

# Center for Integrated Nanotechnologies

Sandia National Laboratories • Los Alamos National Laboratory



## Scientific Thrust Areas

- Center capabilities and expertise
- Building blocks for multidisciplinary projects
- Developed with input from 1st User Workshop

## Core Research Programs

- Joint laboratory nanoscience programs
- Build capabilities and expertise of CINT scientific staff

*“One scientific community focused on nanoscience integration”*



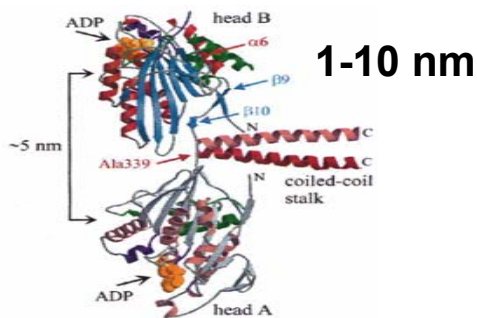
# CINT Scientific Thrust Areas

- Nano-bio-micro Interfaces

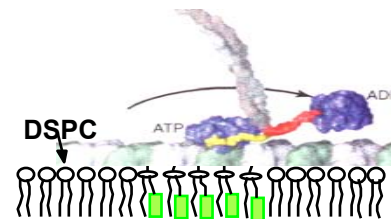
» Import biological principles and functions into artificial biomimetic nano- and micro-systems

Bruce Bunker ([bcbunke@sandia.gov](mailto:bcbunke@sandia.gov))

Andy Shreve ([shreve@lanl.gov](mailto:shreve@lanl.gov))



**motor proteins:**  
molecular biology &  
genetic engineering



Aggregated receptors  
10 -100 nm  
**biomimetic interfaces:**  
complexation chemistry, molecular  
modeling, & self-assembly



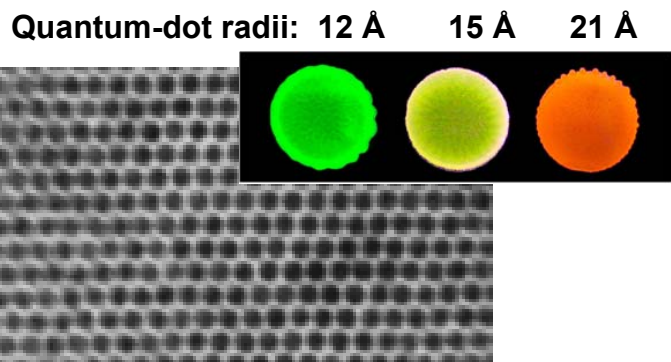
# CINT Scientific Thrust Areas

- Nanophotonics and Nanoelectronics

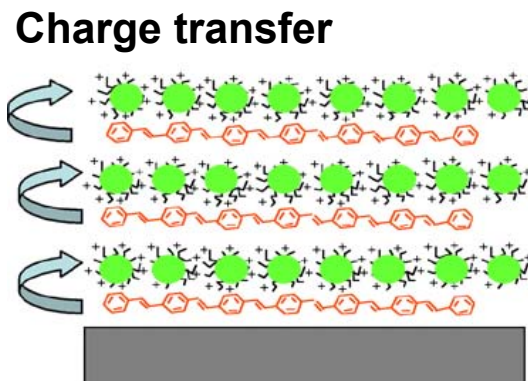
» Control of electronic and photonic properties of nanostructured materials

Victor Klimov ([klimov@lanl.gov](mailto:klimov@lanl.gov))

Jerry Simmons ([jsimmon@sandia.gov](mailto:jsimmon@sandia.gov))



Tunable electronic spectra in Q-dot solids



Organic/inorganic hybrid structures



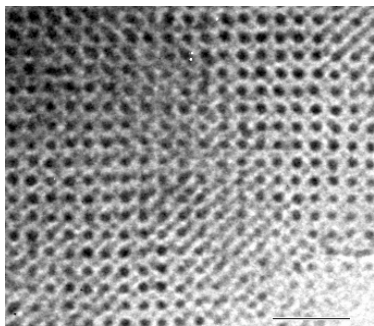
# CINT Scientific Thrust Areas

- **Complex Functional Nanomaterials**

» **Nanoscale materials synthesis, assembly, interfacial science, self-assembly processes and structure-function characterization**

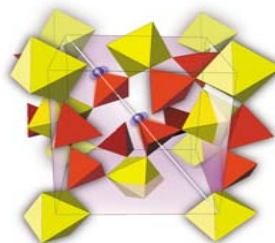
Duane Dimos ([dbdimos@sandia.gov](mailto:dbdimos@sandia.gov))

Toni Taylor ([ttaylor@lanl.gov](mailto:ttaylor@lanl.gov))



Self-Assembly to form  
3-D nanostructures

Unique functionality is often due to  
complex crystal structures



Nanometer Unit Cell-  
 $ZrW_2O_8$

Underconstrained  
lattice – leading to  
Negative Thermal  
Expansion



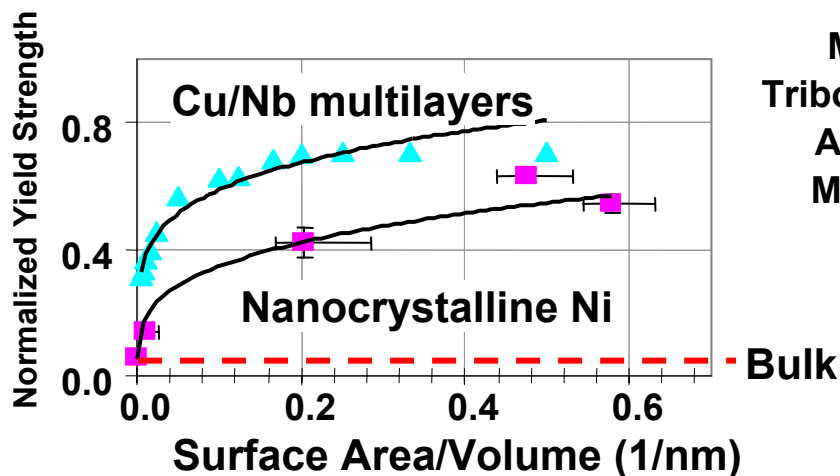
# CINT Scientific Thrust Areas

- Nanomechanics

» Mechanical behavior of nanostructured materials and devices

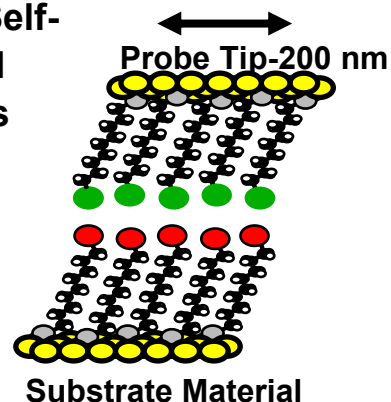
Mike Nastasi ([nasty@lanl.gov](mailto:nasty@lanl.gov))

Charles Barbour ([jcbarbo@sandia.gov](mailto:jcbarbo@sandia.gov))



New Deformation Mechanisms for High Interface/ Volume Ratio

Molecular Tribology of Self-Assembled Monolayers



New Tools: Interfacial Force Microscope



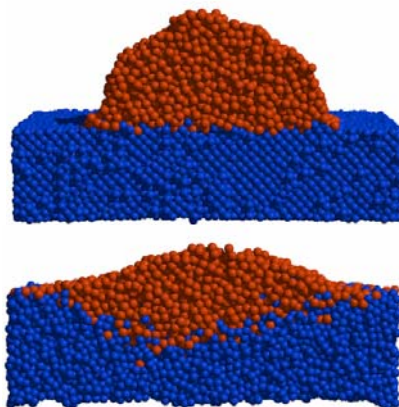
# CINT Scientific Thrust Areas

- Theory and Simulation

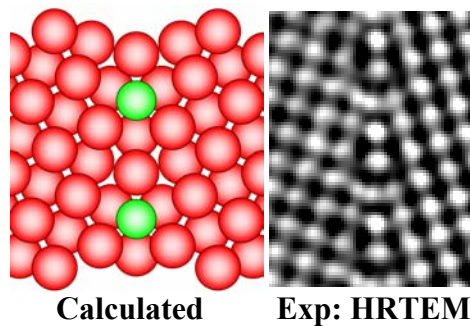
» Capabilities and expertise in theory, modeling and simulation of nano- and meso-scale materials

Eliot Fang ([hefang@sandia.gov](mailto:hefang@sandia.gov))

Tony Redondo ([redondo@lanl.gov](mailto:redondo@lanl.gov))



Wetting Phenomena



Impurity Segregation at GB



# ***Science Programs – Key Challenges***

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- **Integration of top-down fabrication with bottom-up assembly to create new classes of functional materials**
- **Control of optical and electronic energy transfer coupled across multiple length scales**
- **Coupling of mechanical forces across nano, micro and larger length scales, including control of fluidic transport**
- **Integration of biological and synthetic materials, and control of the interface between biological and non-biological components**



# *Science Programs Built to Address Challenges*

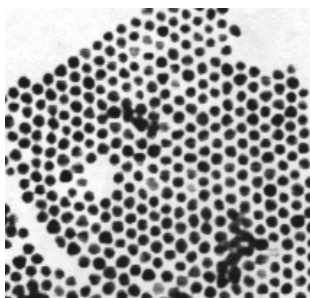
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- **Integrate teams across disciplines and thrust areas**
- **Support the capabilities that are available for users at jump-start**
- **Examples of scientific directions users can interact with**
- **Also see poster session**

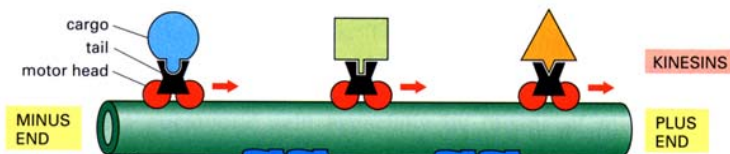




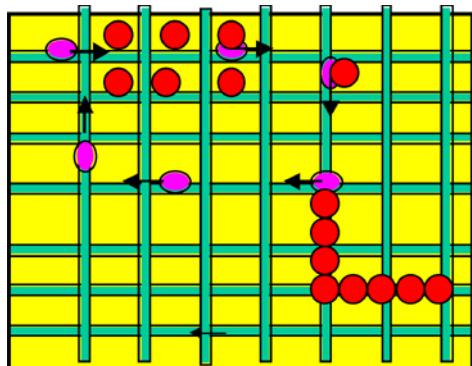
# Assembly and Actuation of Nanomaterials Using Active Biomolecules



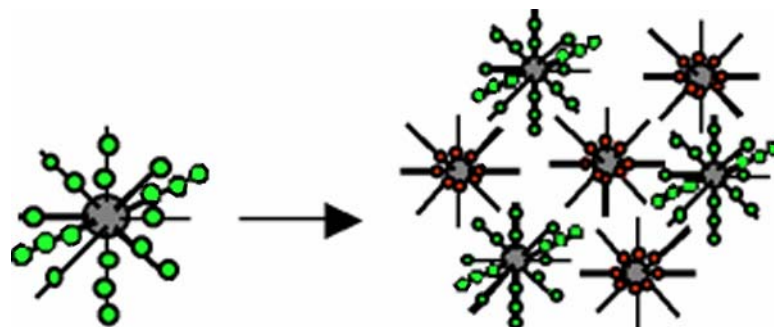
Nanoparticles



Motor Proteins



Nanowires with Programmable Interconnects



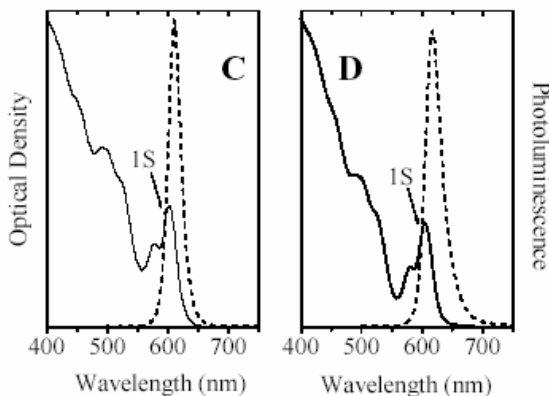
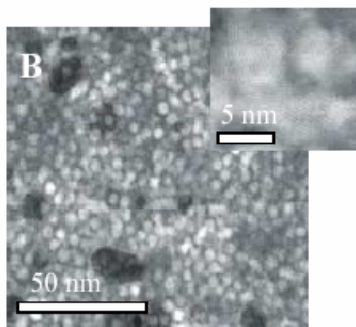
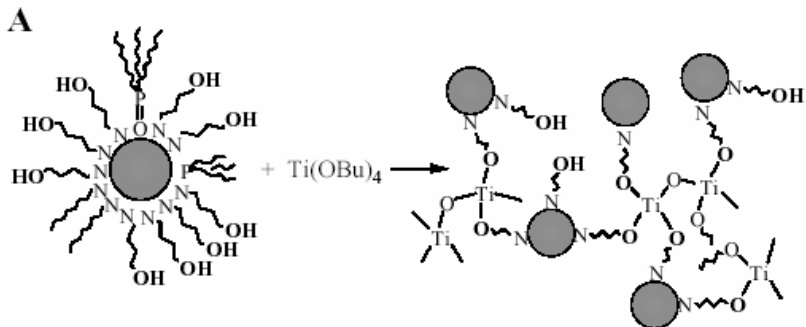
Tunable QD Arrays

- Nano-Bio-Micro Interfaces
- Nanophotonics/Nanoelectronics
- Complex Functional Nanomaterials
- Nanomechanics



# Quantum-dot Nanocomposite Materials For Non-linear Optics and Lasing

■ Partial surface exchange followed by a reaction with a titania precursor

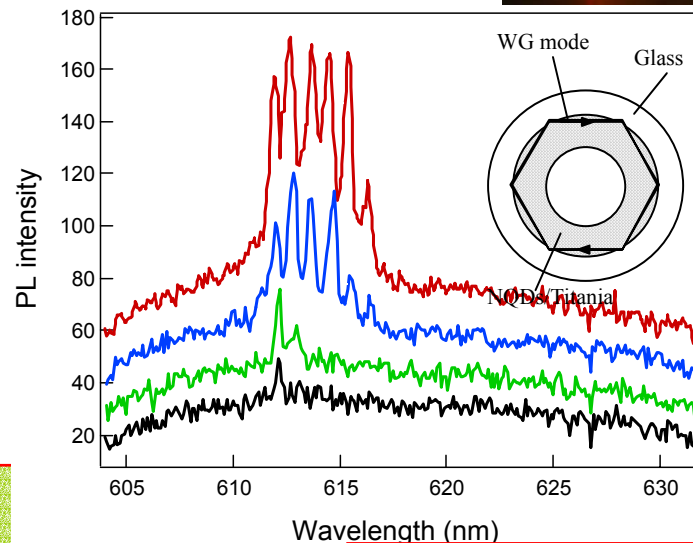
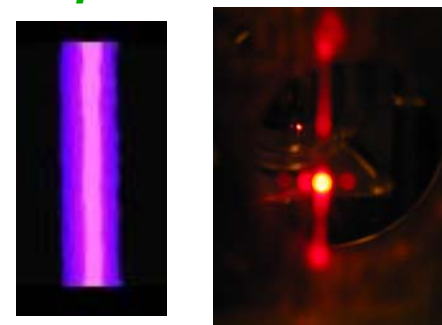


Filling factor: 15 - 20%,  $n = 2.1$   
Modal gain: 100 - 200  $\text{cm}^{-1}$

M. A. Petruska, A. V. Malko, P. M. Voyles, and V. I. Klimov, *Adv. Mater.* **15**, 610 (2003)

■ Sol-gel composites are readily combined with photonic structures

*Q-dot  
Microring  
Laser*

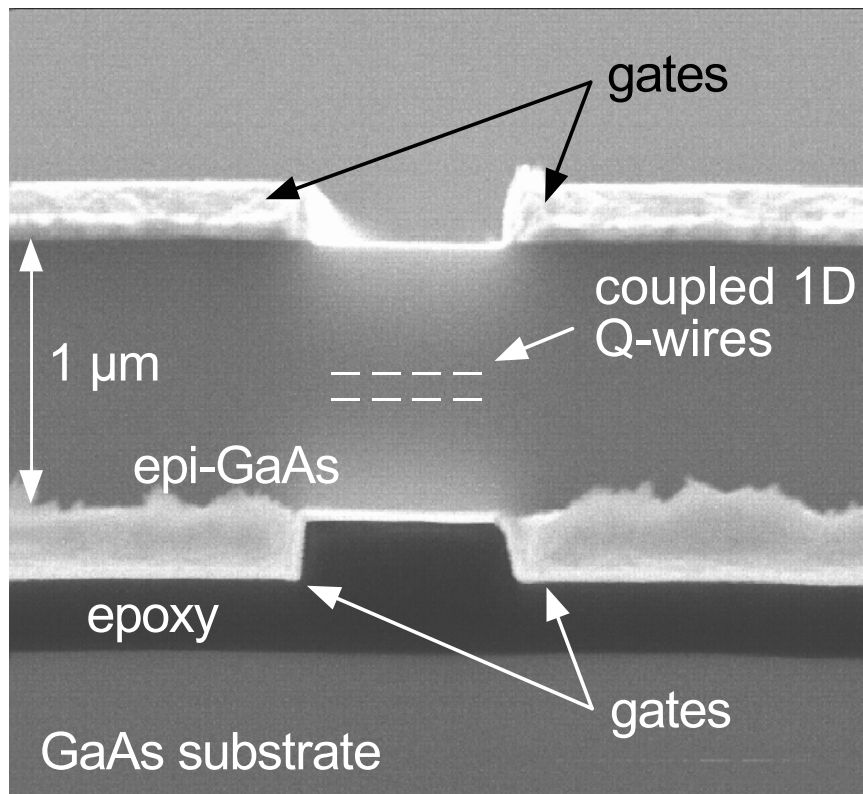


A. V. Malko et al., *Appl. Phys. Lett.* **81**, 1303 (2002)

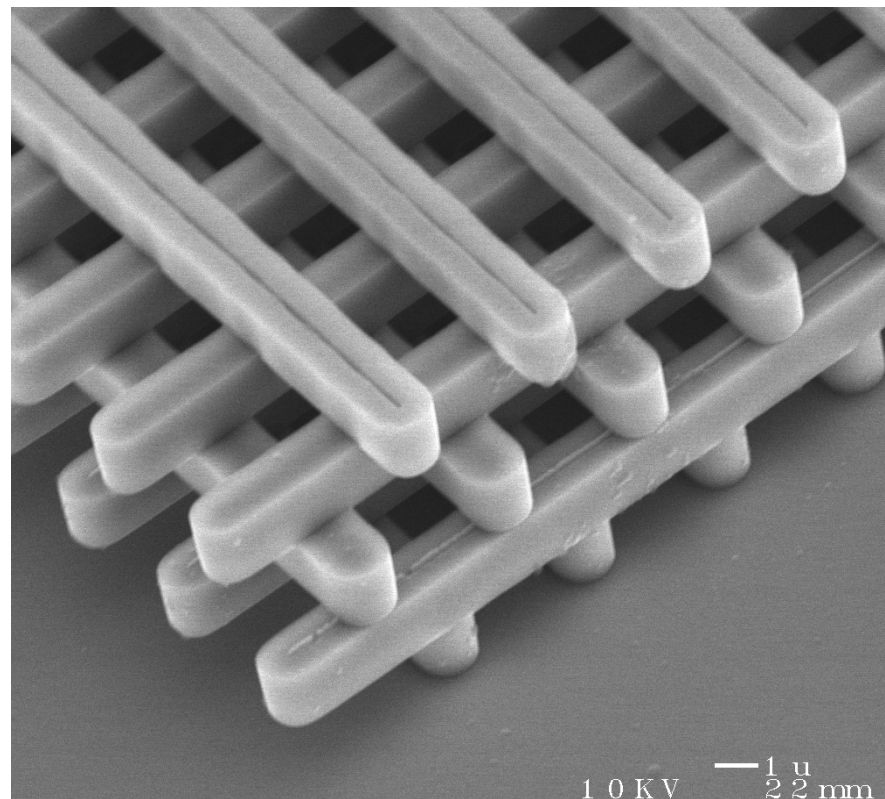
- Nanophotonics/Nanoelectronics
- Complex Functional Nanomaterials



# Fabricated Electronic and Photonic Architectures



Correlated states in coupled Q-wires



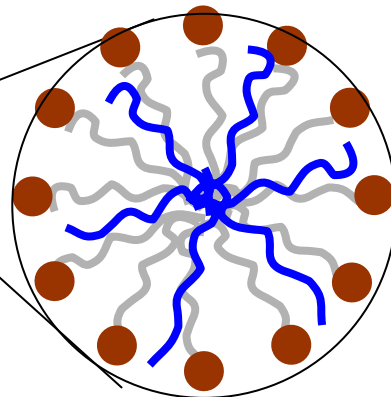
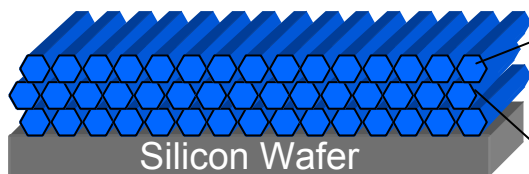
Tunable photon states in photonic structures

- Nanophotonics/Nanoelectronics
- Nanomechanics
- Theory and Simulation

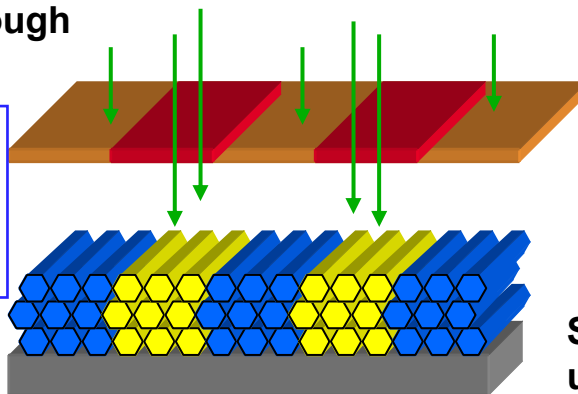


# Thin-Film Self-Assembly of Nanostructured and Composite Materials

Self assembly of photosensitive silica/surfactant mesophase containing a photoacid generator (PAG)



Selective UV exposure through mask



incorporation of the PAG in the micelle

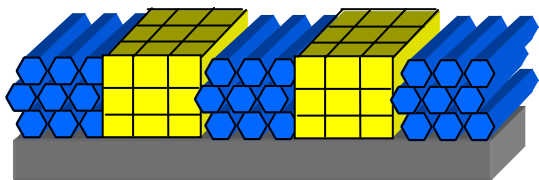
Selective etching of unexposed mesostructure

Compartmentalized production of acid

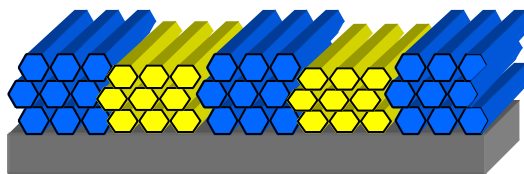
- Nano-bio-micro Interfaces
- Complex Functional Nanomaterials
- Theory and Simulation

(Doshi et al., Science, 2000)

Heat treatment  
 $T > 125\text{ }^{\circ}\text{C}$

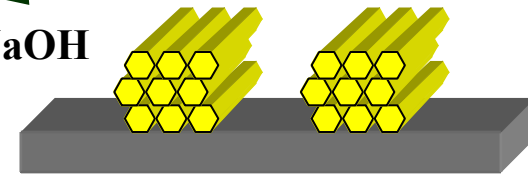


**Nanostructural Lithography**



NaOH

**Patterned Thin Film Mesophase**



J. Brinker, D. Doshi

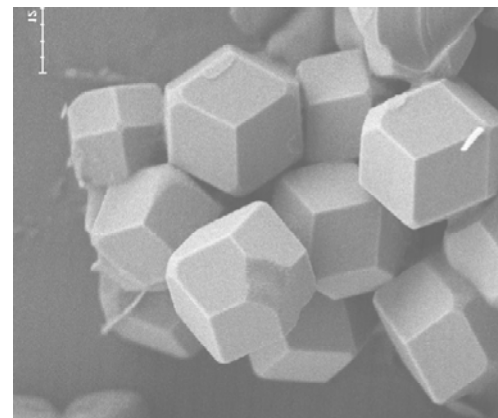
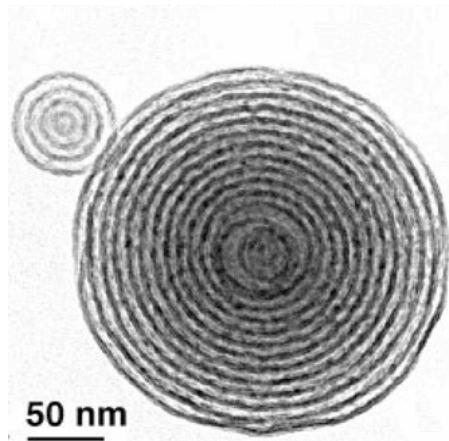
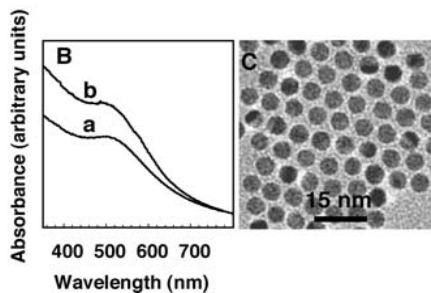
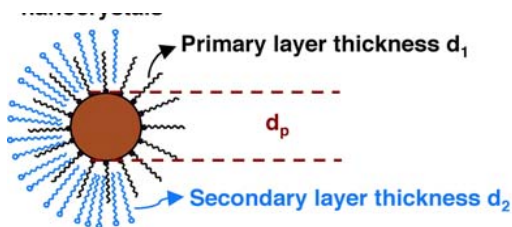


# Processing Methods for Nanomaterials

Race to develop new materials/applications - What will be the bottom line in a few years?

- Scalability?
- Reliability?
- Quality control?
- Functionality?

- Complex Functional Nanomaterials
- Nanomechanics
- Theory and Simulation



**Challenge: Science-based, predictive, robust, scalable processing of nanomaterials**

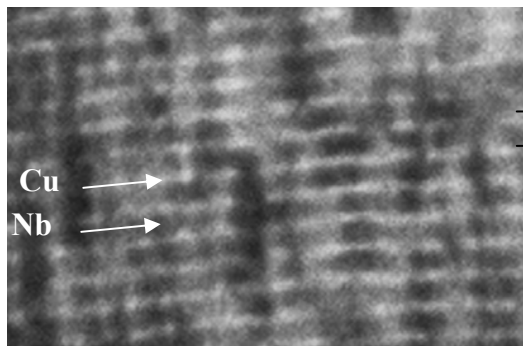
J. Liu, J. Voigt, T. Boyle, J. Brinker



# Mechanical Behavior of Nanomaterials and Nanostructures

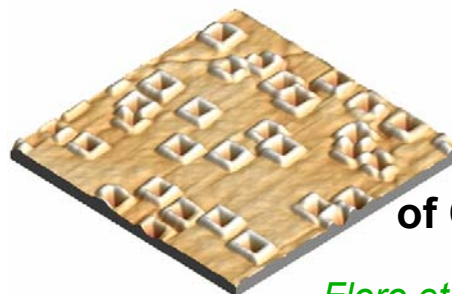
- Mechanical properties of nanostructured materials

- Complex Functional Nanomaterials
- Nanomechanics
- Theory and Simulation



Nanostructures  
Providing  
Extreme  
Strengths

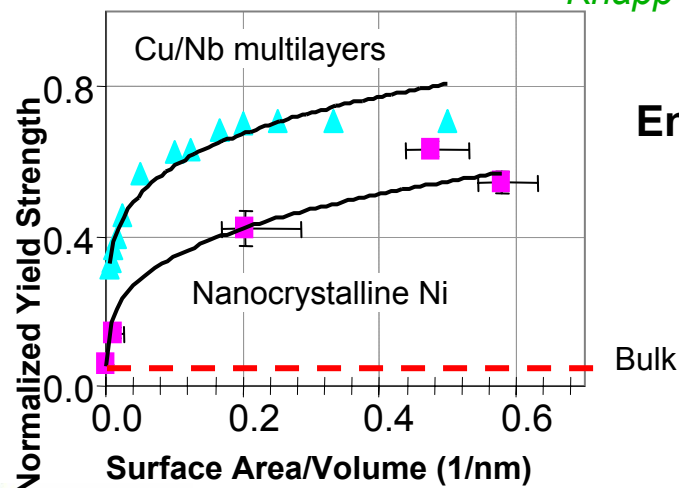
*Misra et al., LANL*  
*Knapp et al., SNL*



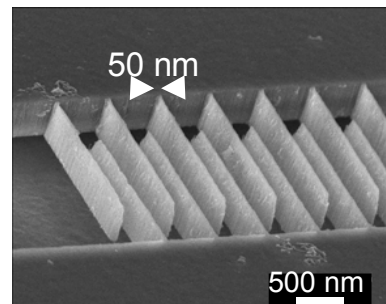
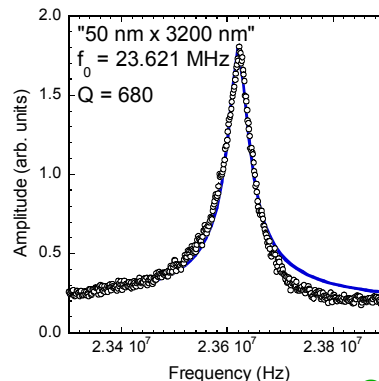
Properties  
of Nanostructures

Strain-layer Self-assembly  
of Quantum Dot Molecules

*Floro et al., SNL*



## Energy Dissipation in Nanomechanical Oscillators

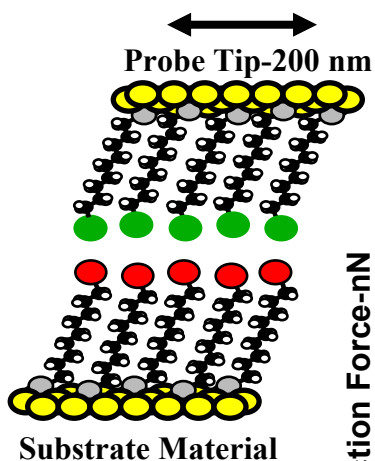


*Sullivan et al., SNL*

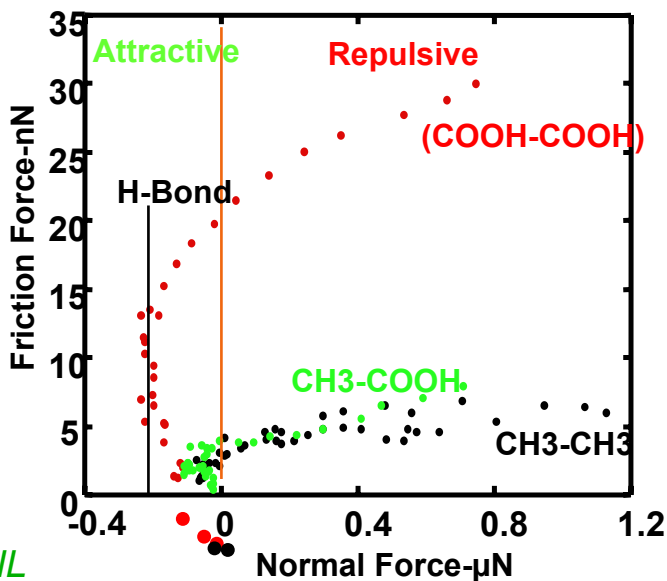


# Surface & Interface Properties, New Techniques and Modeling

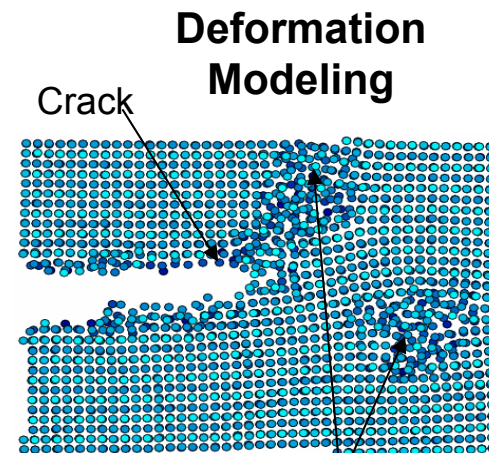
- Mechanical properties derived from surface and interface effects
- Techniques for in-situ mechanical measurement and modeling



Molecular Level Adhesion and Friction



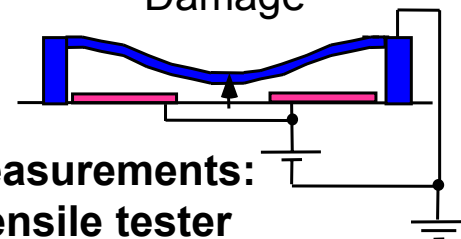
Houston et al., SNL



Deformation Modeling

Swadener et al., LANL

Radiation Damage



In-situ Measurements: MEMS tensile tester

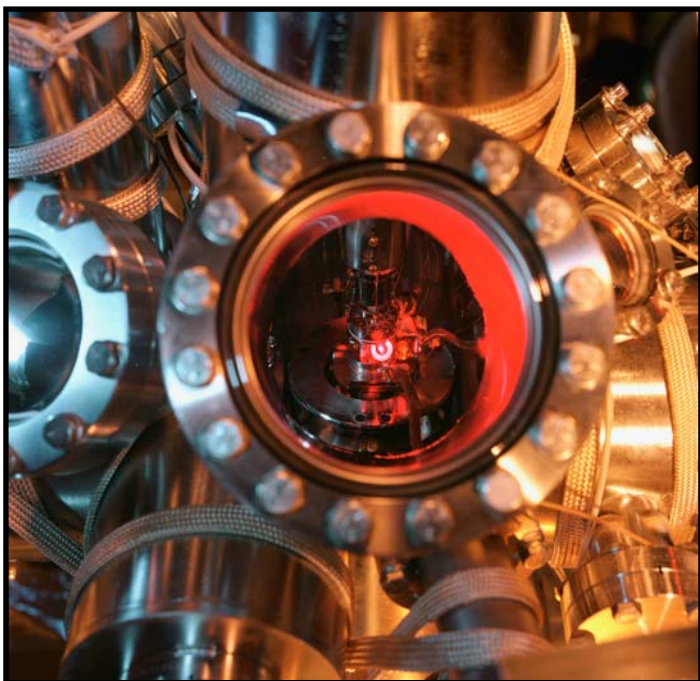
Hearne, de Boer, et al., SNL

- Nano-bio-micro Interfaces
- Complex Functional Nanomaterials
- Nanomechanics
- Theory and Simulation



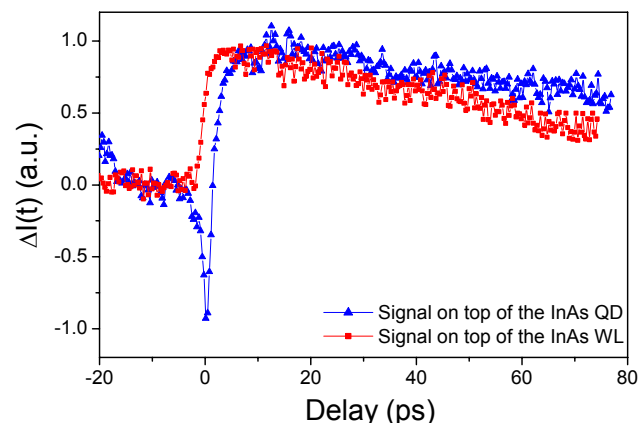
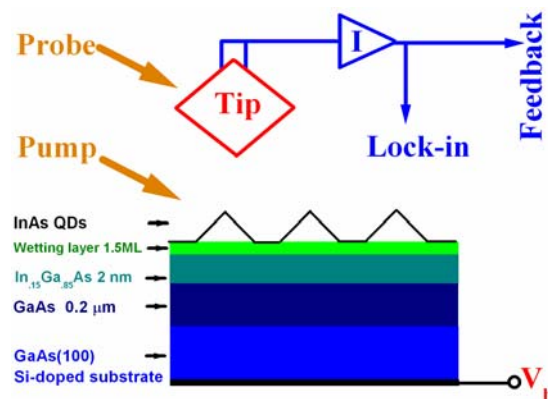
# Capability Development: Ultrafast STM

Spatial and temporal atomic-scale imaging of real space processes and excitations with 20 nm/2 ps resolution.



- Complex Functional Nanomaterials
- Theory and Simulation

## Relaxation dynamics in InAs/GaAs SAQDs



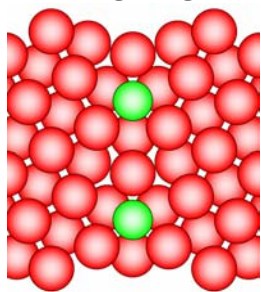
**Ultrafast STM signal from InGaAs SAQD: permits investigation of single quantum dot photoconductivity**



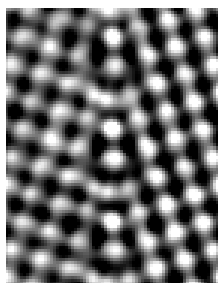


# Atomistic and Mesoscopic Approaches for Theory and Simulation

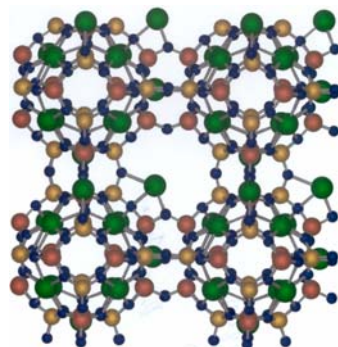
Impurity Segregation at GB



Calculated

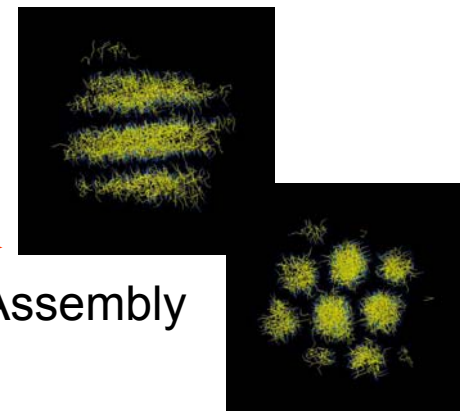


Exp: HRTEM

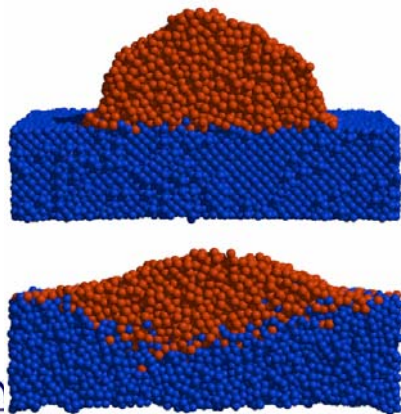


Quantum & Atomistic

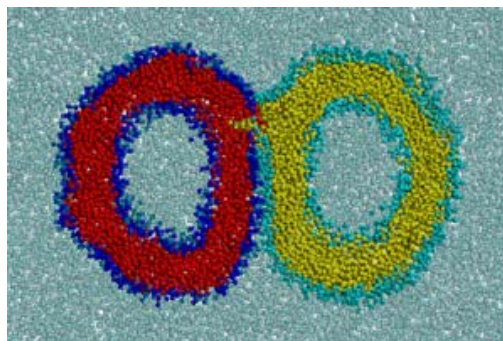
Self Assembly



Nanodroplet at Different Temperatures

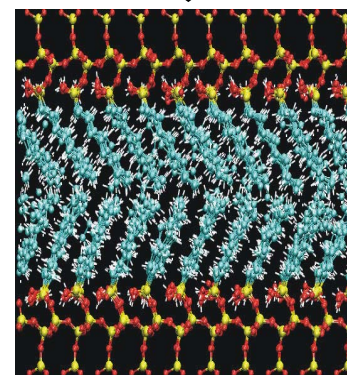
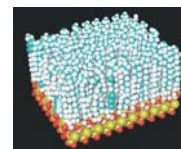


Membrane Fusion



Fusing liposomes

Reliability of MEMS Coating



Si surface

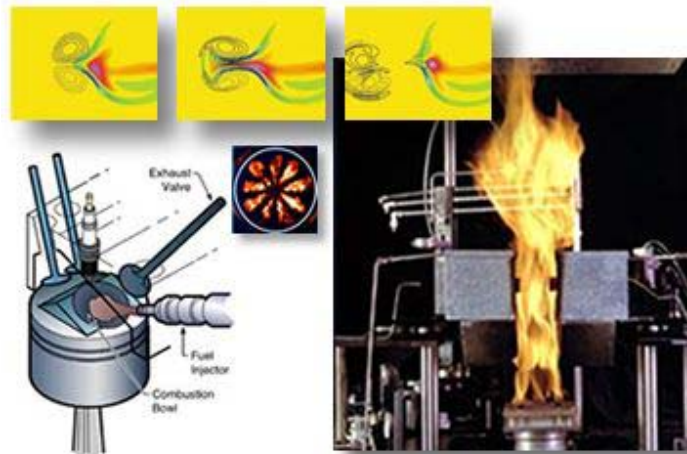
OTS coating



# CINT Connections to National User Facilities



Los Alamos Neutron Science Center  
(<http://lansce.lanl.gov/>)



Combustion Research Facility  
(<http://www.ca.sandia.gov/CRF/>)



National High Magnetic Field Laboratory  
(<http://www.lanl.gov/mst/nhmfl/>)

Additional connections  
to national laboratory  
facilities through  
gateway operations



# *User Workshop Poster Session*

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- **Thirty posters representing ongoing science and thrust area capabilities**
- **Posters representing national user facilities, library resources and overall CINT program**
- **Opportunity to discuss science and develop connections with laboratory scientists (poster presenters and others)**