UT-BATTELLE

Nanoscience Research Opportunities in the Department of Energy

James B. Roberto
Oak Ridge National Laboratory

NIBIB/DOE Workshop on Biomedical Applications of Nanotechnology

Bethesda, Maryland
March 17, 2005

Nanoscience research opportunities in the Department of Energy

- **National context**
- **The nanoscience revolution**
- **DOE capabilities and interests**
- **Nanoscale Science Research Centers**

The National Nanotechnology Initiative (NNI)

1998 Interagency Working Group on Nanoscience, Engineering, and Technology (IWGN) formed

1999 The community speaks: NRC report on condensed matter and materials physics, IWGN workshop report, NSTC nanostructure science and technology report, DOE reports on nanoscale science and complex systems, professional society activities

PCAST responds, recommends proceeding with the NNI

2000 President's FY 2001 budget request includes NNI support

Congress appropriates $465M for the NNI

2001 NNI survives administration change

2003 President signs the 21st Century Nanotechnology Research and Development Act

2004 President requests $982M for NNI in FY 2005, more than double the FY 2001 appropriation

Nanotechnology in the world

Estimated government-sponsored nanoscience R&D in $ millions/year

	1997	2000	2001	2002	2003	2004
Europe	126	200	270	400	650	900
Japan	120	245	465	650	810	920
USA	116	270	465	604	862	961
Others	70	110	380	520	800	920
Total	**432**	**825**	**1580**	**2174**	**3122**	**3701**

U.S. budget by agency

NSF	305
DOD	276
DOE	211
NIH	89
NIST	53
NASA	35
Others	13
FY 05	**$982M**
FY 06	**> $1B**

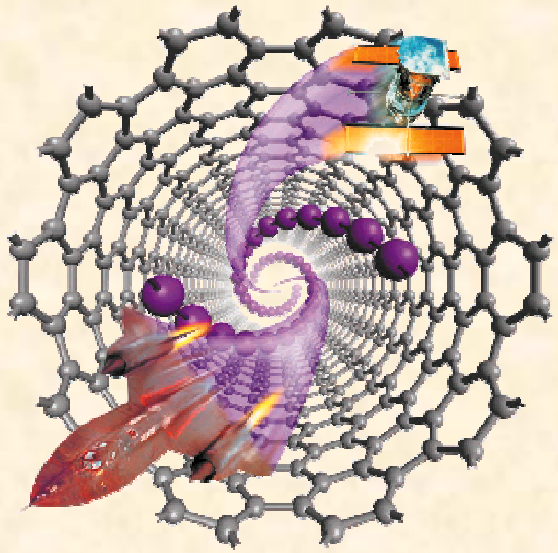
Economic impact of nanotechnology

Market Size Predictions (within a decade)*

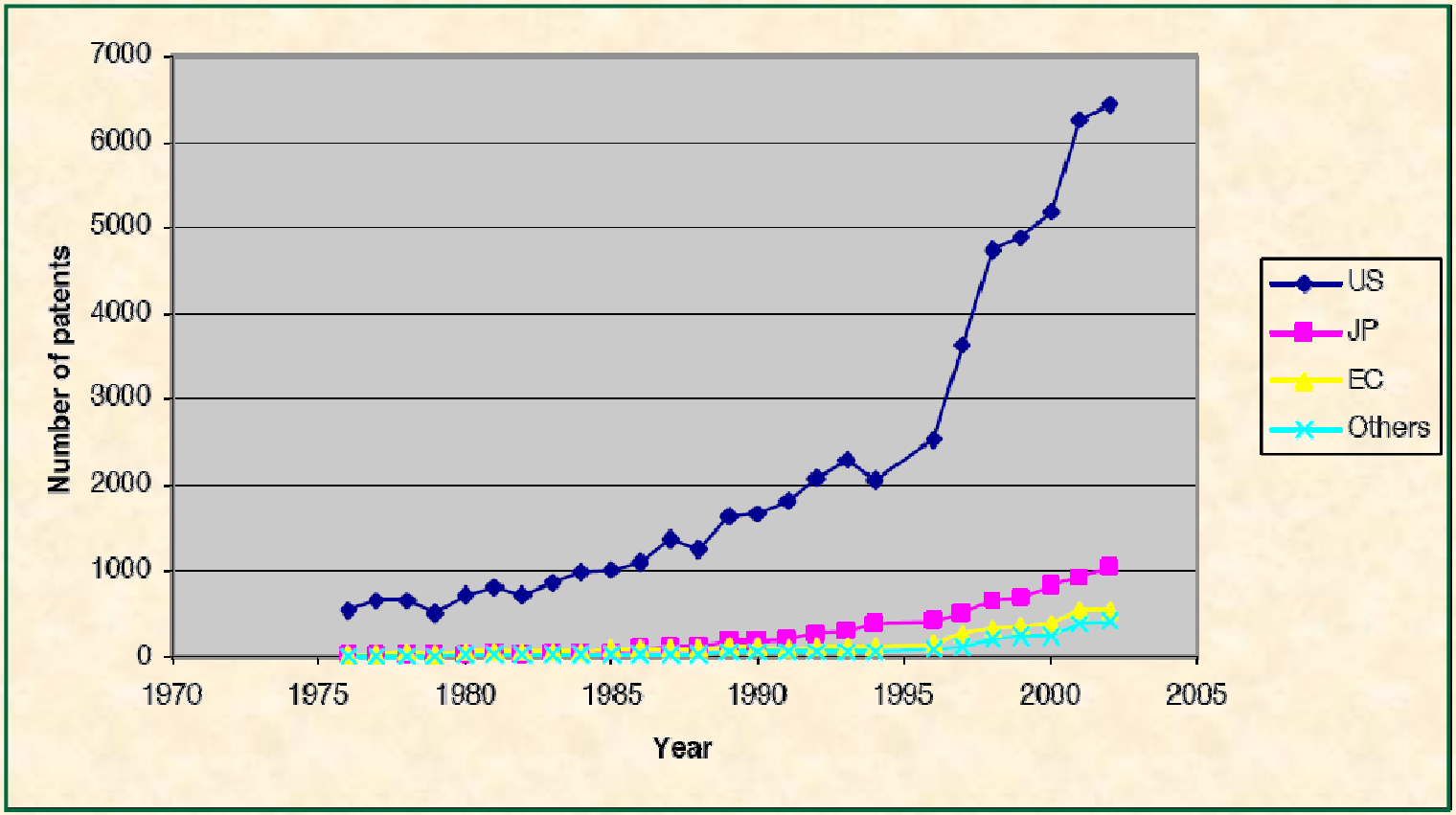
- $340B/yr Materials
- $300B/yr Electronics
- $180B/yr Pharmaceuticals
- $100B/yr Chemical manufacture
- $ 70B/yr Aerospace
- $ 20B/yr Tools
- $ 30B/yr Improved healthcare
- $ 45B/yr Sustainability

$1 Trillion per year by 2015

**Estimates by industry groups, source: NSF*



The U.S. leads the world in nanotechnology patents



www.nsf.gov/nano (from J. of Nanoparticle Research, 2003)

MC. Rocco, 9/07/03

U.S. industry is serious about nanotechnology

General Electric 2003 Annual Report: "To Defeat the Commodity Threat"

"Next Generation Energy"	"Molecular Medicine"	"Nanotechnology"
• Fuel Cells • Hydrogen • Photo voltaics • Turbines	• Molecular diagnostics • Molecular imaging • Molecular knowledge	• Nano for energy • Nano for healthcare • Nano for advanced materials • Nano for transportation

The nanoscience revolution

The challenge

How to use atoms, molecules, and nanoscale materials as building blocks for larger assemblies with new functionalities

20th Century

- **Reducing problems to their ultimate simplicity**
- **Atomic-scale characterization**
- **Elementary excitations**
- **Miniaturization**

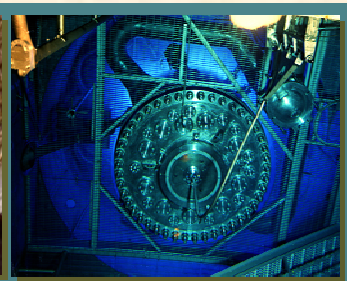
21st Century

- **Embracing complexity**
- **Atomic-scale control**
- **Interactions in complex systems**
- **Self-assembly**

Why now?

- **New tools for atomic-scale characterization**
- **New capabilities for single atom/molecule manipulation**
- **Computational access to large systems of atoms and long time scales**
- **Convergence of scientific-disciplines at the nanoscale**

DOE nanoscience centers



Neutron and synchrotron sources

Ultrascale computing

Nanobiotechnology

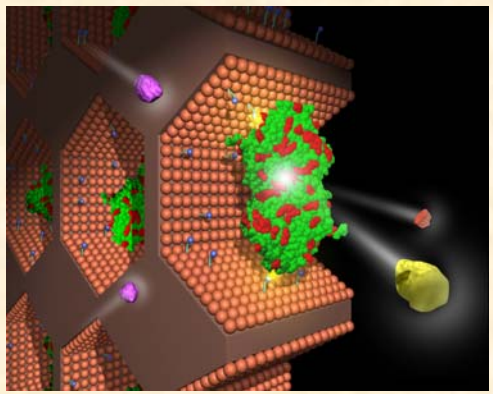
"The physical sciences offer tools for synthesis and fabrication of devices for measuring the characteristics of cells and sub-cellular components, and of materials useful in cell and molecular biology."

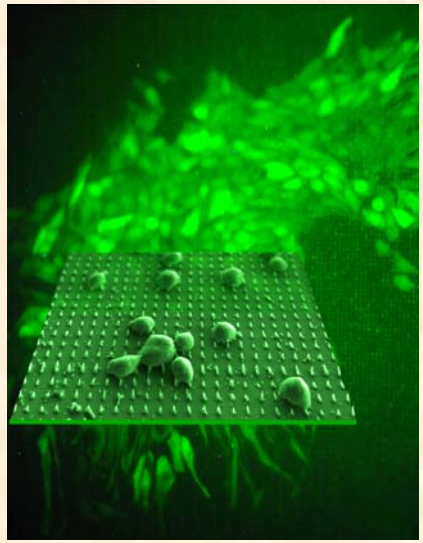
"Biology offers a window into the most sophisticated collection of functional nanostructures that exists."

George Whitesides, *Nature Biotechnology*, Oct 2003

Key questions in fundamental and applied science will be addressed by the overlap of biology, information, and nanoscience

- **Understanding the cell**
- **Self/directed assembly**
- **Materials synthesis**
- **Creating functional materials**
- **Nanomedicine**
- **Biomedical devices**
- **Advanced sensors**
- **Catalysts**



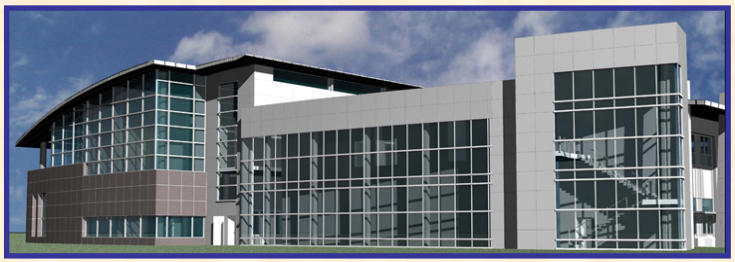


DOE's nanoscience capabilities and interests

- **Nation's largest materials research program**
  - **Unique capabilities in synthesis, characterization, and theory/modeling**
  - **Significant focus on nanoscale materials, macromolecular science, and soft materials**
  - **Emphasis on fundamental understanding**
- **World's most powerful network of materials research facilities**
  - **Synchrotrons, neutron sources, and microscopy centers**
  - **Ultrascale computing capabilities**
  - **Accessible to the scientific user community**
- **Significant biology assets**
  - **Genomics and systems biology**
  - **Connection to physical sciences**
  - **High throughput sequencing**
- **These nanoscience capabilities are focused, integrated, and extended in the DOE Nanoscale Science Research Centers**

Nanotechnology in DOE: The Nanoscale Science Research Centers

- **Complementary capabilities**
- **A capital investment of more than $400M**
- **User centers collocated with major national user facilities (synchrotrons, neutron sources, etc.)**
- **First online in 2005 (CNMS)**

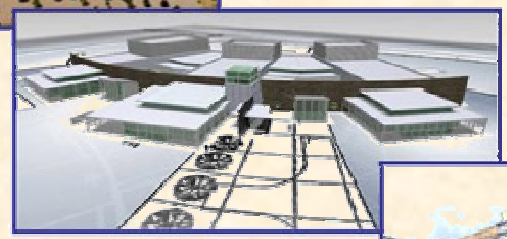


Brookhaven National Laboratory
Center for Functional Nanomaterials

Argonne National Laboratory
Center for Nanoscale Materials

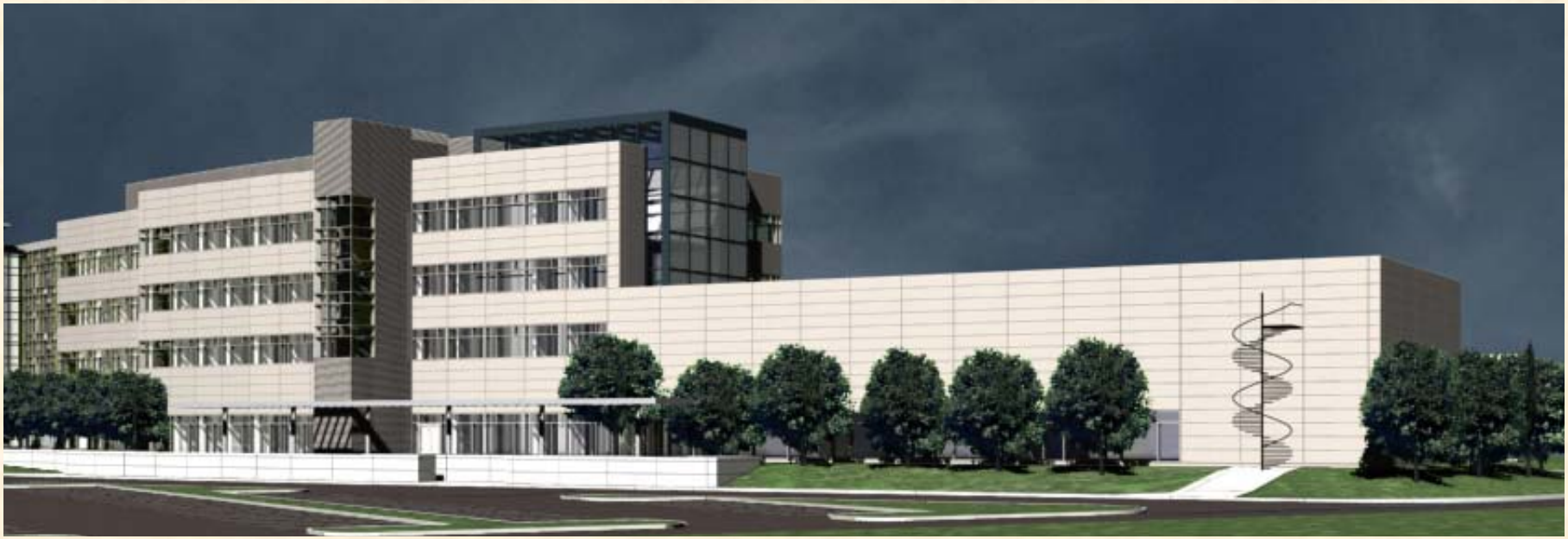
Lawrence Berkeley National Laboratory
Molecular Foundry

Oak Ridge National Laboratory
Center for Nanophase Materials Sciences



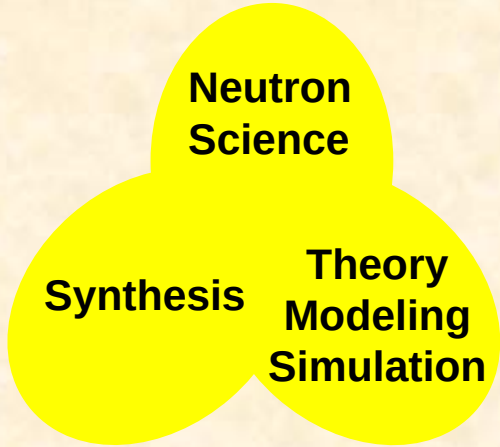
Sandia & Los Alamos National Laboratories
Center for Integrated Nanotechnologies

Oak Ridge National Laboratory Center for Nanophase Materials Sciences (CNMS)



- **DOE's first nanoscience center**
- **$65M in buildings and equipment**
- **State-of-the-art synthesis and characterization of nanoscale materials and structures**
- **Available to universities and industry based on competitive peer review**
- **Open for users October 2005**

CNMS integrates nanoscale science with neutron science, synthesis, and theory/modeling/simulation



- **Neutron Science [Spallation Neutron Source + upgraded HFIR]**
  - **Opportunity to use unique capabilities of neutron scattering to understand nanoscale materials and processes**
  - **Nanoscience focus helps strengthen the U.S.-based neutron science community**
- **Synthesis Science**
  - **Key role of synthesis as enabler of new generations of advanced materials; evolution of synthesis via theory, modeling, and simulation**
  - **More efficient search & discovery; new synthesis pathways**
- **Theory / Modeling / Simulation**
  - **Stimulate U.S. leadership in using theory, modeling and simulation to design new nanomaterials**
  - **Investigate new pathways for materials synthesis**

Scientific themes for CNMS

CNMS' research is organized under seven related scientific themes, selected to address grand challenges to understanding and nanotechnology needs

Macromolecular Complex Systems

Synthetic (polymeric) and bio-inspired materials

Functional Nanomaterials

Nano- tubes, wires, dots, composites; artificial oxide film structures

Nanoscale Magnetism and Transport

Reduced and variable dimensionality; quantum transport

Catalysis and Nano-Building Blocks

Highly selective catalysts; nanoscale synthesis & organization

Nanomaterials Theory Institute: Theory, Modeling, Simulation

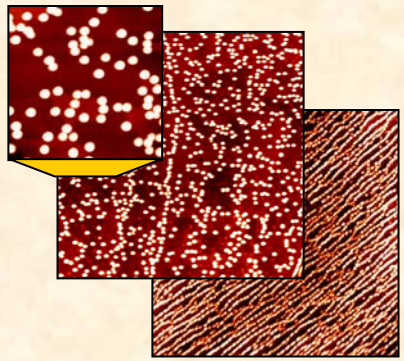
Grand challenges of "computational nanoscience": Multi-scale modeling; nanomaterials design; virtual synthesis

Nanofabrication Research Laboratory

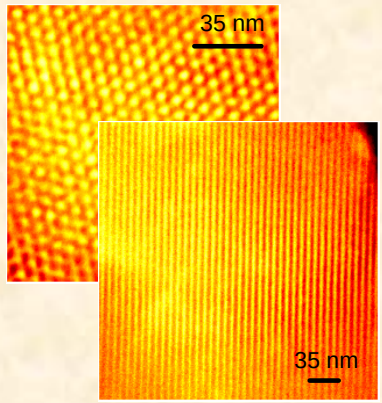
Controlled synthesis & directed assembly; linking nanoscale phenomena to the macroscale; functional integration of "soft" and "hard" materials

Nanoscale Imaging, Characterization, and Manipulation

Unique instruments and methods to characterize and manipulate nanostructures, with simultaneous imaging and environmental control



AFM images of Fe nanodots and nanowires on flat and stepped NaCl surfaces (edge length 750 nanometers)



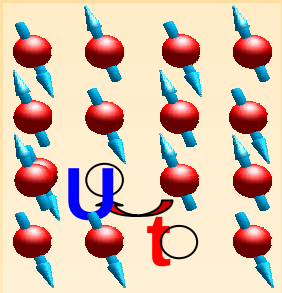
Ordered nanoporous silica synthesized using an organic template

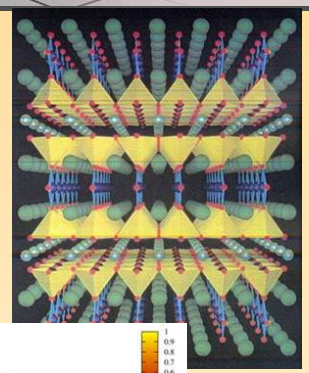
CNMS is located at the Spallation Neutron Source site

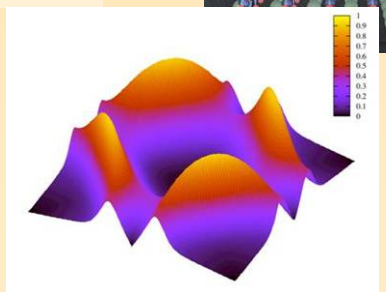
- **Nation’s largest civilian science project**
- **$1.4B in buildings and equipment**
- **World’s most powerful pulsed neutron source**
- **Nanoscale structure and dynamics of materials and biological systems**
- **1500-2000 scientific users annually**

CNMS users will have access to ORNL's leadership-class computing

- **Large-scale simulation needed to predict nanoscale materials properties and trends**
- **We are developing ultrascale computing for grand challenge applications (40 TF by this summer)**
- **Moving toward discovery research in materials, biology, climate, etc.**

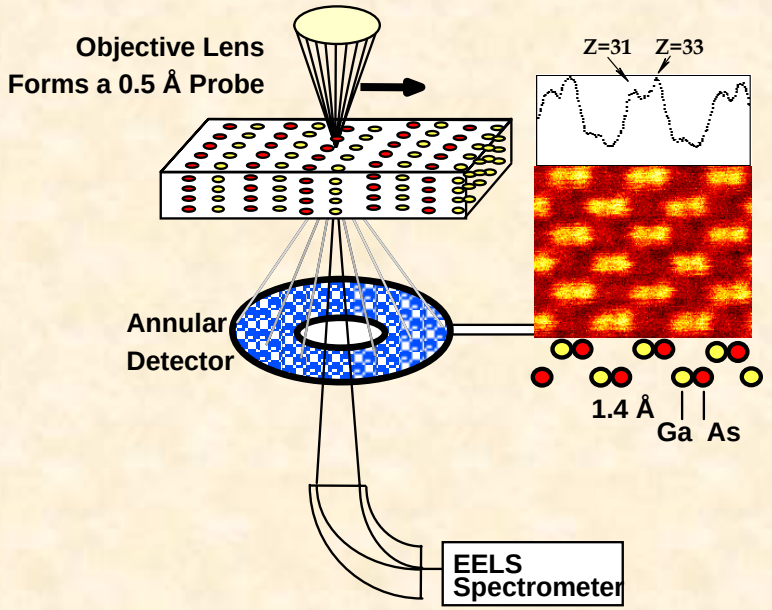






DOE has unique capabilities in nanoscale microscopy

A new era in electron microscopy



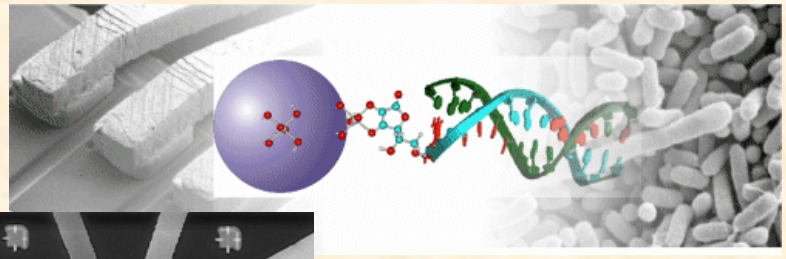
- **Atomic-scale structure and chemistry of materials and interfaces**
- **Single atom sensitivity**
- **Recently established a new world record for electron microscopy (0.6Å resolution)**
- **Next generation capabilities (TEAM project)**

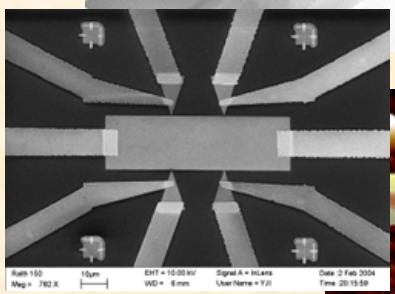
Advanced Microscopy Laboratory

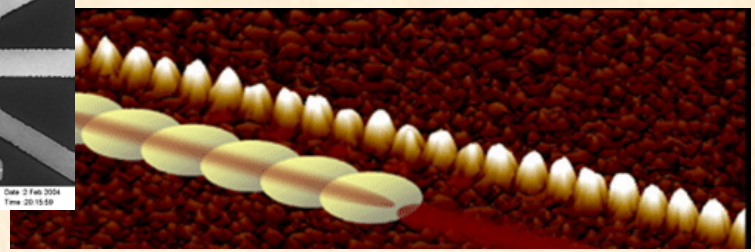
Center for Nanoscale Materials (CNM)
Argonne National Laboratory

Initial CNM user operations Summer 2006

- **CNM building is funded by the State of Illinois**
  - **Adjacent to Advanced Photon Source**
  - **State funds have been appropriated**
  - **Construction has begun**
- **DOE approved through CD-3 as major equipment project**
  - **Nanoprobe beamline in construction**







Scientific Themes

- **Bio-inorganic interface**
- **Complex oxides**
- **Nanocarbon**
- **Nanomagnetism**
- **Nanophotonics**
- **Lithography**
- **Theory and simulation**
- **X-ray nanoprobe**

Center for Functional Nanomaterials (CFM)
Brookhaven National Laboratories

Scientific Thrust Areas

- **Strongly Correlated Oxides**
- **Magnetic Nanoassemblies**
- **Nanocatalyst Materials**
- **Charge Injection and Transport**
- **Nanostructured Organic Films**
- **Applications of Nanoscience**

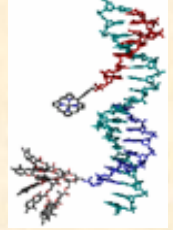
Unique Facilities

- **National Synchrotron Light Source**
- **Transmission Electron Microscopy Facilities**

The latest renderings of the CFN facility

Initial user operations Spring 2007

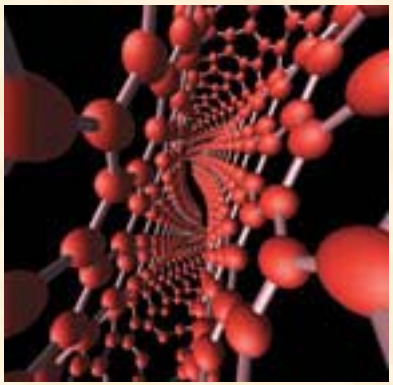
The Molecular Foundry
Lawrence Berkeley National Laboratory

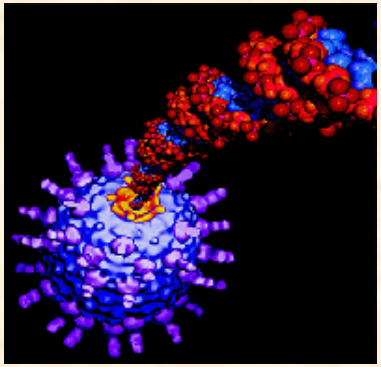


Foundry Building

- Near National Center for Electron Microscopy and Materials Sciences Laboratories
- Under construction
- Full operations Fall 2006

Aug. 26, 2004



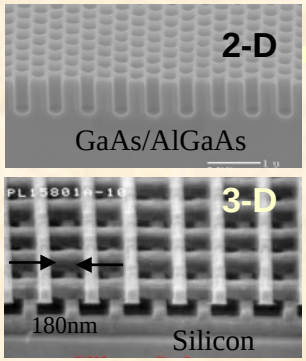


Science

- Inorganic nanostructures
- Nanofabrication
- Organic, polymer/biopolymer synthesis
- Biological nanostructures
- Imaging and manipulation
- Theory

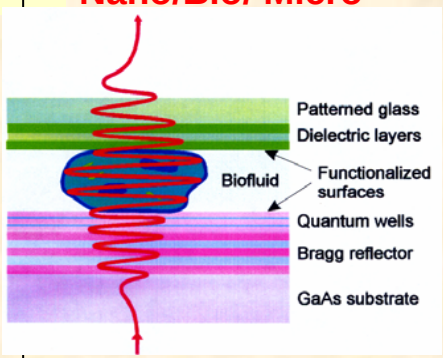
Center for Integrated Nanotechnologies
Sandia and Los Alamos National Laboratories

Nano-Electronics, and Photonics



Photonic Lattices

Nano/Bio/ Micro



Bio-Tailored Surfaces

Initial operations Spring 2006

Science Thrusts

- Nanoelectronics/nanophotonics
- Nano/Bio/Micro Interfaces
- Complex Functional Nanomaterials
- Nanomechanics
- Theory and Simulation

SNL Core Facility

LANL Gateway Facility

The DOE Nanoscale Science Research Centers offer unique capabilities to the scientific community

- **A $400M investment in new construction and state-of-the-art equipment**
- **5 national facilities, each with a distinctive signature**
- **Broad access to universities and industry based on peer review**
- **Coordinated access to $4B national synchrotron, neutron, and computational facilities**
- **Focus on world-class user operation and scientific impact**
- **Partnering opportunities for research and facilities of mutual interest**

All centers can be accessed through the Laboratory websites or the DOE Office of Basic Energy Sciences website