

## Nanotechnology Highlight

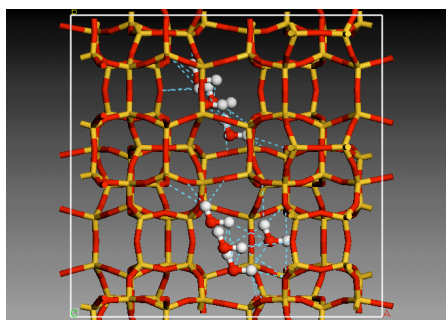
### “NIRT – Collaborative Research: Experimental and Computational Investigations of Fluid Interactions/Transport in Nanodomains and Around Nanoparticles.”

(DMI-0210258)

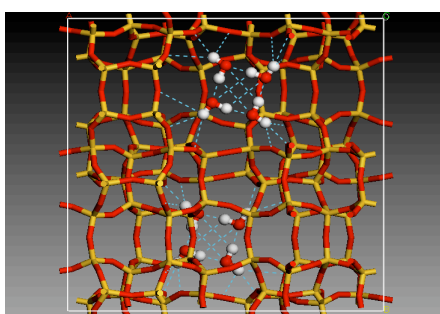
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This research addresses the growing interest in developing manufacturing processes and systems that involve fluids at the nanoscale. There also is continuing evidence that fluid phenomena that occur at the nanoscale are unlike macroscopic behavior. For example, some hydrophobic channels will permit liquid water to exist, while only slightly narrower channels will only permit water vapor to exist. Similar phenomena are expected to manifest when evaluating fluids other than water. The combined experimental, theoretical, and computational investigations focus on the confinement and transport of water, alcohols, amines, and other interesting organic compounds in nanochannels. The generic geometry of the nanofluidic system and fluids to be considered are representative of important manufacturing systems and processes. The outcomes of the research have significance to nano-rheology, nano-lubrication, control of nanosurface properties, modeling and simulation at the nanoscale, lab-on-a-chip technologies, and other nanofluidic devices. Biosystems and environmental processes that involve nanofluidic transport through membranes and channels will also benefit from the expected outcomes. The investigations at WPI are complemented by research on flow behavior of nanoparticles in conventional, rotating and circulating fluidized beds performed by the NIRT group at New Jersey Institute of Technology (NJIT).

We have been studying the ways in which water interacts with pores at the nanoscale, e.g., pores in molecular sieve zeolites. Molecular Dynamics calculations have thus far been carried out in the simulated pores of silicalite and zeolite Y, both assumed to be composed of all silica.



**Figure 1a** Water molecules placed randomly at the intersections between straight and zigzag channels of silicalite-1 before performing an equilibration run.



**Figure 0b** Water molecules rotated and translated from their starting positions in order to reach a local minimum for the total potential energy after the equilibrium run.

of silicalite and zeolite Y, both assumed to be composed of all silica. Self-diffusion rates at various temperatures have been determined, as well as radial distribution functions of intermolecular spacing between oxygen atoms, g<sub>OO</sub>, and oxygen and hydrogen atoms, g<sub>OH</sub>. Currently, adsorption isotherms are being simulated at various temperatures in both structures. In the near future, the structure of the

unit cells of the zeolitic materials will be altered to incorporate small amounts of Al<sup>3+</sup> to investigate its effects on adsorption and transport rates. Figures 1a and 1b show drawings from the MD simulations at the beginning of a simulation and at the conclusion of a simulation in which transport rates were determined. The blue dashed lines represent hydrogen bonds with the zeolite structure.

We also have been developing methods for the synthetic modification of the surfaces of nanodomains, be they zeolites, metals, or silica. We have successfully demonstrated that metal surfaces such as gold can be modified with a variety of ligands with hydrophilic or hydrophobic head groups. This technique involves the deposition of a SAM (self-assembled monolayer) that can act as a template for the subsequent non-covalent deposition of a wide variety of organic groups to form multilayered thin films. We have also recently shown that the same multilayer non-covalent method can be used in the modification of silica surfaces.

We also have been developing a hybrid three-dimensional computational model that combines the molecular and dissipative particle dynamics techniques. This model will capture the multi-scale fluid phenomena at the nanoscale and bridge the gap between the atomic and macroscopic scales.