



BASIC RESEARCH NEEDS FOR ENERGY AND WATER

(Workshop held January 4-6, 2017)

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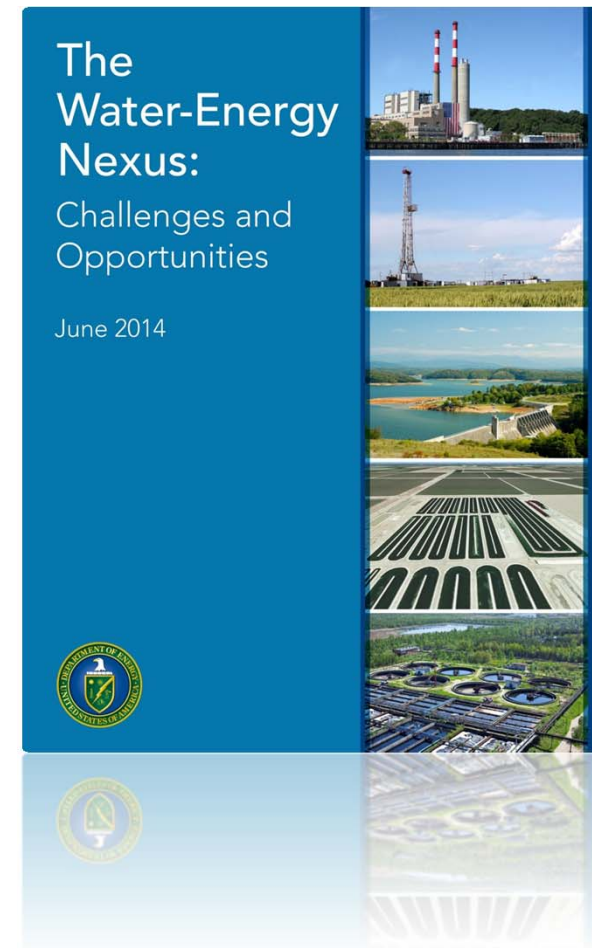
Georgia Tech

AMO Clean Water Workshop

August 2017

DOE AND THE EWN

- DOE emphasis has been on data, modeling, and analysis (DMA) and applied technology research, development, demonstration, and deployment (RDD&D)
- **Pressing need to complement these efforts with a broad suite of basic science programs to extract new insights and discoveries**



PRIORITY RESEARCH DIRECTIONS

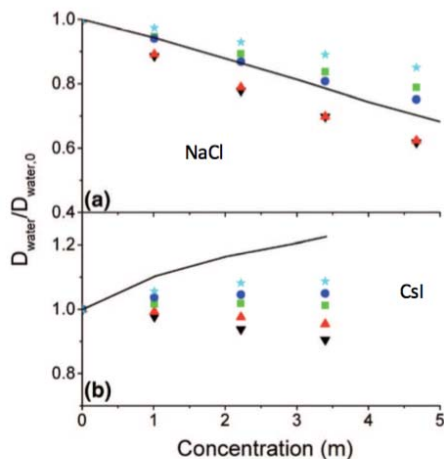
Basic Research Needs for
Energy and Water



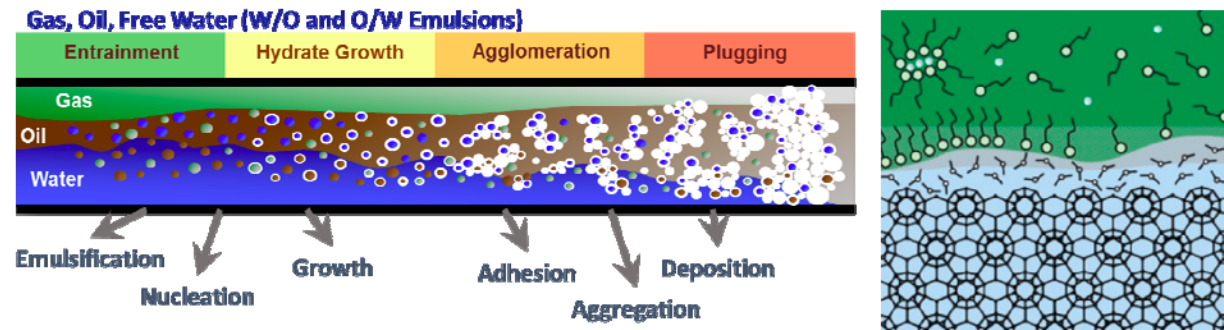
*Energy and Water—Science to Enable Energy-Efficient
Clean Water and Water-Efficient Energy*

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?
- Need to develop understanding of fluids (brines, blends, emulsions) where macroscopic properties—including structure and reactivity under confinement—cannot currently be predicted from first principles



Comparison of measured and calculated water diffusion coefficients in electrolyte solutions [courtesy J. Skinner]

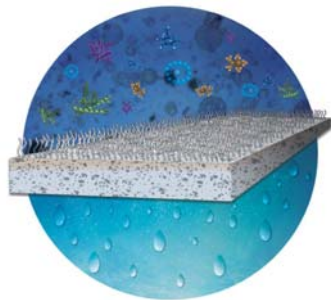


Gas hydrate plugging in an oil pipeline

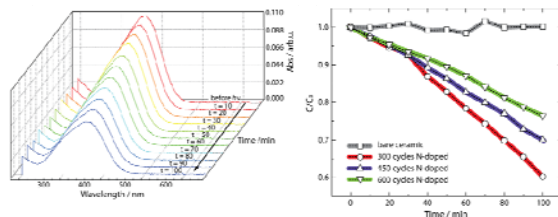
[*Chem. Soc. Rev.* **45** (2016) 1678; *Clathrate Hydrates of Natural Gases*, 2007]

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 role in the diverse transport and reactive processes associated with the energy-water nexus, from water treatment membranes and catalysts to sub-surface resource recovery



Interface fouling
[*Ang. Chemie* **56** (2017) 4662]

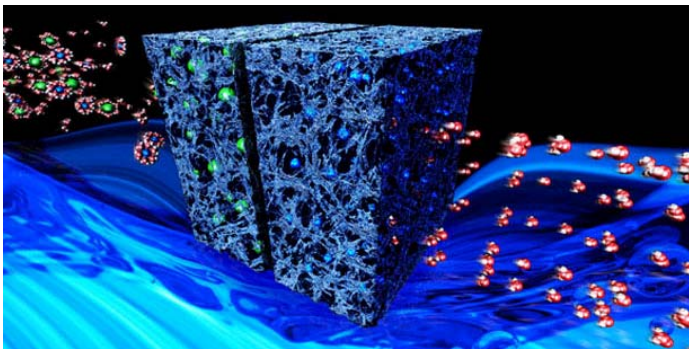


Photocatalytic degradation of organics with novel coatings
[*Adv. Sust. Sys.* **1** (2017) 1600041]

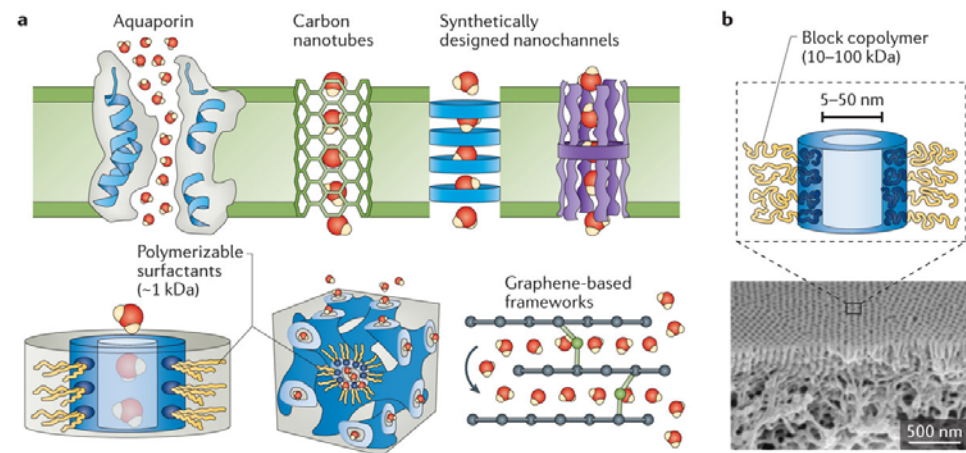


EXPLOIT SPECIFIC MATERIAL-FLUID INTERACTIONS TO DESIGN AND DISCOVER INNOVATIVE FLUIDS AND MATERIALS

- **Key question:** How can we codesign the dynamic interactions between materials and reactive fluids for unprecedented tunability?
- Rational design of new materials to exploit specific material-fluid interactions will enable step-change improvements in tunability and selectivity of purification, transformation, and transport processes



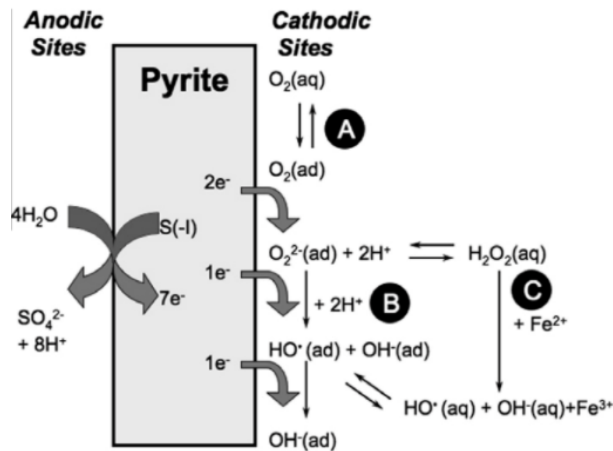
Flow-through capacitive deionization
[*Energy Environ. Sci.* 5 (2012) 9511]



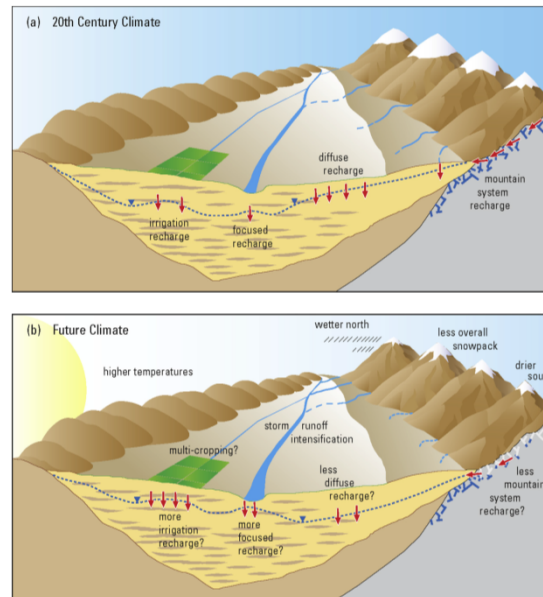
Molecular design of selective membranes
[*Nature Rev. Mater.* 1 (2016) 16018]

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?
- Multiphase flow and reactive transport are non-linear physical, chemical, and biological processes occurring in subsurface systems of tremendous capacity, which can only be effectively utilized with deeper understanding



Mineral-induced reactive oxygen species formation
 [Geochim. Cosmochim. Acta 74 (2010) 4971]



Aquifer recharge mechanisms under current and future climate conditions
 [J. Hydrology 534 (2016) 124]

**BASIC SCIENCE WILL LAY THE GROUNDWORK
FOR ENSURING ROBUST AND SECURE ENERGY-
WATER SYSTEMS IN BOTH NATURAL AND
MANUFACTURED ENVIRONMENTS**