Exploiting Interfacial Water Properties for Desalination and Purification Applications

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Sandia National Laboratories

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Introduction

Goal: Understand how to control water permeation, salt exclusion, and ion exchange in nanoporous spaces

Project Purpose and Approach

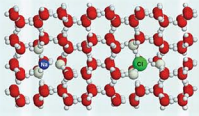
Experimental and computational approach to evaluate molecular controls at aqueous solution-solid interface to enhance solute removal; emphasis on RO membranes (nylon model) and novel inorganic materials (silica membranes and zeolites)

Key Accomplishments

- Vibrational spectroscopies show disruption of ordered water layers adjacent to nylon by solute ions
- Improved DFT models of ice and mica interfaces
- Fabricated synthetic ion channels inspired by efficient biological models; control of pore size, channel length, and surface chemistry
- Water in pores of Nb-based zeolites affected by Ti-substitution; aluminosilicate zeolites exhibit complex mechanisms of ion exchange and hydration

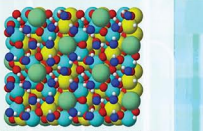
Density Functional Theory Models of Na-Cl Solvation in Ice and Wetting of Muscovite Surface

Ideal solvation geometry found for NaCl in ice Ih



Ions *substitute* for water molecules. Interstitial solvation costs at least 1.5 eV more. You cannot get the right answer unless you ask how many water molecules there should be in the simulation cell.

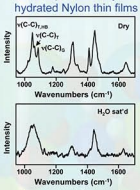
Progress toward understanding the wetting layer muscovite

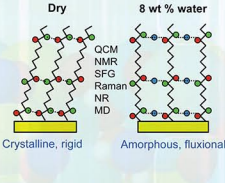


A molecular arrangement intentionally designed to hydrate the K atoms has a lower energy than the best structure obtained from the Parrinello group's *ab initio* simulation. The energetically optimal coverage is less than 1 ML, showing again that a "grand canonical" approach is key to finding the best answer.

Water Restructures Polymer Films

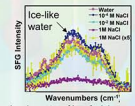
Raman spectra of dry and hydrated Nylon thin films



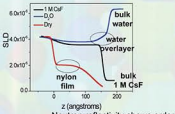


Water disrupts interchain hydrogen bonding and creates a more amorphous, fluxional network that could facilitate water transport

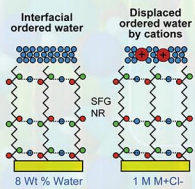
Polymer Films Restructure Interfacial Water



Vibrational spectra of interfacial water shows a high degree of ordering that is disrupted by salt



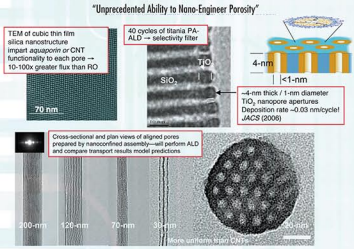
Neutron reflectivity shows ordered water extends ~5 nm from the polymer surface



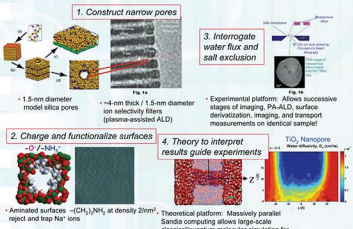
Water ordering may influence the partitioning of salts for reverse osmosis membranes

Self-Assembly, Nano-Confined Assembly, and Atomic Layer Deposition

"Unprecedented Ability to Nano-Engineer Porosity"

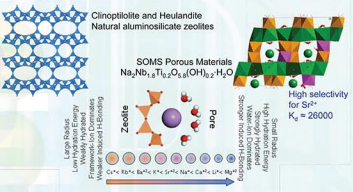


Nanopores: Convergence of Theory and Experiment



Behavior of Water in Nanopores

- Water treatment materials and residual waste storage
- Characterize fundamental interactions of hydration within pores
- Development of improved materials for enhanced ion exchange and selectivity

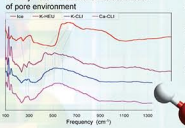


Behavior of Water in Nanopores

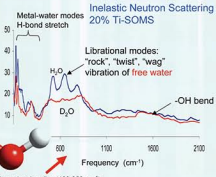
Synthesis of ion exchangeable frameworks and fully characterize **water in pores** using synthesis, ^{1}H MAS NMR, inelastic neutron vibrational spectroscopy, DFT, MD, plus TPD, TGA/DTA, FTIR, Raman, and BET analysis

Inelastic Neutron Scattering Clinoptilolite and Heulandite

Identify water librational shifts as function of pore environment



Inelastic Neutron Scattering 20% Ti-SOMS



Aquo complexes: H_2O is bound to metal ion by partial covalent bonding (100-350 cm^{-1})
Lattice water: H_2O oxygen is bound to metal in ionic bond, water molecule may be considered rigid or ice-like (300-600 cm^{-1})

Inelastic Neutron Scattering data from LANSCE (LANL)

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