Exploiting Interfacial Water Properties for Desalination and Purification Applications

by **P. J. Feibelman (with R. T. Cygan, B. C. Bunker, C. J. Brinker, and T. M. Nenoff)**

Motivation—Dearth of potable water plagues half the world's population, causing death, disease, and international political tension. Improved understanding of water behavior in porous purification systems will have a profound impact on water supply, decontamination, and desalination technologies. Significant improvements over conventional water treatment processes will, however, require novel approaches, based on fundamental understanding of nanoscale and atomic interactions at interfaces between aqueous solution and materials. A group of about 20 Sandia scientists has accordingly formed to study how the structure and composition of materials surfaces affect the molecular arrangement, transport and chemistry of adjacent, impure water, and how confinement in pores modifies these properties.

Accomplishment—We held a workshop in April 2005, aimed at identifying key unresolved scientific issues and fostering collaborations. A summary of discussions and key conclusions, by R. T Cygan and J. A. Greathouse, is available at www.sandia.gov/water/waterworkshop.

Research now begun is divided into 2- and 3-dimensional components. The 2D work (Fig. 1) takes advantage of the ability to "see" what is happening at a water interface with a flat, high quality surface, and to use the high degree of control in a "surface science" environment to isolate the surface properties that control interfacial water structure and transport. By applying a wide range of analytical techniques, now being tested, we have a reasonable chance of discovering the nature of what we know to be a very complicated interfacial environment.

Our 3D work focuses on understanding how interplay of pore structure and composition controls pore function. (Fig. 2) One thread is to use SNL expertise in synthesis to fabricate model pores of desired size, shape and surface-functionality, allowing quasi-realistic tests of concepts for improved purification. Another involves synthesizing "molecular sieves," and systematically relating composition and structure to ion-exchange capabilities.

The broad range of expertise at Sandia is critical to eventual success. Currently, we are building and validating 2-d approaches based on NMR, non-linear optics (sum-frequency generation), interfacial-force, atomic-force and scanning-tunneling microscopies. 3-d efforts involve self-assembly, focused particle beam lithographies, and atomic layer deposition to create the membrane platform allowing structural and functional characterization of individual nanopores. Neutron spectroscopy is our key probe of water behavior in zeolite membranes.
Analyzing our results via ab-initio and classical simulations is a common theme of our group project. Theorists, working closely with our experimenters, will support data interpretation, suggest experimental directions and develop new concepts.

Significance—Learning to increase water flux through porous membranes by even one order of magnitude would have worldwide impact on desalination and purification technologies. By establishing a scientific basis for identifying and overcoming the critical roadblocks to improved purity and flow, we will guide R&D efforts to optimal impact.

Sponsors for various phases of this work include: Laboratory Directed Research & Development

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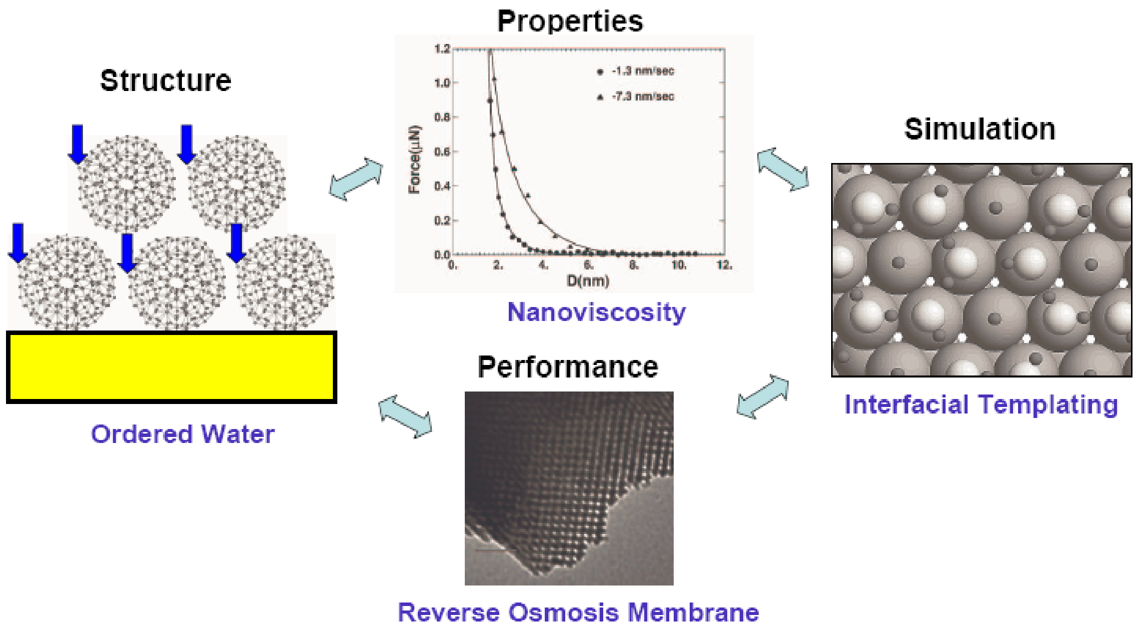

Figure 1. To learn how surface structure and properties affect water treatment technologies, 2D studies of "interfacial water" and its behavior will be conducted on model surfaces whose structure and chemistry can be systematically varied.

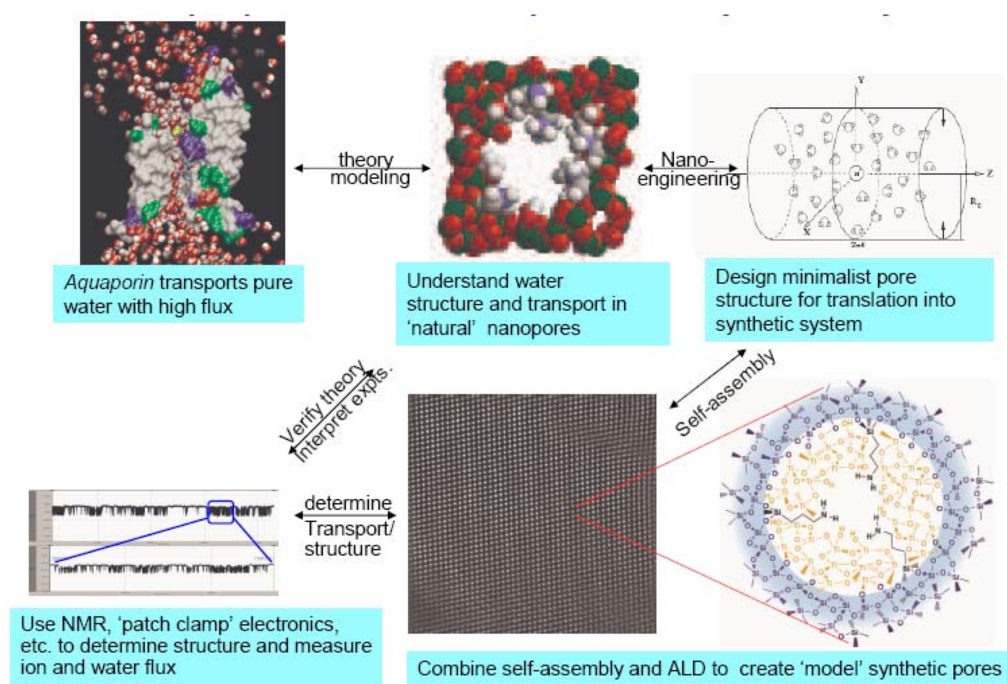

Figure 2. 3D studies will combine theory, modeling, synthesis and characterization to teach us how to embody properties of natural pores in synthetic systems.