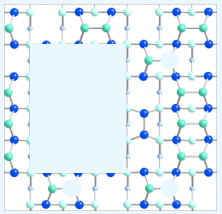
Understanding Nanomaterials & Nanoscale Phenomena

SAND2006-5132P

Example Research Directions

Understanding Atomic Scale Images



As
In or Ga
Lone Pair
from As

STM image

calculated structure
(Modine)

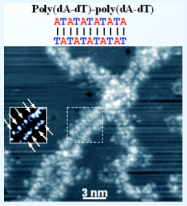
Quantum calculations produce a proposed structure for mysterious coexisting structures in a semiconductor.

Image at left show proposed (4X3) reconstruction coexisting with (2X4) reconstructions on InGaAs.

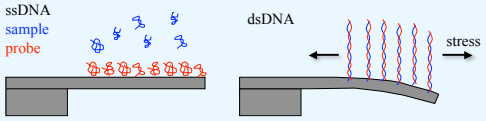
DNA can be a conducting molecule. Because of all the complex chemical binding aspects of DNA, this provides intriguing possibilities for complex conducting structures.

SNL-LANL effort has begun on calculating the STM images of DNA.

Images of DNA from Tanaka *et al.*



Coupling between nanomaterials and biomaterials
Example: cantilever sensors



coupling of stress in dsDNA layer
bend cantilever beam

The binding of sample ssDNA to the probe ssDNA produces a monolayer of dsDNA on the cantilever. The lateral stress in the dsDNA monolayer is different than in the ssDNA monolayer. This stress difference causes the cantilever to bend, which can be detected and a signal generated.

What is the source of the stress coupling in the DNA system? Other systems?

How can we have *both* the biomolecular and the silicon components interact with each other? In other words, how can we pass information in both directions?

Combining Capabilities & Research

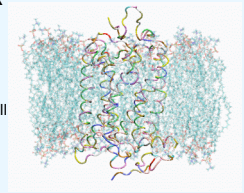
Molecular Dynamics Simulations

A key aspect of understanding molecular systems is simulating the sequence of molecular events that yield the functional dynamics of a material or system. At Sandia, we have a molecular dynamics code that runs on our massively parallel computers and enables us to perform simulations a new level.

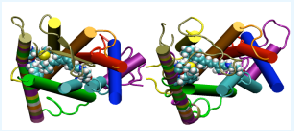
Ex: Seeing molecular events combine like clockwork

Rhodopsin is the protein in your eye that
- •absorbs light
- •straightens retinal chain
- •which moves rhodopsin helices
- •which alters the structure at the other end, inside the cell
- •which starts signaling cascade that results in our vision

We now can simulate the initial 'clockwork' in rhodopsin.



rhodopsin protein in membrane

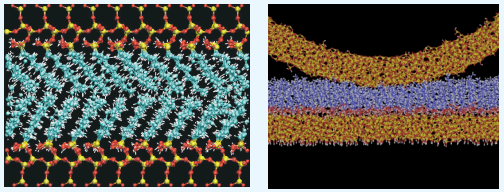


before after
isomerization

Nanomechanics of Interfaces

At the nanoscale interfaces are common and influence material properties strongly. Interfaces present challenges to our theoretical methods.

Self-assembled monolayers are archtypical nanomaterials. We have recently developed the capability to perform molecular dynamics simulations that explicitly treat the tip of a force microscope. This is revealing details of the molecular events involved in nanoscale adhesion and friction.



Images from simulations of two self-assembled monolayers on crystal silica under shear and load (left). A tip pushing down on a coated amorphous surface (right).

Selected Capabilities

Quantum Simulations

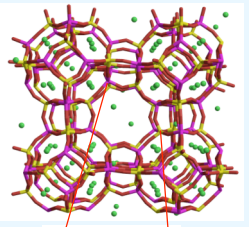
A characteristic of the nanoscale is the transition from classical to quantum dynamics as the scale decreases.

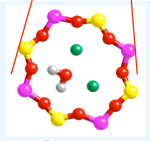
SOCORRO:Quantum code
- Kohn-Sham Density Functional Theory
- Provides
  1. Structures, Energetics, Transition States, MD
  2. Electronic Densities and Wavefunctions
- Capabilities
  1. Projector Augmented Wavefunction Method
  2. Exact Exchange (Available Fall 2006)
  3. Gnu Public License

Hybrid Combined Quantum/Classical (QM/MM) Capability
- Embed a region represented with DFT within a system represented with classical potentials
- Based on Socorro and LAMMPS

(Modine)

Classical



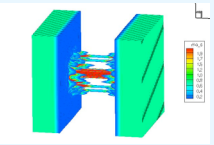


Quantum

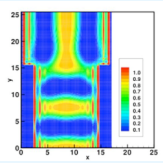
Molecular Theory Code

A characteristic of nanomaterials is self-assembly of the molecules into ordered structures.

We can compute these structures based on the molecular interactions using the molecular theory code TRAMONTO. This is a unique, massively parallel 3D code developed at Sandia.



Density of solvent outside a lipid bilayer and in a pore created by an assembly of peptides in the bilayer (L.J.D. Frink).



A confined diblock copolymer, showing two different microphase-separated patterns depending on channel width (A.L. Frischknecht et al.).

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