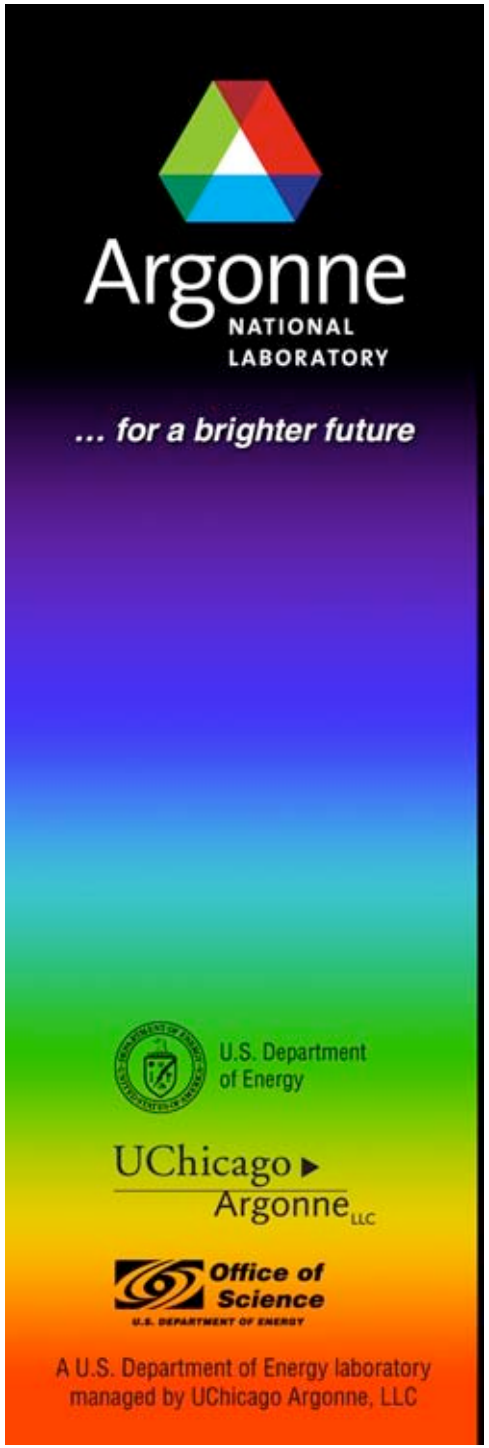
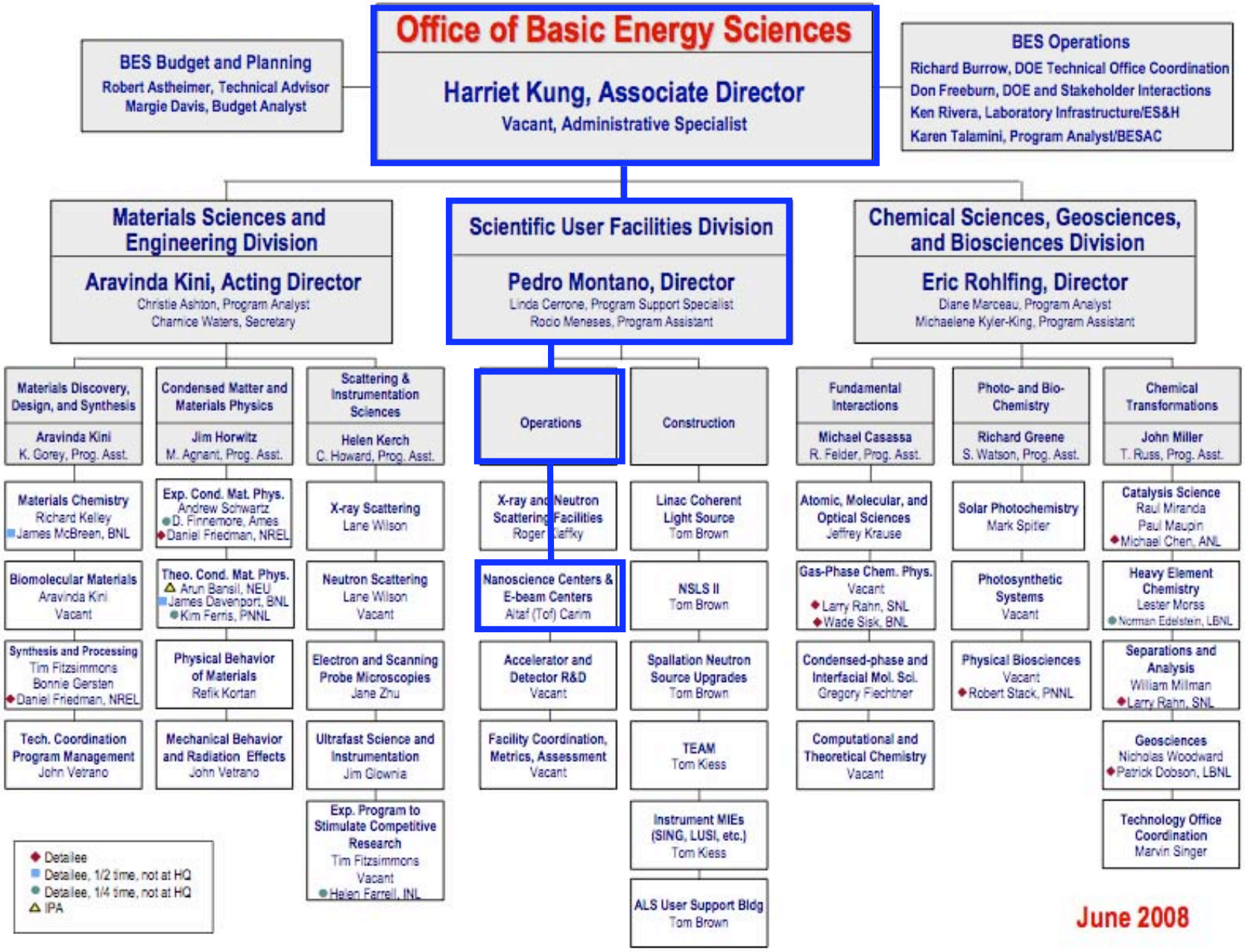


DOE Nanoscale Science Research Centers (NSRCs): User Facilities for the Broad Scientific Community

Dr. Kathleen Carrado Gregar
Manager, User & Outreach Programs
Center for Nanoscale Materials
Argonne National Laboratory

DOE EPSCoR Meeting, Oak Ridge, TN, July 22-24, 2008

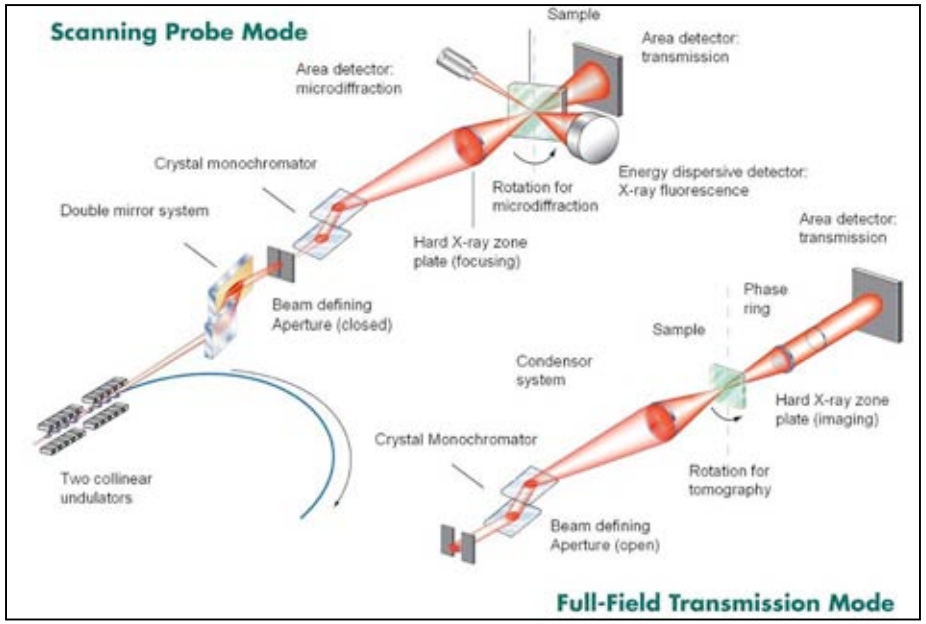

Office of Basic Energy Sciences
Harriet Kung, Associate Director
Vacant, Administrative Specialist
BES Budget and Planning
Robert Astheimer, Technical Advisor
Margie Davis, Budget Analyst
BES Operations
Richard Burrow, DOE Technical Office Coordination
Don Freeburn, DOE and Stakeholder Interactions
Ken Rivera, Laboratory Infrastructure/ES&H
Karen Talamini, Program Analyst/BESAC
Materials Sciences and Engineering Division
Aravinda Kini, Acting Director
Christie Ashton, Program Analyst
Charnice Waters, Secretary
Scientific User Facilities Division
Pedro Montano, Director
Linda Cerrone, Program Support Specialist
Rocio Meneses, Program Assistant
Chemical Sciences, Geosciences, and Biosciences Division
Eric Rohlfing, Director
Diane Marceau, Program Analyst
Michaelene Kyler-King, Program Assistant
Materials Discovery, Design, and Synthesis
Aravinda Kini
K. Gorey, Prog. Asst.
Materials Chemistry
Richard Kelley
James McBreen, BNL
Biomolecular Materials
Aravinda Kini
Vacant
Synthesis and Processing
Tim Fitzsimmons
Bonnie Gersten
Daniel Friedman, NREL
Tech. Coordination Program Management
John Vetrano
Condensed Matter and Materials Physics
Jim Horwitz
M. Agnant, Prog. Asst.
Exp. Cond. Mat. Phys.
Andrew Schwartz
D. Finnemore, Ames
Daniel Friedman, NREL
Theo. Cond. Mat. Phys.
Arun Bansil, NEU
James Davenport, BNL
Kim Ferris, PNNL
Physical Behavior of Materials
Refik Kortan
Mechanical Behavior and Radiation Effects
John Vetrano
Scattering & Instrumentation Sciences
Helen Kerch
C. Howard, Prog. Asst.
X-ray Scattering
Lane Wilson
Neutron Scattering
Lane Wilson
Vacant
Electron and Scanning Probe Microscopies
Jane Zhu
Ultrafast Science and Instrumentation
Jim Glownia
Exp. Program to Stimulate Competitive Research
Tim Fitzsimmons
Vacant
Helen Farrell, INL
Operations
X-ray and Neutron Scattering Facilities
Roger Kaffky
Nanoscience Centers & E-beam Centers
Altaf (Tof) Carim
Accelerator and Detector R&D
Vacant
Facility Coordination, Metrics, Assessment
Vacant
Construction
Linac Coherent Light Source
Tom Brown
NSLS II
Tom Brown
Spallation Neutron Source Upgrades
Tom Brown
TEAM
Tom Kiess
Instrument MIEs (SING, LUSI, etc.)
Tom Kiess
ALS User Support Bldg
Tom Brown
Fundamental Interactions
Michael Casassa
R. Felder, Prog. Asst.
Atomic, Molecular, and Optical Sciences
Jeffrey Krause
Gas-Phase Chem. Phys.
Vacant
Larry Rahn, SNL
Wade Sisk, BNL
Condensed-phase and Interfacial Mol. Sci.
Gregory Fiechtner
Computational and Theoretical Chemistry
Vacant
Photo- and Bio-Chemistry
Richard Greene
S. Watson, Prog. Asst.
Solar Photochemistry
Mark Spitler
Photosynthetic Systems
Vacant
Physical Biosciences
Vacant
Robert Stack, PNNL
Chemical Transformations
John Miller
T. Russ, Prog. Asst.
Catalysis Science
Raul Miranda
Paul Maupin
Michael Chen, ANL
Heavy Element Chemistry
Lester Morss
Norman Edelstein, LBNL
Separations and Analysis
William Millman
Larry Rahn, SNL
Geosciences
Nicholas Woodward
Patrick Dobson, LBNL
Technology Office Coordination
Marvin Singer
Detailee
Detailee, 1/2 time, not at HQ
Detailee, 1/4 time, not at HQ
IPA
June 2008


Center for Nanoscale Materials
Argonne National Laboratory
Molecular Foundry
Lawrence Berkeley National Laboratory
Center for Functional Nanomaterials
Brookhaven National Laboratory
Center for Nanophase Materials Sciences
Oak Ridge National Laboratory
Center for Integrated Nanotechnologies
Los Alamos National Laboratory &
Sandia National Laboratory

NRSC's – New DOE User Facilities

- Opened 2006 - 2008
- Operate as user facilities
  - available to all researchers
  - access determined by external peer review of proposals
  - no cost for research published in the open literature; proprietary access - full cost recovery
  - provide specialized equipment and scientific expertise
- Similar staffing and budgets
- Co-located with existing DOE user facilities (synchrotrons, neutron scattering facilities, etc.)
- Multidisciplinary – materials science, chemistry, physics, computational, biology, engineering,….
- Provide extraordinary characterization and analysis capabilities
- "Nano" environment, safety, and health concerns are a priority

NSRCs provide new kinds of capabilities

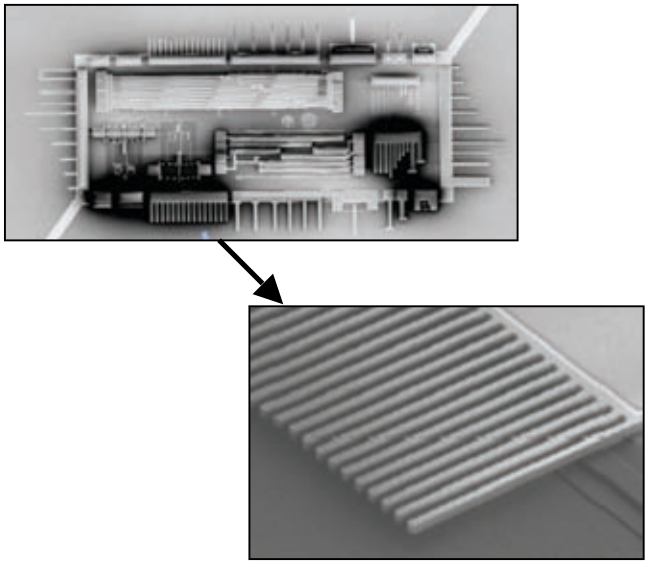


X-Ray Synchrotron Beamlines with Nanoscale Resolution (CNM)

- *Unique instruments to study individual nanostructures*
- *Quantitative structure, strain, orientation imaging*
- *Sensitive trace element and chemical state analysis*

"Discovery Platforms": modular micro-laboratories for nanoscience (CINT)

- *Standardized and batch fabricated*
- *Access to a range of diagnostic and characterization tools*



Cantilever Array (mechanics at nanoscale)

Scientific Capabilities of the NSRCs (2008)

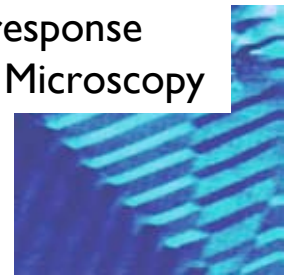
- **CNMS (ORNL)**
  - Nanomaterials theory institute
  - Bio-inspired nanomaterials
  - Macro-molecular nanomaterials
  - Scanning probes & nanoscale physics
  - Nanofabrication
  - Catalytic nanosystems
  - Functional hybrid nanostructures
  - Electron microscopy, neutron & x-ray scattering
- **Foundry (LBNL)**
  - Theory of nanostructured materials
  - Biological nanostructures
  - Organic & mac-romolecular synthesis
  - Imaging and manipulation of nanostructures
  - Nanofabrication
  - Inorganic nanostructures
- **CINT (SNL/LANL)**
  - Theory & simulation
  - Soft, Biological & Composite Nanomaterials
  - Nanophotonics & optical nanomaterials
  - Nanoelectronics & mechanics
- **CNM (ANL)**
  - Theory & modeling
  - Nanobio interfaces
  - Electronic & magnetic materials & devices
  - X-ray microscopy
  - Nanofabrication
  - Nanophotonics
- **CFN (BNL)**
  - Theory & computation
  - Soft & biological nanomaterials
  - Electronic nanomaterials
  - Interface science & catalysis
  - Electron microscopy

http://www.sc.doe.gov/bes/BESfacilities.htm

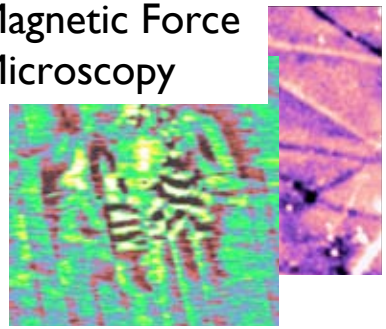
Proximal Probes: SPM, STM, NSOM, etc.

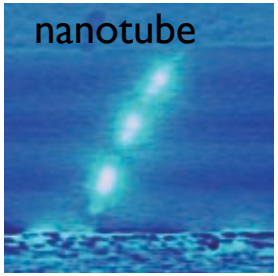
Advanced SPM: imaging, conductivity, ferromagnetism, ferroelectricity, catalysis

Piezoresponse Force Microscopy

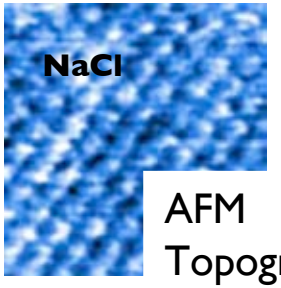


Magnetic Force Microscopy

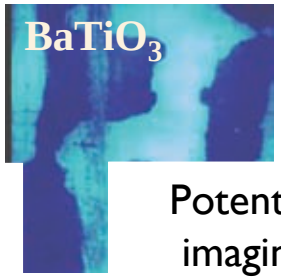




Transport



AFM Topography



Potential imaging

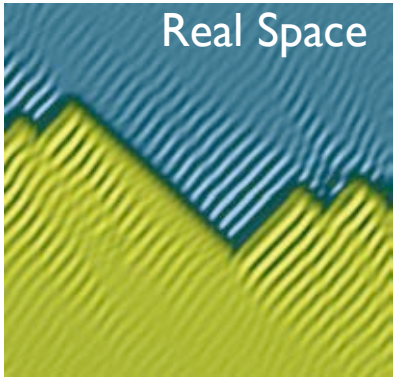
Low Temperature-High Field STM

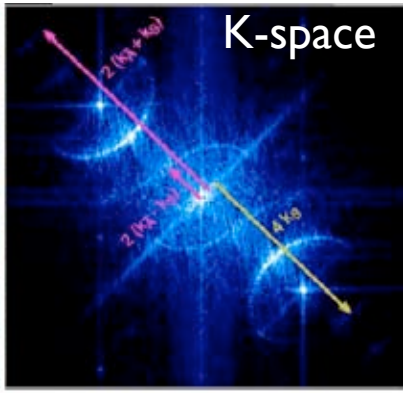
Scientific Drivers

- atomically-resolved topography and spectroscopy maps
- quantum response at low T and high B
- real Space – K-space
- single molecule spectroscopy

Capabilities

- low T - 300 mK
- rotates in magnetic field
- optical access to sample
- high resolution
- cryogenic UHV cleaving
- sample fabrication in UHV

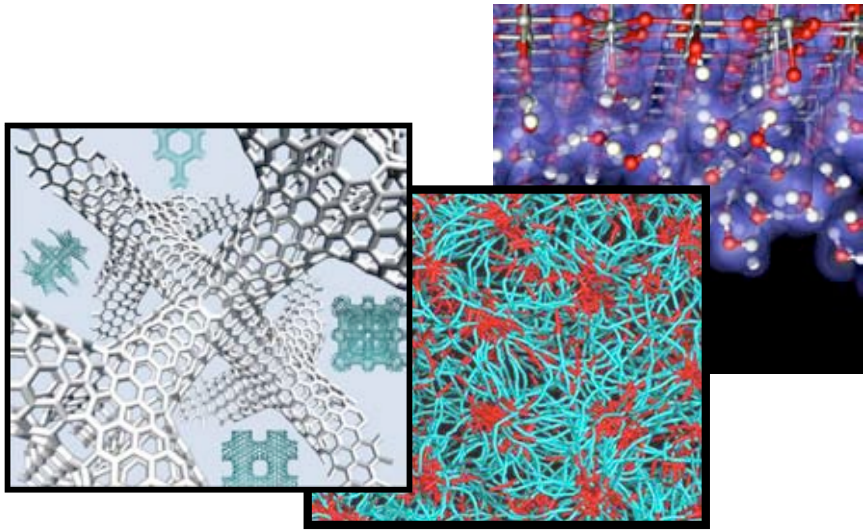




Computation and Visualization

- NSRC Cluster examples
  - 10 Tflop (CNM)
  - 5 Tflop (CNMS)

- Access to CNMS 250 Tflop Leadership Class Computer



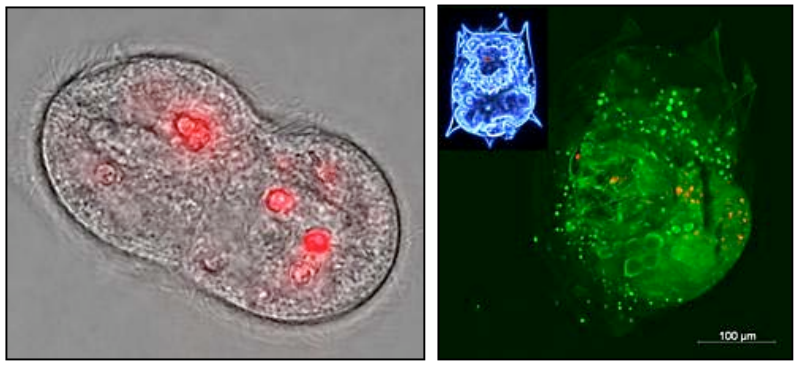
Challenges: Environment, Health, and Safety

- Research needs for risk analysis and mitigation
- Occupational health and safety
- Consumer health and safety
- DOE & 5 NSRC's hosted:

  "Safe Handling of Engineered Nanoscale Materials",

  July 7-9, 2008 at Argonne

  http://nano.anl.gov/events



User Agreements and Intellectual property

- User agreements available for:
  - Non-proprietary, essentially non-collaborative work
  - Proprietary, non-collaborative work (full cost recovery)
  - "Precompetitive", non-proprietary, collaborative work
- Case-by-case basis for proprietary, collaborative work (CRADAs, WFO, etc.)
- DOE is currently evaluating User Agreements for uniformity across all Labs

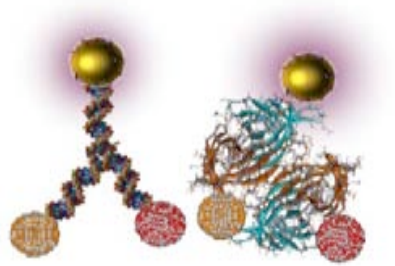
Center for Nanoscale Materials at Argonne National Laboratory

http://nano.anl.gov

cnm_useroffice@anl.gov

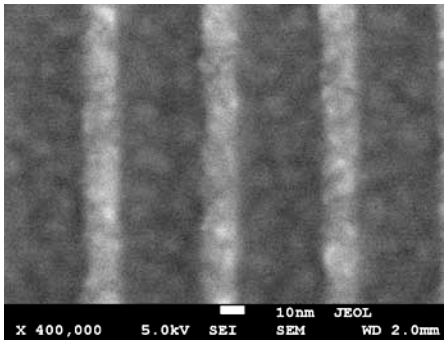
CNM: Six Integrated Scientific Themes

NanoBio Interfaces



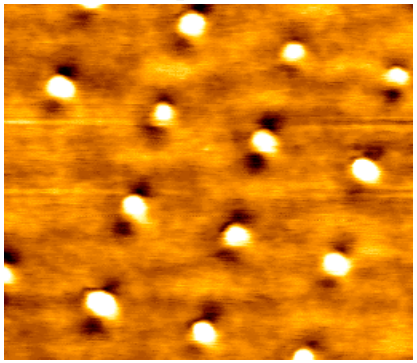
Create bio-inspired materials and processes for energy transduction

Nanofabrication



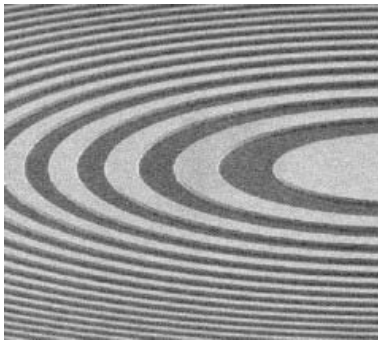
Discover new paths for nanostructured materials, including below 10 nm

Nanophotonics



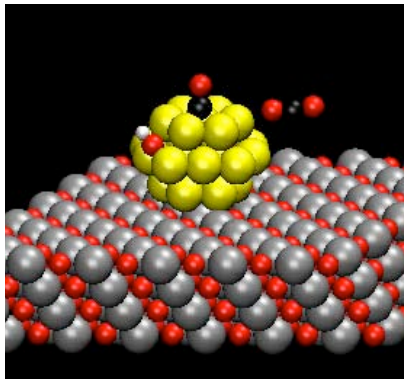
Understand and control optical energy pathways

X-ray Microscopy



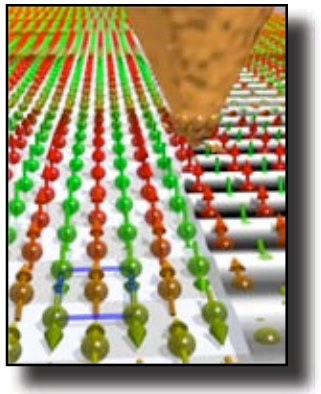
Create images of the nanoworld with hard x-rays

Theory & Modeling



Towards the 'virtual fab lab'

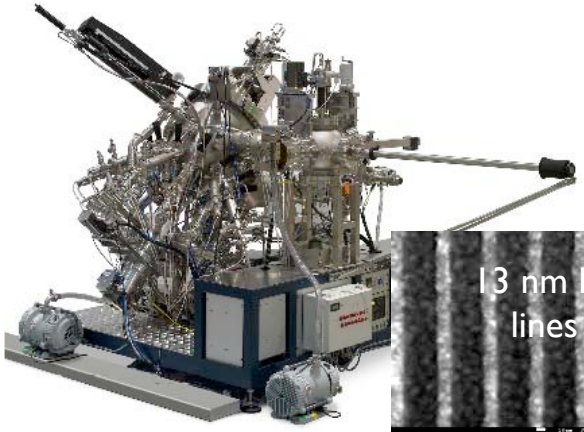
Electronic & Magnetic Materials & Devices

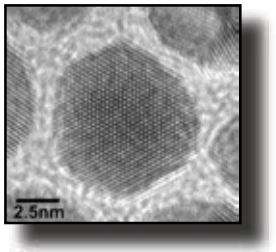


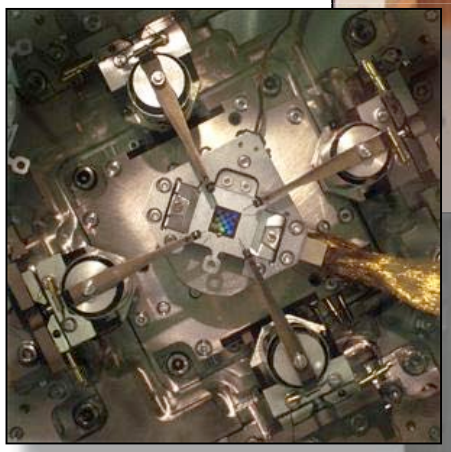
Understand and control charge and spin-based materials for energy and information transport

CNM: Enabling Science Through Technical Capabilities

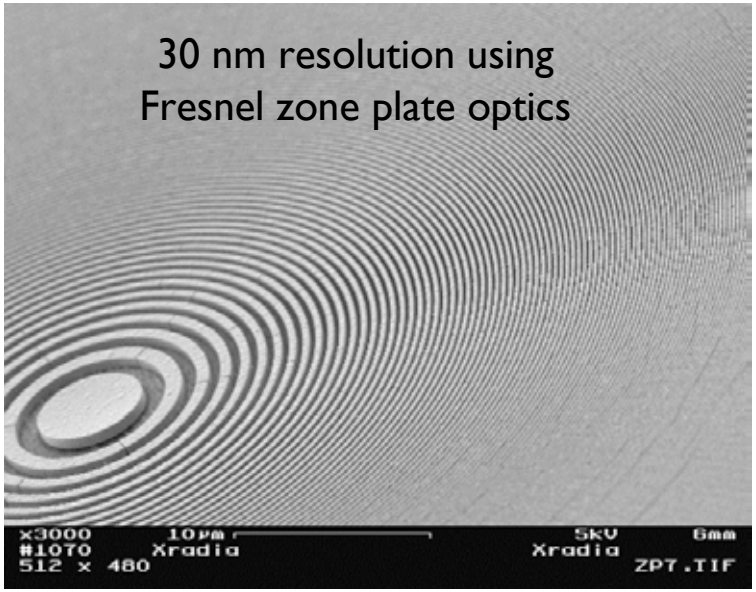
- **Materials Synthesis**
  - Polymeric templating
  - Colloidal nanoparticle synthesis
  - Peptide/DNA synthesis methods
  - Complex oxide molecular beam epitaxy
  - PECVD nanocrystalline diamond
  - Thin films by sputtering and evapoaration
- **Nanofabrication Research**
  - Electron-beam lithography (JEOL 9300, Raith)
  - Focused ion beam processing (FEI Nova)
  - Nanoimprint patterning methods (Nanonex)
  - Optical lithography
- **Characterization**
  - Proximal Probes: AFM, NSOM, UHV VT-STM/AFM
  - SEM, FESEM, STM/SEM
  - Magnetometry and electrical characterization
  - Optical microscopy and spectroscopy
  - Thermal analysis, Diffractometry
- **Computational Nanoscience**
  - 1152 node cluster with compute capacity of 10 Tflops, ~11M CPU hr/yr
- **Hard X-Ray Nanoprobe Beamline at APS**



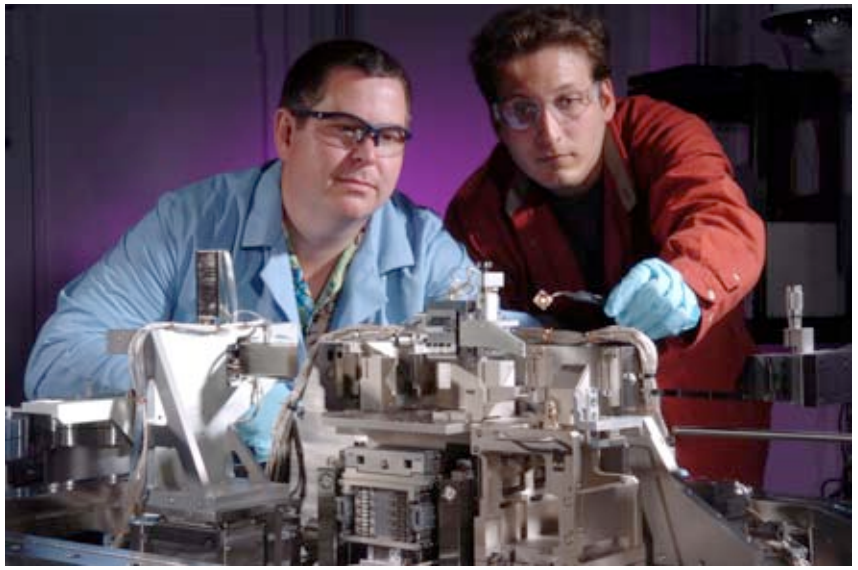




CNM Nanoprobe at the Advanced Photon Source

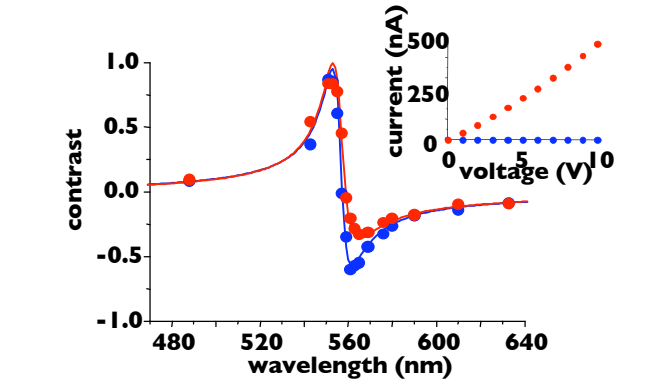


- X-ray optics
- Nano-diffraction
- Transmision imaging
- Fluorescence microscopy
- Dynamics



CNM Scientific Highlights

User: Optical probe of graphene sheets



Jung, et al, *Nano Letters*, **7**, 3569 (2007)

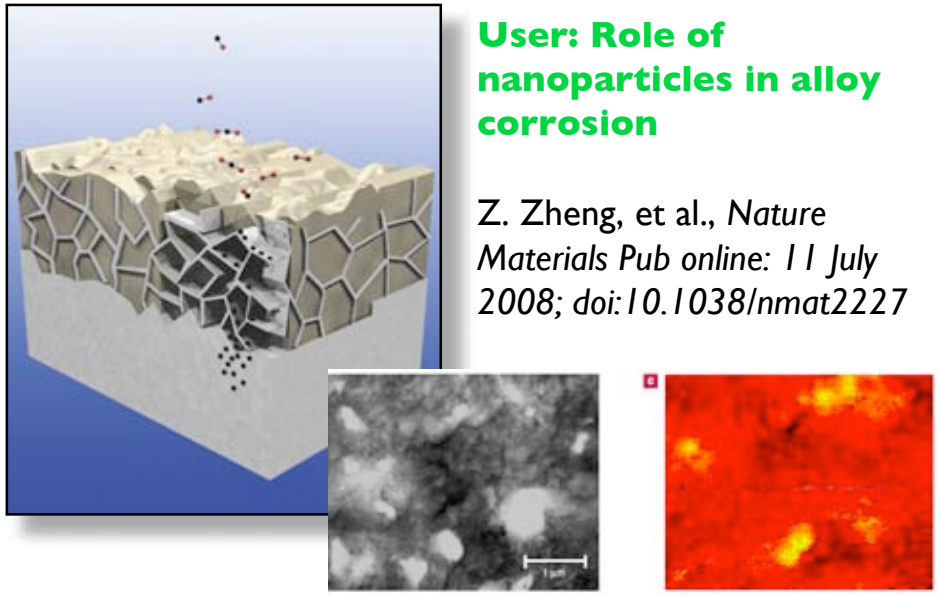
Staff: Ordering in polymer systems

Ramanathan & Darling
Wired Magazine 4•25•08
http://www.wired.com/science/discoveries/multimedia/2008/04/gallery_nano_art

Staff: Novel metal nanoplates for energy conversion

Y. Sun & Wiederrecht, *Small* ***3***, *1964 (2007)*

200 nm Ag(0) on GaAs



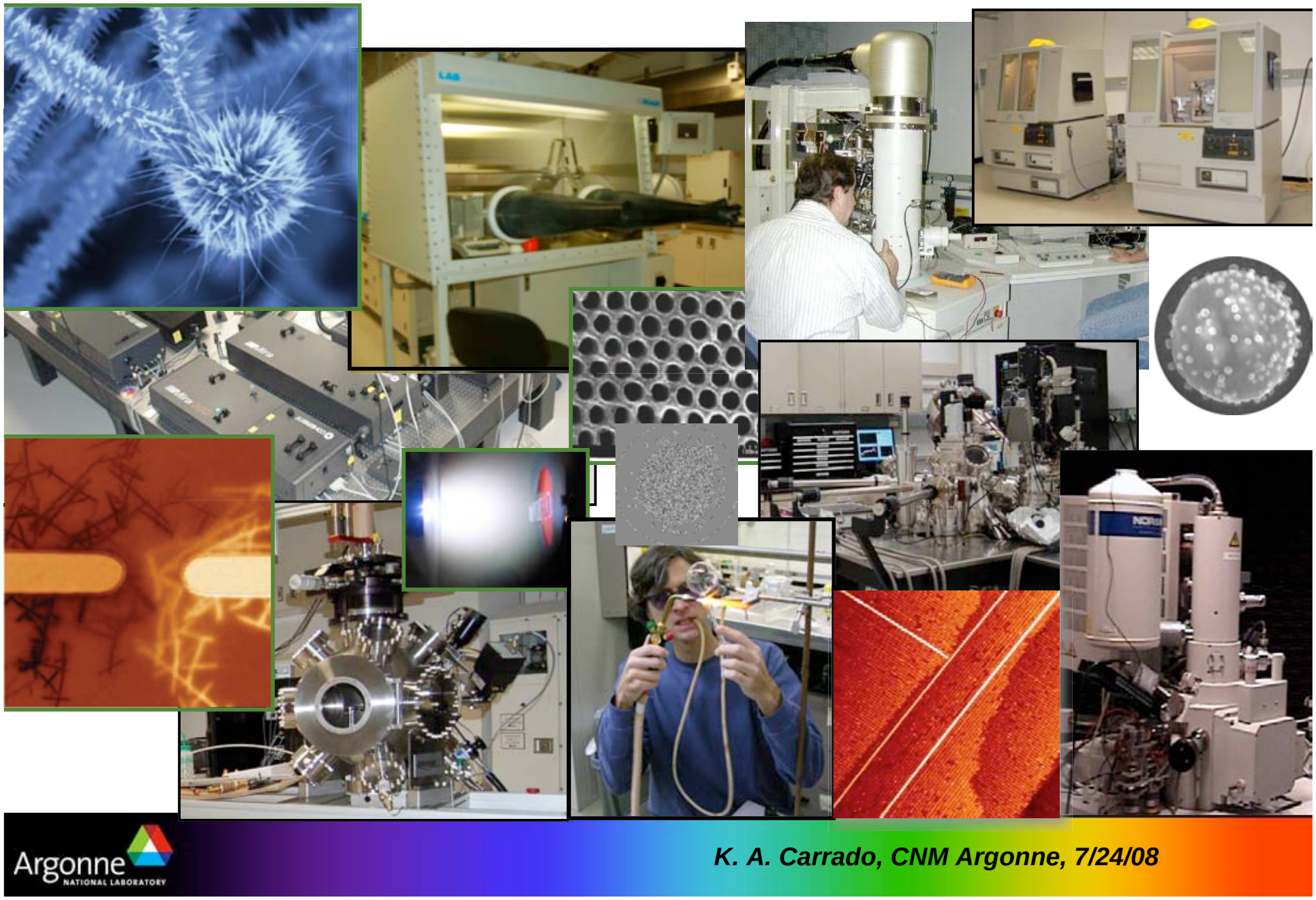
User: Role of nanoparticles in alloy corrosion

Z. Zheng, et al., *Nature Materials Pub online: 11 July 2008; doi:10.1038/nmat2227*

CNMS: Center for Nanophase Materials Sciences
Oak Ridge National Laboratory

facilitates links with
Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFER)
for neutron studies of nanomaterials
www.cnms.ornl.gov

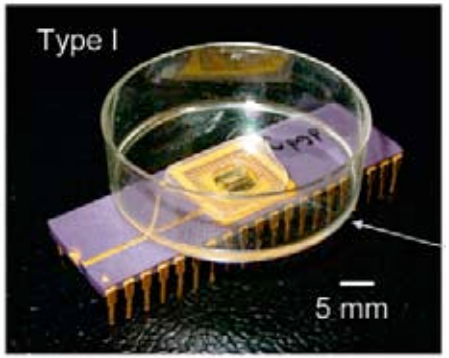
CNMS: Key Synthesis & Characterization Capabilities

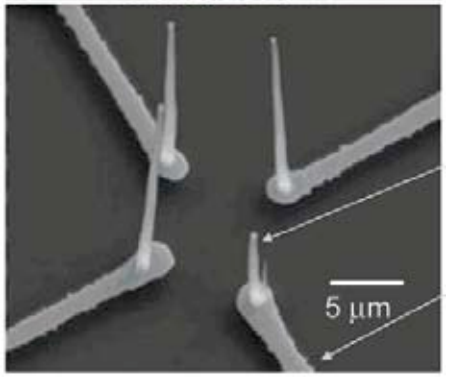


CNMS Nanofabrication Research

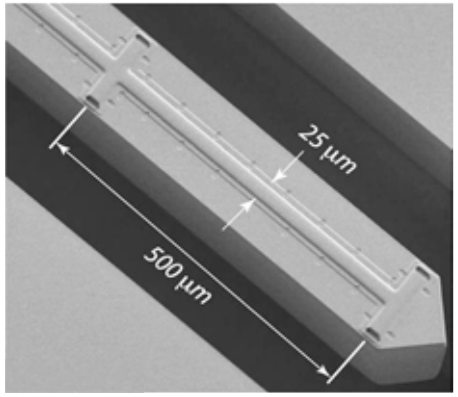
Thin Film Deposition and Characterization
- **Chemical and physical vapor deposition**
- **High temperature growth and annealing**
- **SEM, SPM and optical visualization**

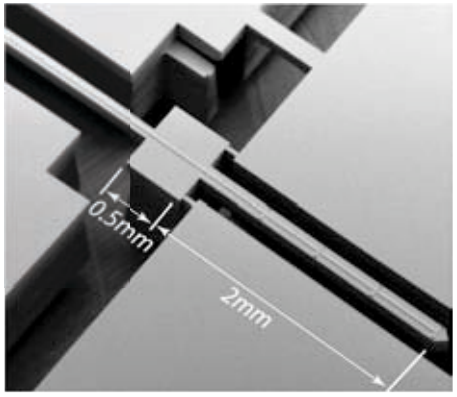
- **Multiscale Lithography**
  - **Optical and electron beam lithography**
- **Material Removal**
  - **Dry etching and ablation**
  - **Wet chemical etching**

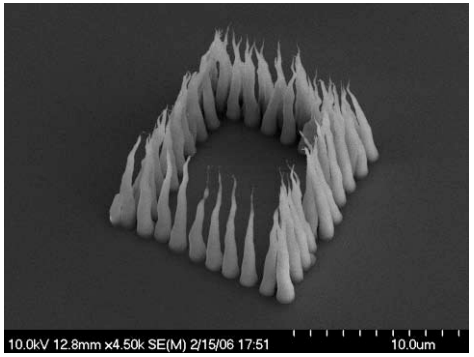




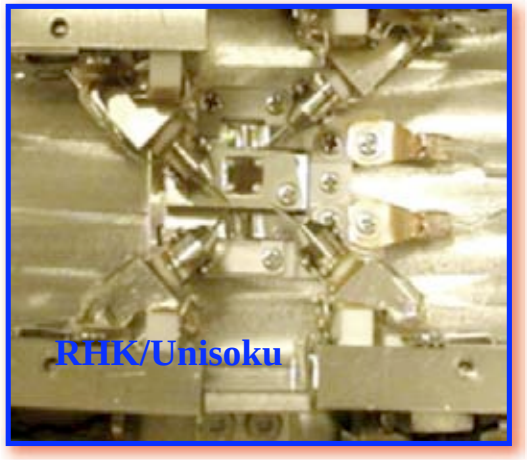
McKnight et al.
CNMS2003-042





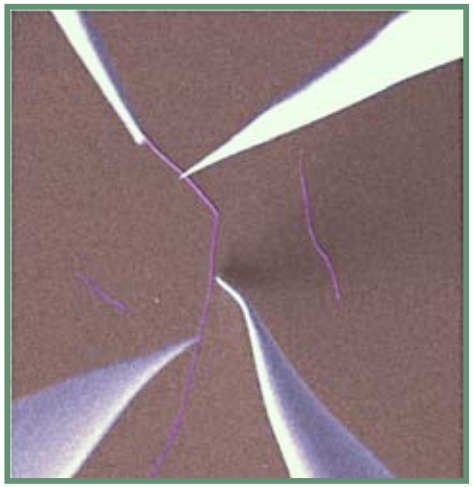


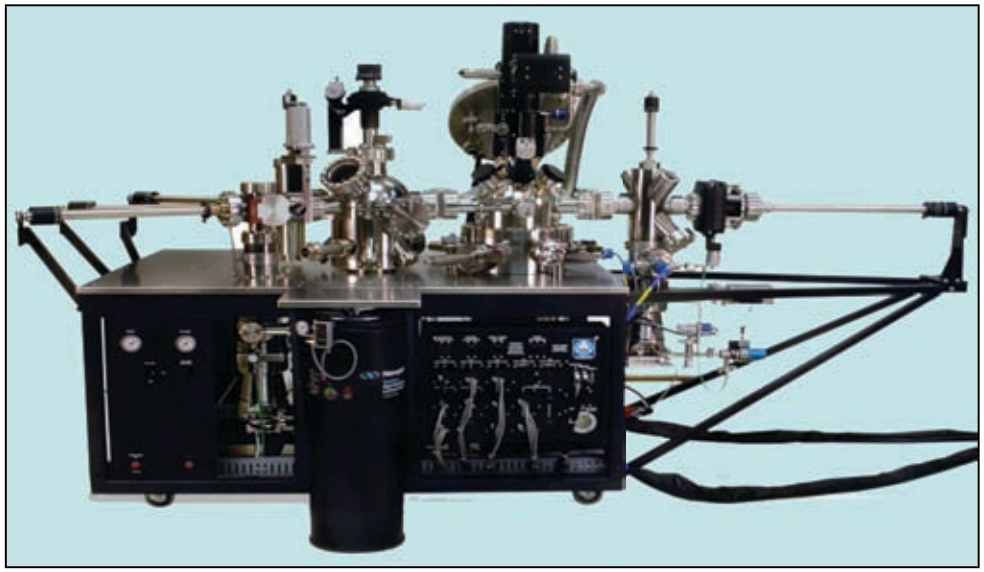
CNMS: 4 probe Scanning Tunneling Microscope with SEM/SAM



Scientific Drivers

- Nanoscale electrical transport as a function of temperature
- Nanofabrication and manipulation
- Elemental identification





Capabilities

Four probe STM
- independent operation
- in situ amplifiers for transport
- 10-300 K

Scanning Electron Microscopy
- 7 nm resolution
- accurate positioning of four tips
- electron beam induced current

Scanning Auger Microscopy

Sample preparation
- MBE growth - sputtering, cleaving

CNMS: Where high-resolution experiment and large scale calculations meet… …and succeed

PHYSICAL REVIEW LETTERS

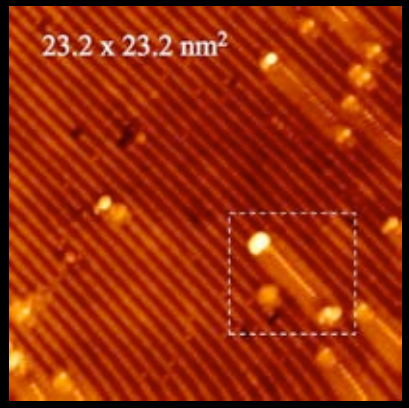
Surface Reconstructions of TiO_2(110) Driven by Suboxides

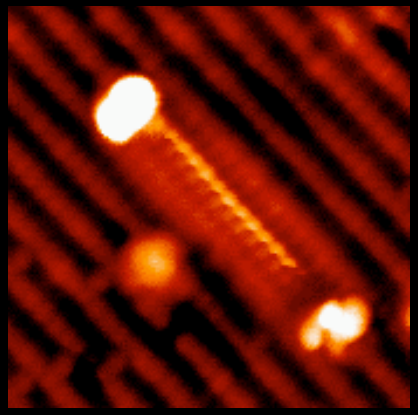
K. T. Park,[1,2] M. H. Pan,[3,4] V. Meunier,[5,3] and E. W. Plummer[2,4,3]

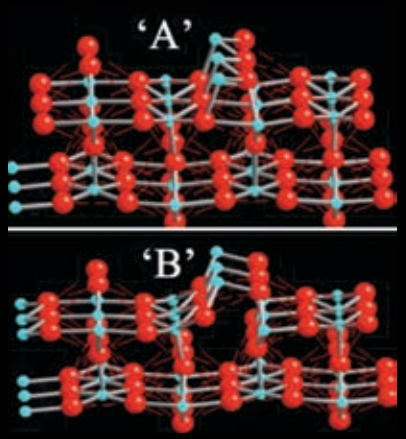
(Received 9 March 2006)

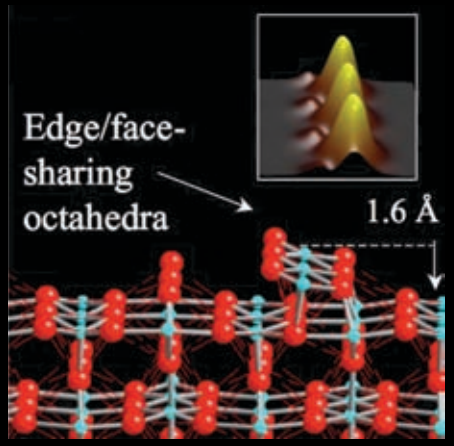
Scanning tunneling microscopy and density functional theory are used to develop a new structural model for surface reconstructions driven by Ti interstitials on TiO_2(110). Ti interstitials form the edge- or face-sharing octahedra that serve as building blocks for (1 × 1) reconstruction. Thus, contrary to conventional wisdom, the 1 × 1 periodicity is insufficient to establish the correct surface stoichiometry. Furthermore, in our structural and compositional model the reversible oxidation or reduction between (1 × 1) and (1 × 2) is entirely achieved by transfer of the added rows.

High resolution Experiment…









… and first principles theory

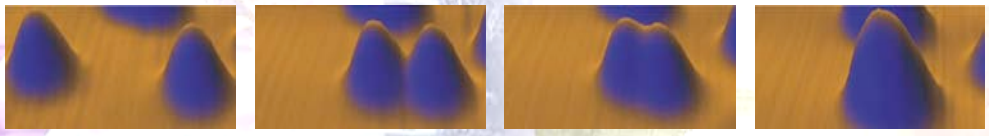
In close collaboration with Minghu Pan

Molecular FOUNDRY
A NANOSTRUCTURES USER LABORATORY

THE MOLECULAR FOUNDRY

A DOE User Facility
for Nanoscale Science Research
at Lawrence Berkeley National Lab

Jim De Yoreo, Deputy Director for Research

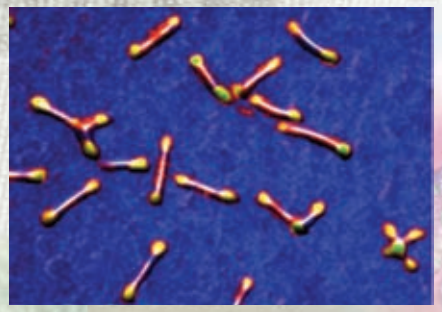


Office of Science

The Molecular Foundry is at LBNL above UC Berkeley Campus

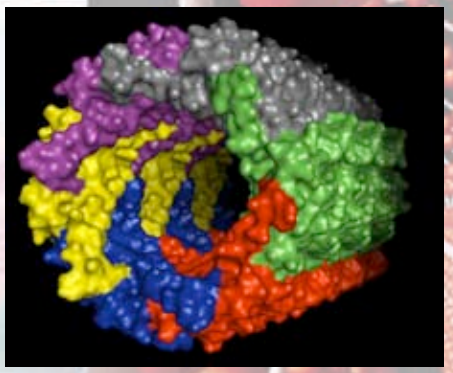
Molecular Foundry - six facilities, one team

Inorganic Nanostructures



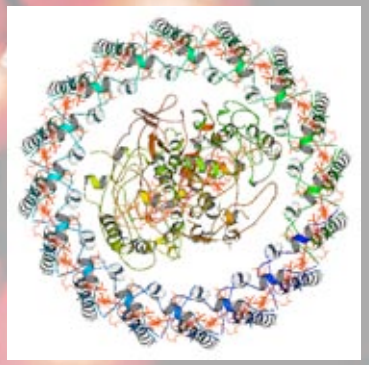
A. Paul Alivisatos

Biological Nanostructures



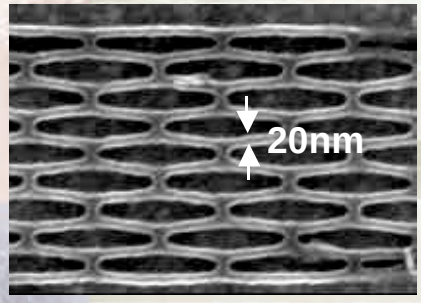
Carolyn Bertozzi

Organic and Macro-molecular Synthesis



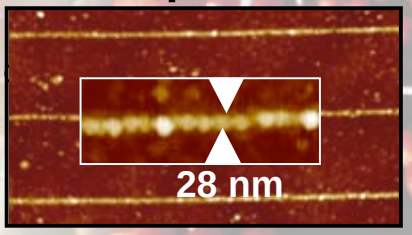
Jean Fréchet

Nanofabrication



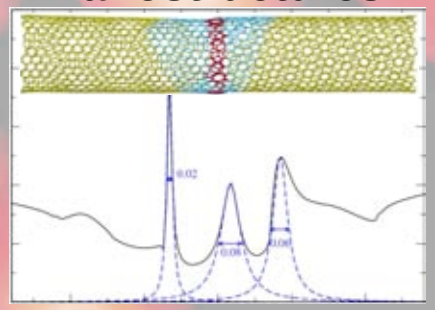
Jeffrey Bokor

Imaging and Manipulation



Miquel Salmeron

Theory of Nanostructures

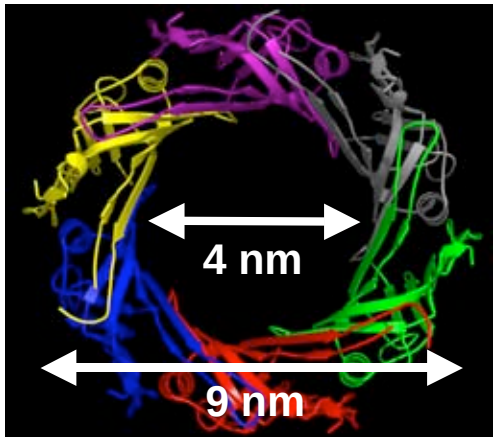


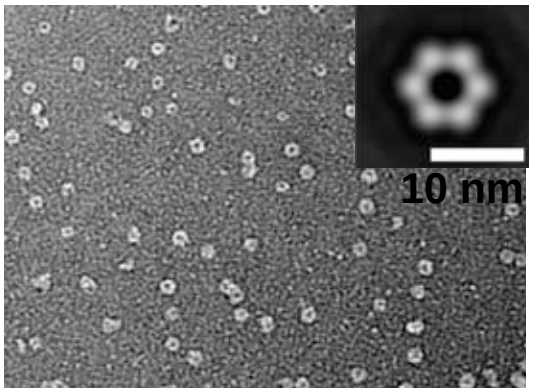
Steven G. Louie

Office of Science

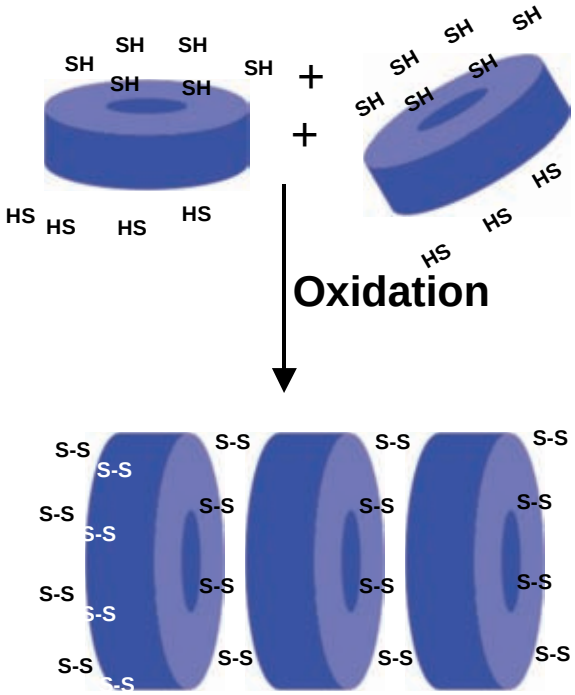
Protein subunits as building blocks

Hcp1 protein forms a ring-shaped hexamer

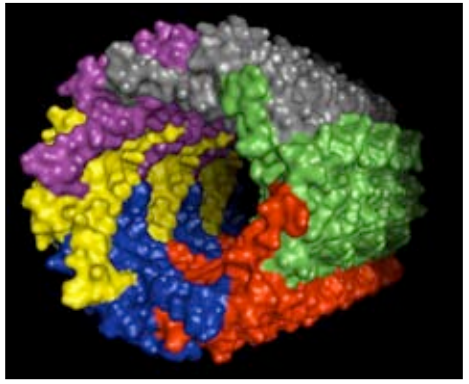


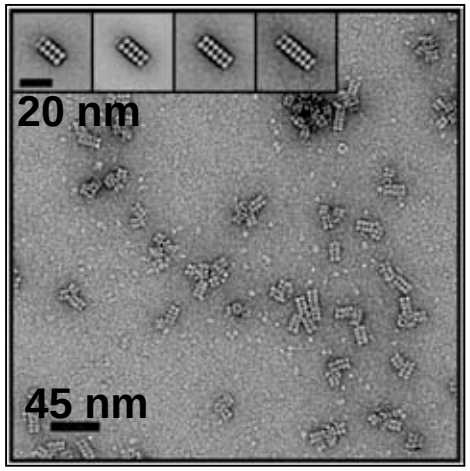


6 cysteines were introduced into each ring face



Rings self-assemble into covalent nanotubes





Can rings be engineered to self- assemble into tubes?

"Single digit" nano

- **Drug delivery**
- **Ion selection**
- **Structural scaffolds**

Foundry User: Joe Mougous **Foundry Staff: Ron Zuckerman**

Ballister et al., *PNAS* (2008)

Center for Integrated Nanotechnologies

Sandia National Laboratories • Los Alamos National Laboratory

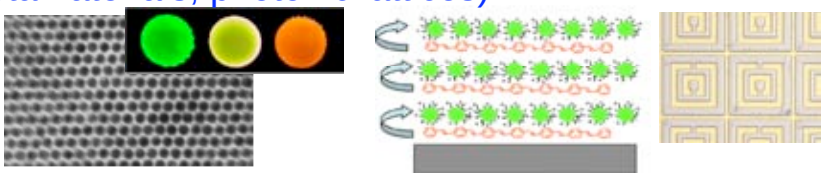
- Highly collaborative U.S. Dept. of Energy User Facility
- Access to tools and expertise
- Pre-competitive and proprietary research options
- Focused on nanoscience integration

"One scientific community focused on nanoscience integration"

Science Thrusts provide relevant expertise

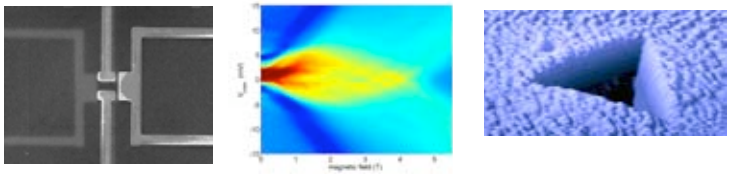
Nanophotonics & Optical Nanomaterials

Synthesis, excitation and energy transformations of optically active nanomaterials and collective or emergent electromagnetic phenomena (plasmonics, metamaterials, photonic lattices)



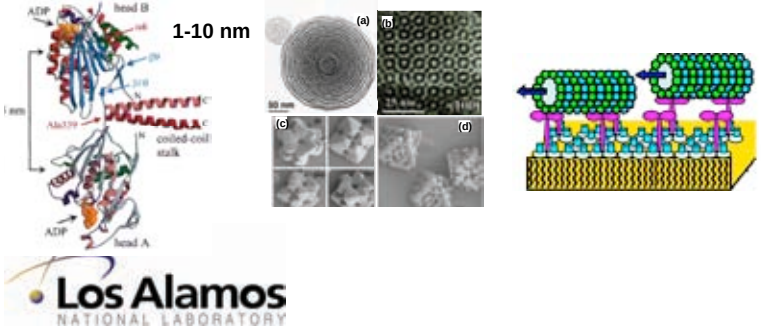
Nanoscale Electronics and Mechanics

Control of electronic transport and wavefunctions, and mechanical coupling and properties using nanomaterials and integrated nanosystems



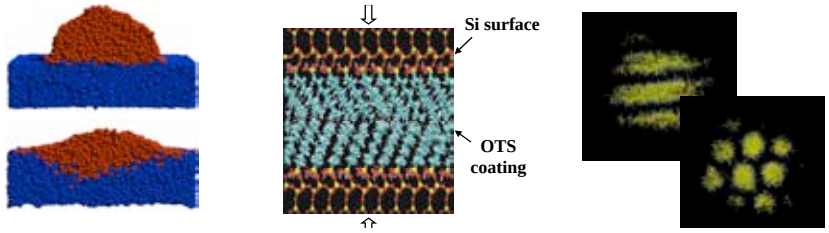
Soft, Biological, & Composite Nanomaterials

Solution-based materials synthesis and assembly of soft, composite and artificial bio-mimetic nanosystems



Theory & Simulation of Nanoscale Phenomena

Assembly, interfacial interactions, and emergent properties of nanoscale systems, including their electronic, magnetic, and optical properties



Los Alamos NATIONAL LABORATORY

Sandia National Laboratories

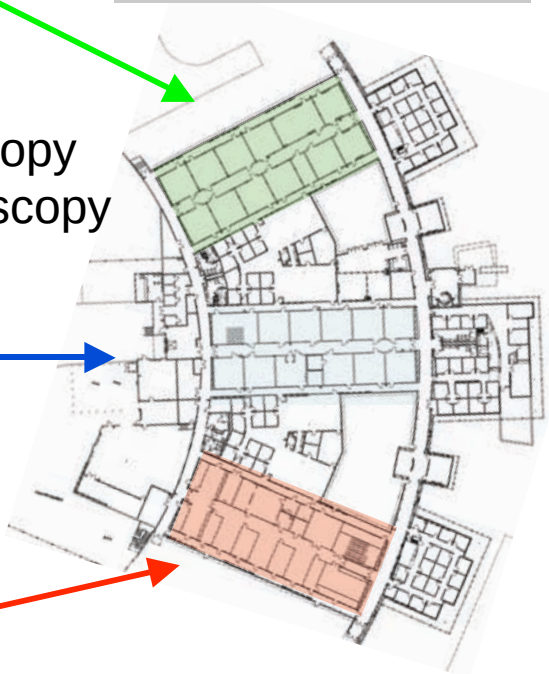
CINT has capabilities for synthesis, characterization and integration

Characterization Wing
- TEM, SEM
- Low Temp Transport
- Scanning Probe Microscopy
- Ultra-fast Laser Spectroscopy

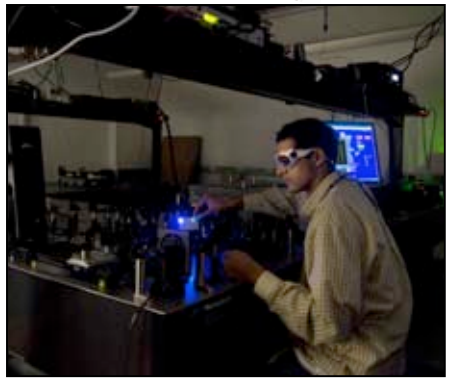
Synthesis Wing
- Molecular Beam Epitaxy
- Chem & Bio labs
- Molecular films

Integration Lab
- E-beam lithography
- Photolithography
- Deposition & Etch
- SEM/FIB

Core Facility



Gateway to Los Alamos
- NSOM, AFM
- Environmental SEM
- Nano-indenter
- Pulsed Laser Dep.
- Ultra-fast Spectroscopy
- Computer Cluster
- Visualization Lab



Los Alamos NATIONAL LABORATORY

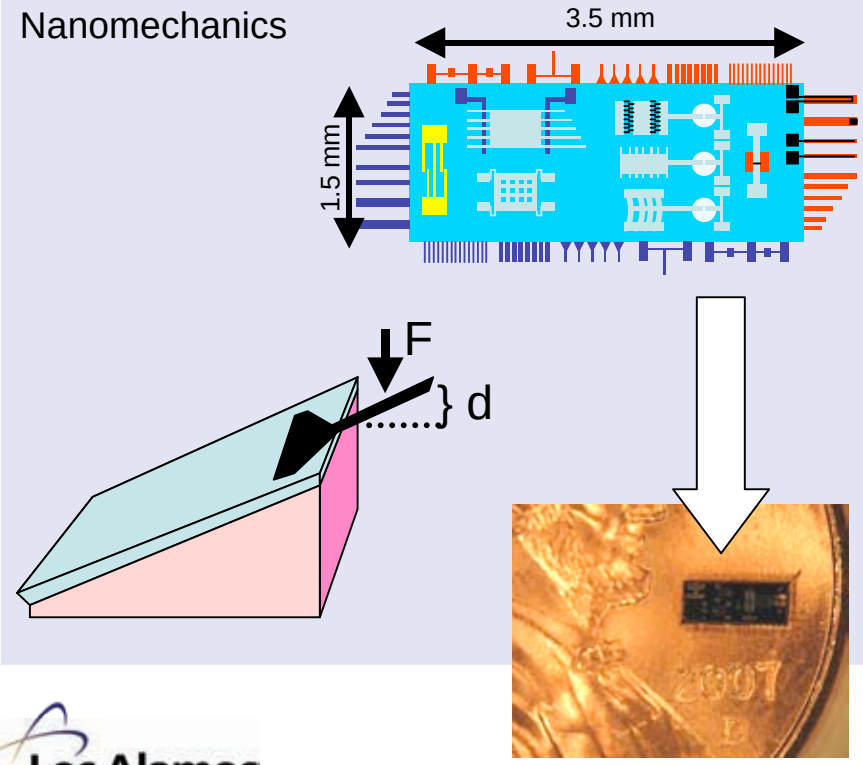
Sandia National Laboratories

CINT Discovery Platforms™: micro-labs for nanoscience exploration

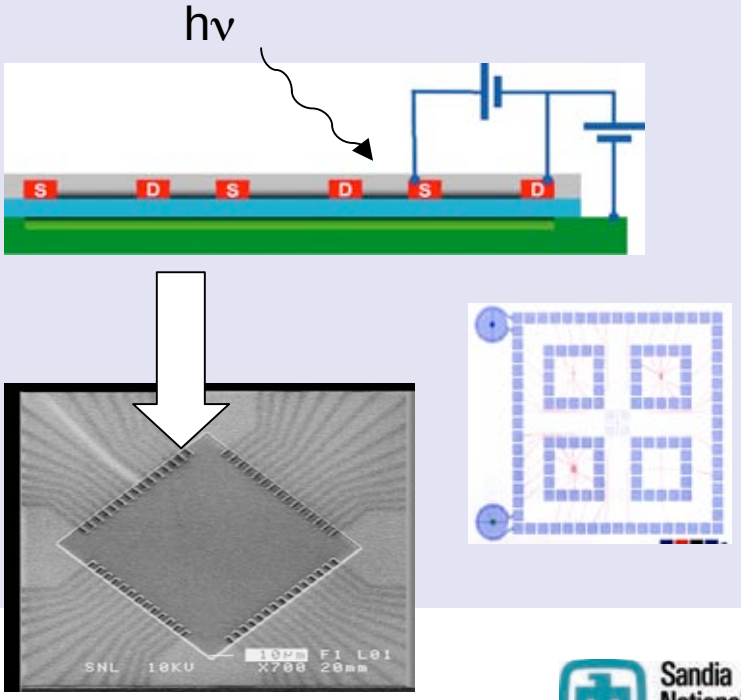
Stimulate, interrogate and exploit
nanoscale materials in a microsystem environment

CINT provides the platforms… for user-inspired problems.

Nanomechanics



Transport

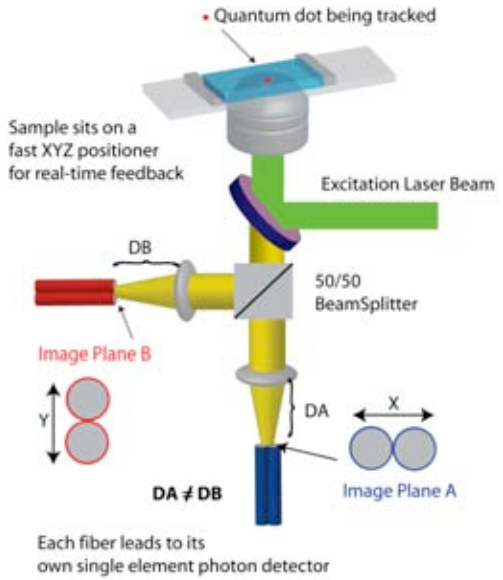


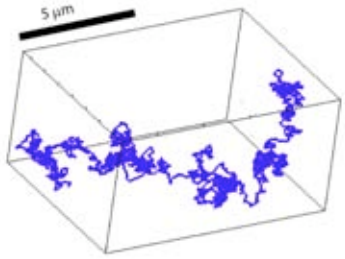
Los Alamos NATIONAL LABORATORY

Sandia National Laboratories

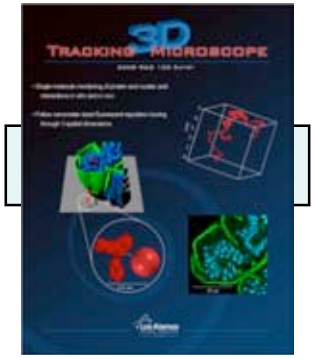
3D Tracking of Individual Quantum Dots

Advanced Instrument Development……..





2008 R&D 100 Award



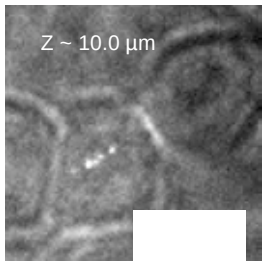
"Three dimensional tracking of individual quantum dots"
Applied Physics Letters 91 2224106 (2007).
GA Lessard, PM Goodwin, JH Werner

"Confocal, 3D tracking of individual quantum dots in high background environments"
Submitted to *Optics Letters*
NP Wells, GA Lessard, JH Werner

"*Method and Apparatus for Tracking a Molecule or Particle in Three Dimensions"*
US Patent Application 20080085550
JH Werner, GA Lessard, PM Goodwin

Los Alamos NATIONAL LABORATORY

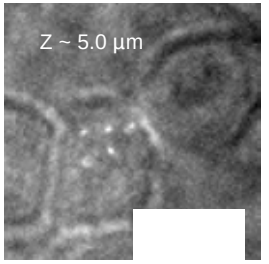
Leads to Unique CINT Science



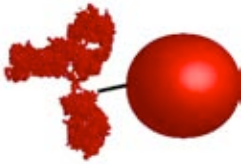
Following three dimensional intracellular transport of quantum dot labeled IgE, an important signaling molecule for the allergic response

top membrane

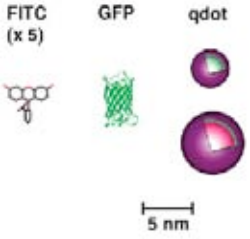
cell interior



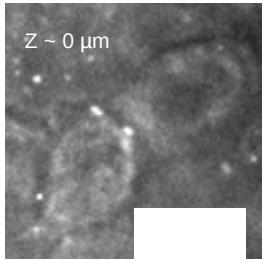
10 nm



qdot labeled IgE



bottom membrane



"Probing the 3D nano-environment of cells molecule by molecule"
CINT User Proposal U2008A062
Diane Lidke, University of New Mexico Cellular Pathology Department

Sandia National Laboratories

Center for Functional Nanomaterials
at Brookhaven National Laboratory

A User-Oriented Research Center

Focus on Functional Nanomaterials for Energy-relevant Applications

CFN Scientific Themes

CFN-Based Research:

- **Nanocatalysis** (Peter Sutter, psutter@bnl.gov)
- **Electronic Nanomaterials** (Charles Black, ctblack@bnl.gov)
- **Soft- & Biological Nanomaterials** (Oleg Gang, ogang@bnl.gov)
- **Electron Microscopy** (Yimei Zhu, zhu@bnl.gov)
- **Theory & Computation** (Mark Hybertsen, mhyberts@bnl.gov)

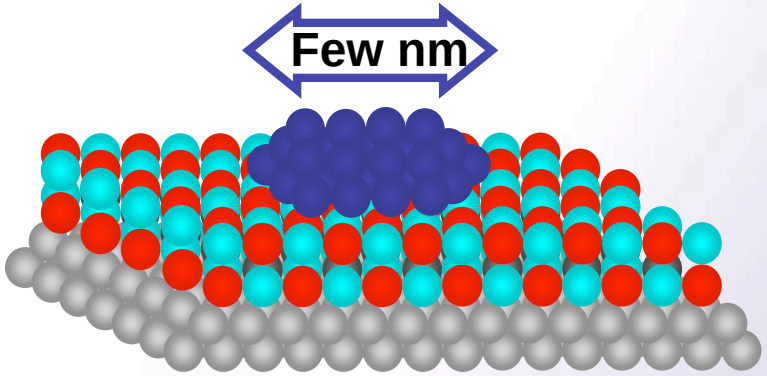
Focus - **Energy Applications:** Functional nanomaterials for exploiting renewable energy sources, energy storage, utilization.

Nanocatalysis

Leader: Peter Sutter (psutter@bnl.gov)

Nano-Catalysis - utilize phenomena at the nanoscale to achieve improved activity, selectivity, resistance to poisoning.

- Increased surface/volume ratio.
- **Electronic** structure**, charging**.
- Availability of specific **active sites**.
- **Dynamically changing** active sites.
- Alloying, tuning of composition, strain.
- Cooperative/proximity effects, spill-over.



Focus - In-Situ Microscopes & Probes

Interrogate individual nanostructures …

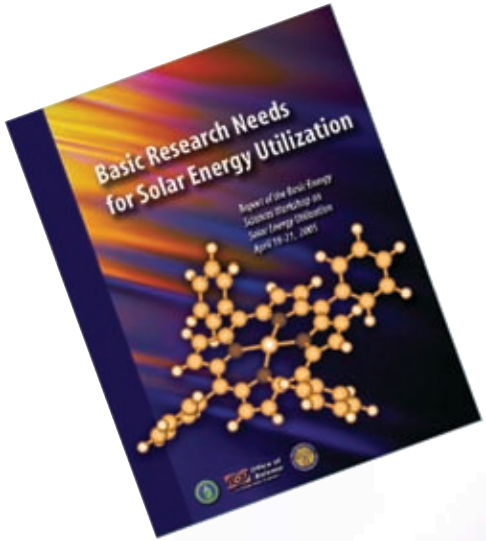
- In relevant environments: realistic pressures & temperatures.
- With combined spatial, temporal, and spectral resolution.

Electronic Nanomaterials

Leader: Charles Black (ctblack@bnl.gov)

Explore nanostructured materials for enhanced or novel optical/electronic properties (esp. *energy conversion*)

- **Science program:**
  - Photovoltaics
  - Photochemistry
  - Nanoplasmonic structures



http://www.sc.doe.gov/bes/reports/abstracts.html

"The Sun is a singular solution to our future energy needs"

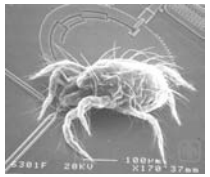
- **But:** Enormous gap between potential and current use of solar energy
- ⇒ Need conceptual breakthroughs through high risk/high payoff research

CFN Facilities

- **Materials synthesis**: Chemical vapor deposition and other synthesis methods for the growth of nanowires and quantum dots; biofunctionalization of nano-objects and surfaces
- **Nanofabrication**: Nanopatterning via optical, electron-beam and nanoimprint lithography; wet or reactive-ion etching, focused ion-beam, thin-film deposition by evaporation and sputtering for materials processing and device fabrication in a class-100 facility
- **Proximal probes**: An array of scanning probe tunneling and atomic force microscopies for advanced surface and interface analysis
- **Electron microscopy**: Most advanced transmission electron microscopy; allows the study of electronic, magnetic and optical properties at the atomic level
- **Optical spectroscopy**: CW and ultrafast spectroscopy tools for the study of optical processes, and their dynamics, in nanomaterials, down to single molecules
- **Dedicated beamline at the NSLS**: Especially designed for small- and large-angle x-ray scattering and ideally suited for the study of soft materials and interfaces
- **Theory & computation**: Staff and computational tools directed to understanding the formation and structure of nanoscale materials and associated electronic, optical and chemical phenomena

The Scale of Things

Things Natural

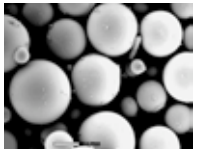


Dust mite

200 µm

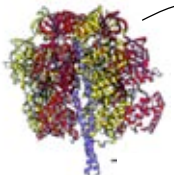
Human hair
~ 60-120 µm wide

Ant
~ 5 mm

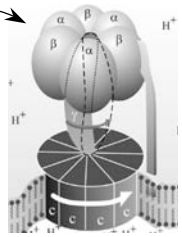


Fly ash
~ 10-20 µm

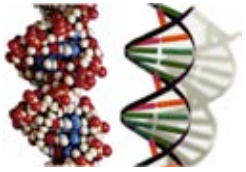
Red blood cells
(~7-8 µm)



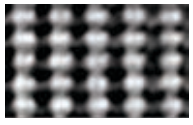
~10 nm diameter



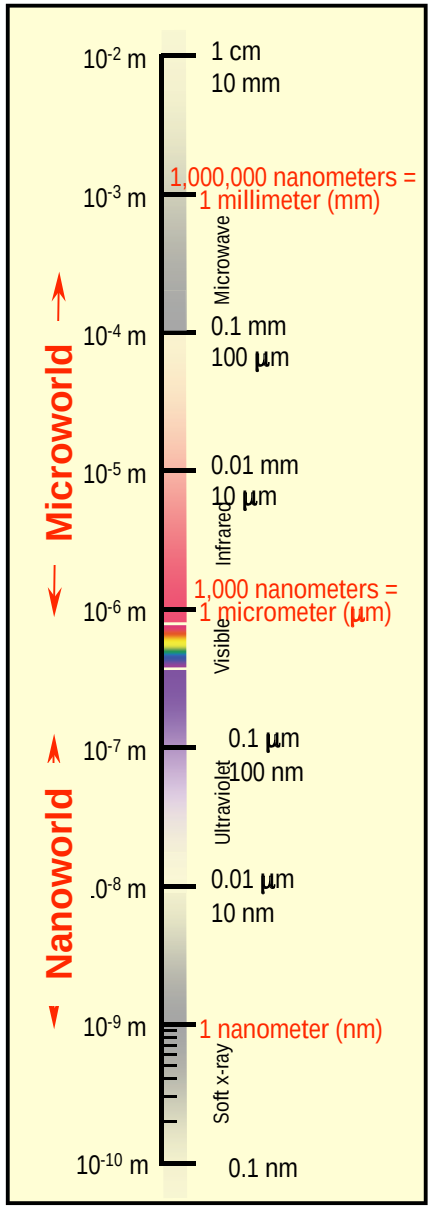
ATP synthase



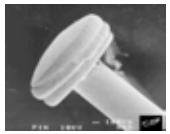
DNA
~2-1/2 nm diameter



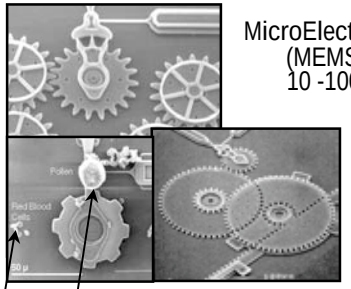
Atoms of silicon
spacing
0.078 nm



Things Manmade



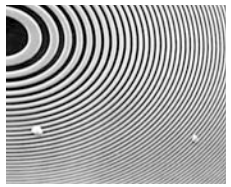
Head of a pin
1-2 mm

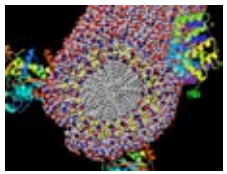


MicroElectroMechanical
(MEMS) devices
10 -100 µm wide

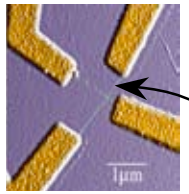
Pollen grain
Red blood cells

Zone plate x-ray "lens"
Outer ring spacing ~35 nm

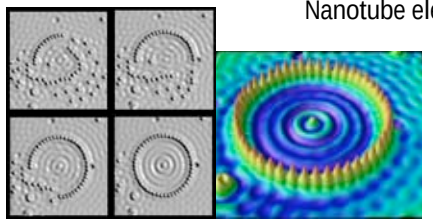




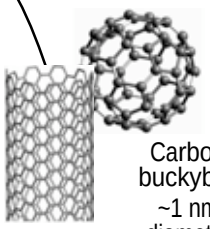
Self-assembled,
Nature-inspired structure
Many 10s of nm



Nanotube electrode



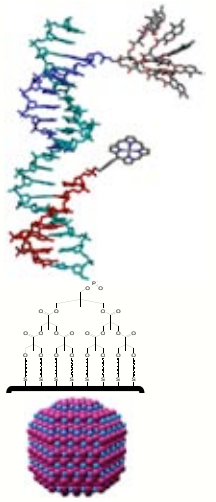
Quantum corral of 48 iron atoms on copper surface
positioned one at a time with an STM tip
Corral diameter 14 nm



Carbon nanotube
~1.3 nm diameter

Carbon
buckyball
~1 nm
diameter

The Challenge



Fabricate and combine nanoscale building blocks to make useful devices, e.g., a photosynthetic reaction center with integral semiconductor storage.

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