resources from the earth make up a significant fraction of water use. Conversely, water treatment, distribution, and use are large consumers of energy.

The connection between water and energy means that issues in one area—for instance, too much or too little water—can profoundly affect the other. The looming challenge is to address the coupled needs of sufficient energy and clean water for a thriving economy and national security.

This challenge presents an enormous opportunity for fundamental energy science. Fertile basic research opportunities, ripe for exploration, span disciplines—such as chemistry, geosciences, biosciences, and materials sciences—and scales, starting with molecular phenomena. Energy–water systems, whether manufactured or part of the natural world, exhibit extraordinary dynamics and complexities. The “water” is not simply water—it is typically a complex fluid with multiple chemical, particulate, and biological components. The molecular interactions of water with these components, with other fluids, and at material interfaces are still a mystery. Basic science is essential to solve this and other mysteries related to energy and water.

A report from a 2017 Basic Research Needs workshop identifies four priority research directions to understand the chemical processes and materials underlying the interdependence of energy and water and to harness the potential for technological impact. The full report will be available at <https://science.energy.gov/bes/community-resources/reports/>.



Priority Research Directions

- **Predict static and dynamic properties of multicomponent fluids**

Key question: *How can we predict and control molecular-to-macroscopic properties and behavior of complex, multicomponent fluids?*

Many aspects of energy–water systems involve the interactions of multicomponent aqueous solutions and other complex fluids. The ability to reliably predict and control the emergence of structures and phases in these fluids requires fundamental knowledge of the underlying mechanisms that demands a molecular-level understanding of the interactions between the components.

- **Achieve mechanistic control of interfaces and transport in complex and extreme environments**

Key question: *What are the underlying mechanisms of affinity and reactivity at interfaces in aqueous systems?*

Interfaces—and confinement by interfaces—play a central, often dominant, role in the diverse transport and reactive processes associated with energy–water systems, from water treatment membranes and catalysts to subsurface resource recovery.

- **Exploit specific material–fluid interactions to design and discover innovative fluids and materials**

Key question: *How can we codesign the dynamic interactions between materials and reactive fluids for unprecedented tunability?*

The codesign of new materials and fluids to exploit specific material–fluid interactions will enable step-change improvements in the design and selectivity for purification, transformation, and transport processes in energy–water systems.

- **Advance science to harness the subsurface for a transformational impact on water**

Key question: *How do we develop the ability to predict and control multiscale, multiphase, multiphysics subsurface properties?*

Reactive natural and engineered subsurface materials offer tremendous potential for water storage and treatment. Realizing this potential will require revolutionary advances in approaches to quantify, sense, predict, and manipulate coupled physical, chemical, and biological processes occurring in complex subsurface systems.



Summary

The connection between energy and water is a multifaceted part of our everyday life. Today's water and energy practices rely largely on empirical or engineering approaches. For the future, basic research will play a vital role in fostering innovation to address the ongoing demand for robust, efficient energy–water systems. Many of the needed advances will result through a powerful convergence of expertise across basic energy sciences and draw upon forefront capabilities at scientific user facilities.

The identified priority research directions will provide the fundamental scientific underpinnings needed to address challenges facing energy and water. New insights inspired by uncovering how water behaves and reacts with other fluids and materials can enable novel approaches and technologies for energy and water. New membranes can offer selective filtration of targeted contaminants with minimal energy consumption. Determining fluid transport and reactivity in subsurface processes can enable enhanced recovery of energy resources. Inventive separations techniques can improve use of wastewater as a valuable resource as well as reduce the amount of water needed for energy production and use. Through a better understanding of the fundamental phenomena associated with energy–water systems, science can ensure a future with even greater economic and energy security.



Image courtesy of Argonne National Laboratory.

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