Nanoscale Science, Engineering, and Technology in DOE's Office of Basic Energy Sciences

Research Directions and Nanoscale Science Research Centers

Office of Science
U.S. DEPARTMENT OF ENERGY

Nanoscale Science, Engineering, and Technology in the Office of Basic Energy Sciences (BES) of the U.S. Department of Energy (DOE)

Research Directions and Nanoscale Science Research Centers

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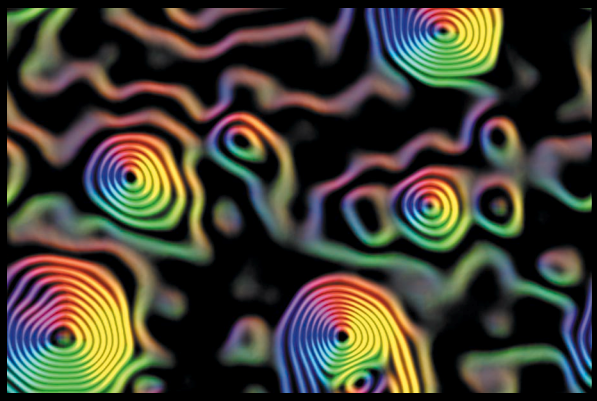


Map showing magnetic flux lines for nickel nanoparticles. These studies provide insight into magnetism at the nanoscale and may revolutionize data storage media of the future. (Area shown is 30 x 45 nanometers.)

In his address to the 2002 meeting of the American Association for the Advancement of Science, Dr. Jack Marburger, President Bush's Science Advisor, declared that we are in the early stage of a revolution in science. "The revolution I am describing," he said, "is one in which the notion that everything is made of atoms finally becomes operational."

The development of what Dr. Marburger called "the atom-by-atom understanding of functional matter" opens a dazzling array of possibilities for observing the functioning of living systems, modifying the fundamental properties of materials, and designing atomic-scale structures with entirely new properties, leading to fresh opportunities for advances in science and technology.

Our ability to work with structures whose dimensions are measured in billionths of a meter, or nanometers, is emerging from a coordinated national program of investment in science and technology over the past few decades. This investment has supported a variety of research activities, facilities, and tools for understanding, probing, and beginning to manipulate matter at the nanoscale.

The resulting advances include laptop computers more powerful than the mainframe systems that supported the Apollo lunar missions, superconducting materials for high-efficiency transmission of electricity, composites ten times as strong as steel, and the ability to engineer genes, visualize individual atoms, and put lasers on chips for portable CD players. But the future promises to be even more amazing. New tools, new understanding, and integration across all of the disciplines anchored in the nanoscale — physics, chemistry, materials science, biology, computation, and engineering — will enable us to build on our 20th century successes and begin to ask and answer 21st century questions.

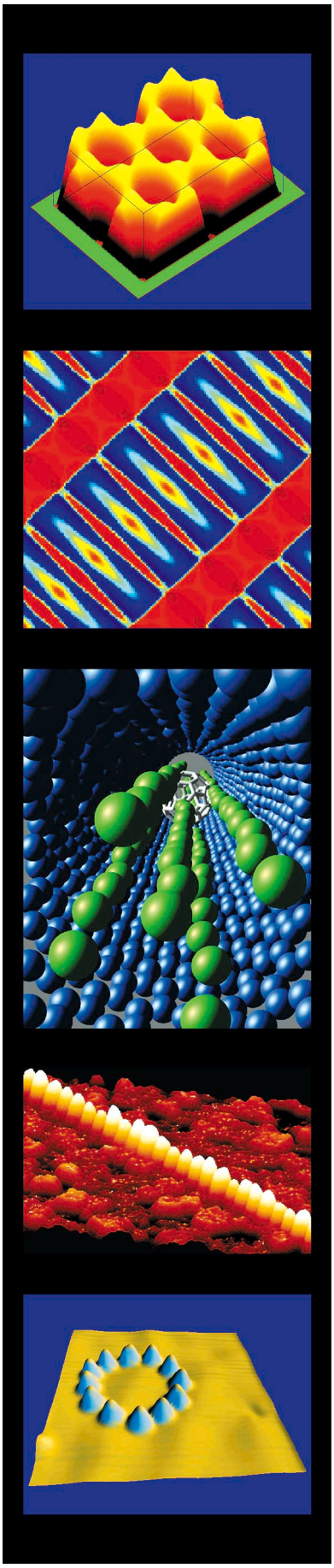
The Department of Energy's Office of Science has played a major role, indeed often *the* major role, in developing facilities and tools for nanoscale research. These include X-ray, neutron, and electron scattering facilities; atomic probe microscopies; instruments for single-molecule spectroscopy; and high-performance computers. Within the Office of Science, the Office of Basic Energy Sciences (BES) leads a broad program of fundamental research that applies these resources to the challenges of science at the nanoscale.

In this brochure, we briefly discuss these challenges and DOE's role in addressing them. We describe the BES research program, and we introduce our new Nanoscale Science Research Centers. These user facilities will provide the Nation's research community with world-class resources for the synthesis, processing, fabrication, and analysis of materials at the nanoscale.

Each Center will be housed in a new building located near one or more existing BES user facilities. Research thrusts and instrument suites for the Centers have been determined in consultation with the nanoscale research community, largely through workshops that have drawn nearly 2,000 participants from industry, universities, and national laboratories.

User programs are being initiated at the Centers to give the research community immediate access to their emerging capabilities. Access will be through submission of proposals for peer review. Information on how to apply to the user programs is included in this brochure.

As the Centers evolve and mature over the next few years, BES will continue to rely on the research community for guidance. Additional workshops will be held, and direct input is welcome. Contact information for each Center and for BES is provided on the back cover.



What Is Nanoscale Research?

Nanoscale research refers to science, engineering, and technology at the level of atoms and molecules, with a length scale of 1 to 100 nanometers. A nanometer is one billionth of a meter. For perspective, a row of 10 hydrogen atoms would span about 1 nanometer, and the width of a human hair is about 50,000 to 150,000 nanometers.

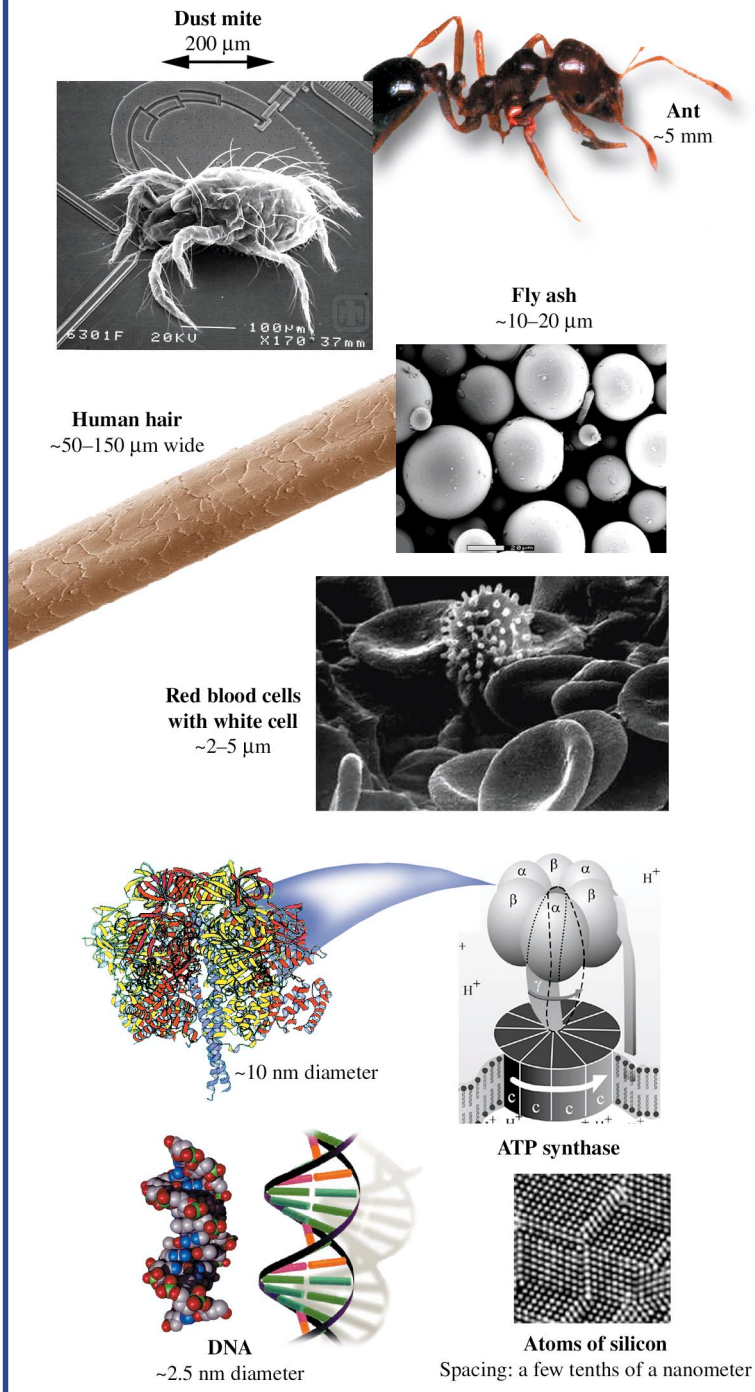
The nanoscale is the scale at which the fundamental properties of materials and systems are established. Melting temperature, magnetic properties, charge capacity, and even color are dictated by the arrangement of nanoscale structures. The realm of molecular biology also operates largely at the nanoscale.

Much is known about the physical properties and behavior of isolated molecules and bulk materials. The properties of matter at the nanoscale, however, cannot necessarily be predicted from those observed at larger or smaller scales. Instead, they exhibit important differences that cannot be explained by traditional models and theories.

Some of these differences result from continuous modification of characteristics with changing size. Others represent totally new phenomena, such as quantum size confinement, wave-like transport, and the predominance of interfacial phenomena. Beginning at the molecular level, new chemical and physical properties emerge as cooperative interactions begin to dominate the behavior of nanoscale molecular complexes. The ability to understand, design, and control these properties will lead to a whole new world of functional molecular assemblies.

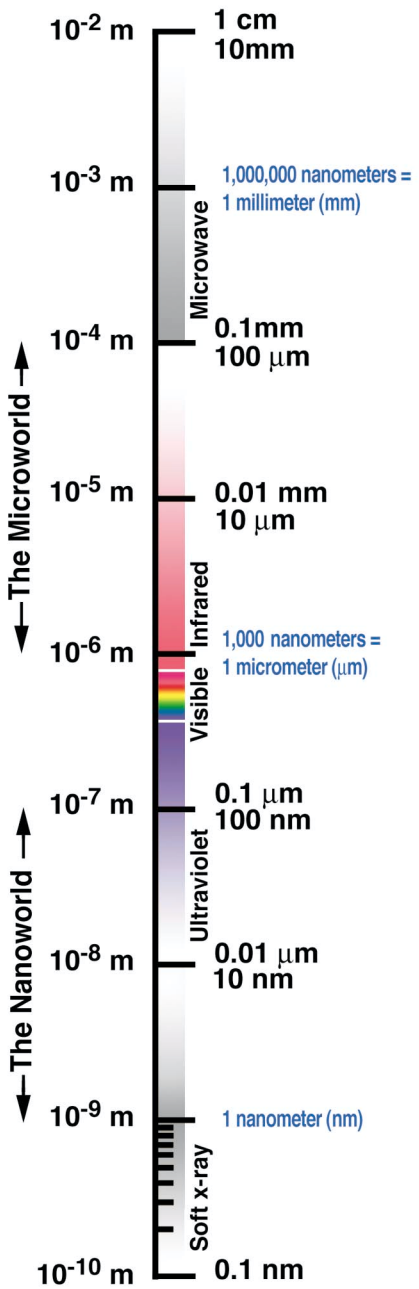
the Scale of things . . .

things Natural



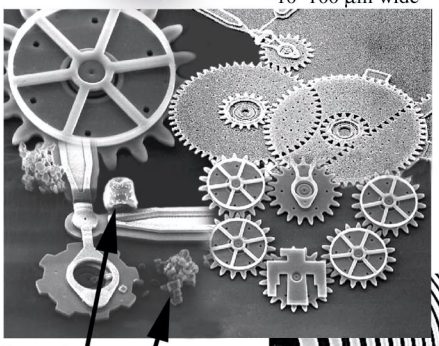
Nanometers & More

things Manmade

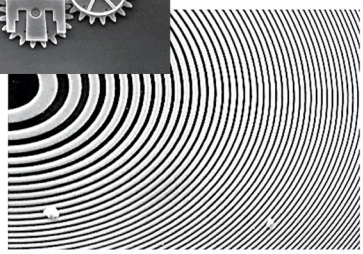


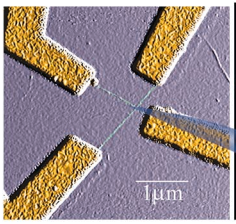
Head of a pin
1–2 mm

Microelectromechanical devices
~10–100 µm wide

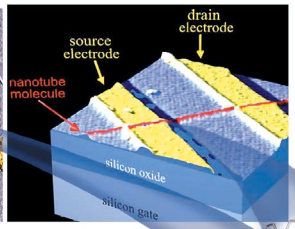


Zone plate X-ray "lens"
Outermost ring spacing
~35 nm

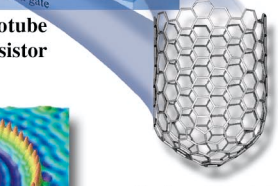




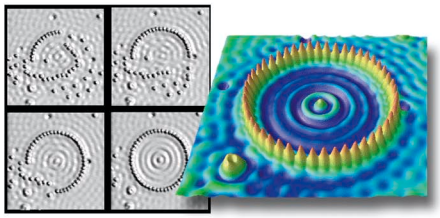
Nanotube electrode



Nanotube transistor



Carbon nanotube
~2 nm in diameter



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

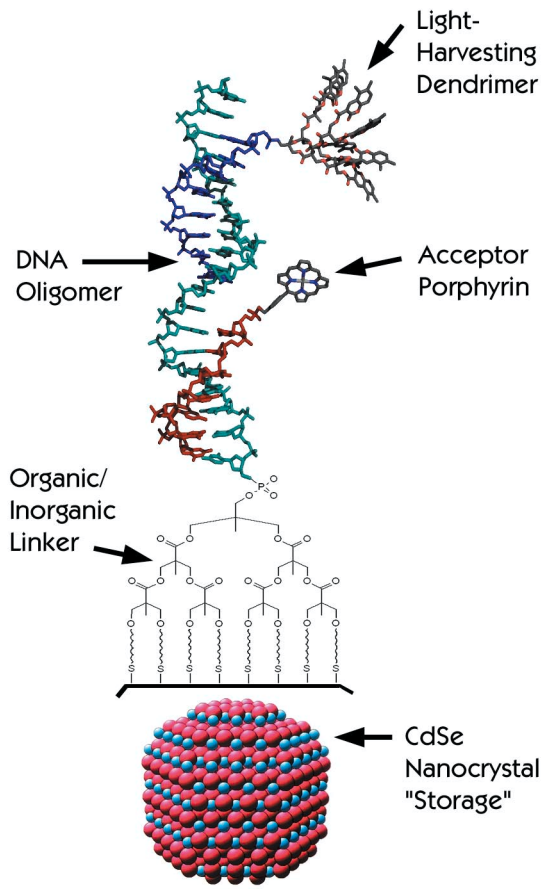
Why Do Nanoscale Research?

Research at the nanoscale will provide both a fundamental understanding of the unique physical, chemical, and biological properties and phenomena that emerge at this length scale and the ability to tailor these properties and phenomena to produce new materials and technologies. The potential benefits of nanoscale research reach into electronics, biotechnology, medicine, transportation, agriculture, environment, national security, and other fields.

For example, we should be able to design highly specific and efficient catalysts, sensors for the detection of biological and chemical substances, nanoscale signal processors, and functional nanodevices that use solar photons or molecular energy sources to generate motion or drive chemical reactions.

Realizing the promise of nanoscale research, however, will require much more fundamental scientific knowledge and technological know-how. This includes a detailed understanding of the processes by which molecules organize and assemble themselves, the construction of quantum devices, and the operation of complex nanostructured systems. We also must find new ways to think about all aspects of materials and device fabrication. In the future, we will be building things from the bottom up as well as from the top down.

Realizing the nanoscale revolution:



Nanoscale building blocks can be combined to make novel functional devices, such as this design for a photosynthetic reaction center with integral semiconductor storage.

DOE's Role in Nanoscale Research

The U.S. Department of Energy (DOE) is the Nation's largest sponsor of research in the physical sciences and ranks fourth among all Federal agencies in support for basic research. Its Office of Science funds extensive programs of research supporting DOE missions in science, energy, national security, and the environment.

Developments at the nanoscale are expected to make major contributions to meeting DOE's applied mission needs:

- Strong, tough, ductile, lightweight materials with low failure rates will improve the fuel efficiency and safety of ground and air transportation.
- Low-loss, high-performance magnets will make motors more efficient.
- Layered structures will provide efficient, low-power, solid-state lighting.
- Hardened alloys and ceramics for cutting tools will improve manufacturing efficiency.
- Surface tailoring of materials will reduce friction and increase resistance to wear, thus cutting fuel consumption.
- Smart materials will range from paints that change color with temperature to windows that respond to thermal inputs and improve energy efficiency.
- Nanostructured catalysts will lead to cleaner, less expensive, more environmentally friendly petroleum refining; better batteries and fuel cells; and improved chemical and product manufacturing.
- Innovative systems for harvesting light and storing energy will dramatically improve solar energy conversion.

For this reason, the Office of Science maintains an impressive portfolio of research and scientific user facilities devoted to exploring the challenges of nanoscale research with applications in energy, national security, and the environment, with an emphasis on research relating to the generation, conversion, storage, transmission, and clean and efficient use of energy.

Much of this portfolio is managed by the Office of Basic Energy Sciences (BES). With support from BES, hundreds of researchers at academic institutions throughout the nation and at DOE's national laboratories are working to visualize, characterize, and control the nanoworld. Current work spans photovoltaic materials development, photo-biochemical solar energy conversion, catalysis, solid-state lighting, self-assembled composite materials, developments in molecular electronics, and a host of other topics with important ramifications for energy use, storage, and generation.

Office of Science facilities and tools supporting this research include

- X-ray, neutron, and electron scattering user facilities;
- atomic probe microscopies;
- instruments for single-molecule spectroscopy; and
- high-performance computers.

These programs, facilities, and tools for nanoscale research are integrated into the National Nanotechnology Initiative (NNI). Launched by the U.S. Government in FY 2001, the NNI is focused on accelerating the pace of revolutionary discoveries in nanoscale science, engineering, and technology and facilitating their incorporation into beneficial technologies. The NNI is an interagency effort that supports a broad program of nanoscale research in materials science, physics, chemistry, biology, and engineering, with an emphasis on interdisciplinary work.

In support of the NNI, DOE has established, as its signature activity in nanoscale research, five new Nanoscale Science Research Centers designed to transform the Nation's approach to nanoscale science.

DOE's Nanoscale Science Research Centers

The cornerstone of the BES effort in nanoscience is the development and operation of five new Nanoscale Science Research Centers to support the synthesis, processing, fabrication, and analysis of materials at the nanoscale:

- The Center for Functional Nanomaterials at Brookhaven National Laboratory in New York
- The Center for Integrated Nanotechnologies at Sandia National Laboratories and Los Alamos National Laboratory in New Mexico
- The Center for Nanophase Materials Sciences at Oak Ridge National Laboratory in Tennessee
- The Center for Nanoscale Materials at Argonne National Laboratory in Illinois
- The Molecular Foundry at Lawrence Berkeley National Laboratory in California

These facilities are designed to be the Nation's premier user centers for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. Together, the Centers provide a gateway to existing major BES user facilities for X-ray, neutron, and electron scattering.

Each Center will focus on a different area of nanoscale research, such as materials derived from or inspired by nature; hard and crystalline materials, including the structure of macromolecules; magnetic and soft materials, including polymers and ordered structures in fluids; and nanotechnology integration.

Planning for the Centers, including the selection of research thrusts and instrument suites, drew on substantial participation by the research community, largely through a series of widely advertised open workshops. Nearly 2,000 researchers attended these workshops, about half of them from the academic community.

Each Center will be housed in a new laboratory building near one or more existing BES facilities for X-ray, neutron, or electron scattering. These new buildings will contain

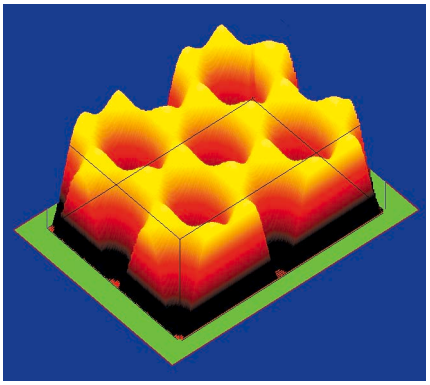
- clean rooms;
- laboratories for nanofabrication;
- one-of-a-kind signature instruments; and
- other instruments (e.g., nanopatterning tools and research-grade probe microscopes) not generally available except at major user facilities.

As with the existing BES user facilities, access will be through submission of proposals that will be reviewed by independent proposal evaluation boards. In response to the requests of prospective users who attended the initial workshops, each Center will begin a limited-scope user program in FY 2003. Details of these programs are available at the Center Web sites (addresses are provided in each Center's description and listed on the back cover of this brochure).

Center for Functional Nanomaterials

The Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory (BNL) will provide state-of-the-art capabilities for the fabrication and study of nanoscale materials, with an emphasis on atomic-level tailoring of nanomaterials to achieve desired properties and functions. Its focus is to achieve a basic understanding of how functional materials, which exhibit a predetermined chemical or physical response to external stimuli, respond when in nanoscale form.

As a premier user facility for conducting interdisciplinary research on a variety of functional nanomaterials, the CFN will serve as a focal point and enabler of advanced materials research in the northeastern United States.

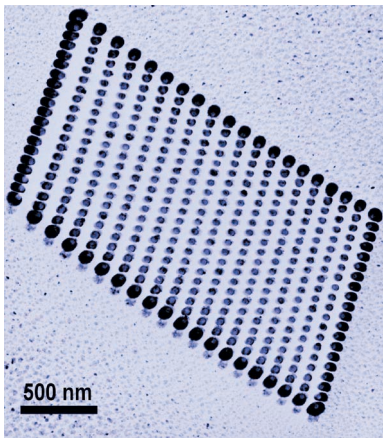


Distribution of electrons between boron atoms (yellow peaks) and magnesium atoms (orange valleys) in magnesium diboride, an unusual superconducting material discovered in 2001.

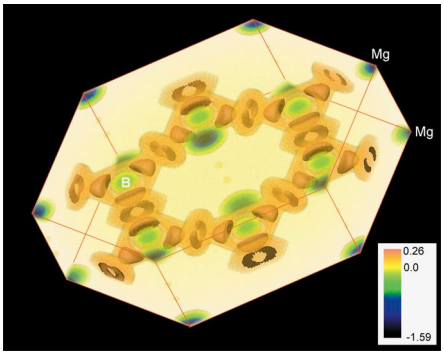
Scientific Themes

Initially, the CFN will focus on six scientific areas.

- **Strongly correlated oxides:** Examining changes in the electronic response of metal oxide nanomaterials.
- **Magnetic nanoassemblies:** Investigating magnetic interactions in nanomaterials.
- **Nanocatalysts:** Studying ways to form catalysts (materials used to speed chemical reactions) and examining their electronic structure and reactivity.
- **Charge injection and transport:** Studying electronic conduction in molecular wires, nanocrystals, and nanodots.
- **Nanometer-thick organic films:** Investigating how thin organic films self-assemble into structures that have better mechanical, electronic, and optical properties, and how these films could be used as lubricants and adhesives and to enhance chemical selectivity.
- **Nanoscience applications:** Building new devices, such as nanoscale electronic materials, ultrathin-film optical devices, and advanced fuel cell catalysts.



Array of nickel nanoparticles observed with an electron microscope.



Valence electron orbitals responsible for superconductivity in magnesium diboride.

Facilities and Capabilities

The CFN will be housed in a new building consisting of offices and laboratories, located next to the National Synchrotron Light Source (NSLS). The centerpiece of the facility will be composed of five state-of-the-art groups of laboratories called Laboratory Clusters, a Theory and Computation Center, and a set of advanced endstations on beamlines at the NSLS.

The Laboratory Clusters will include forefront capabilities in nanopatterning, transmission electron microscopy, nanomaterials synthesis, ultrafast laser sources, and powerful probes to image atomic and molecular structure, together with clean rooms and other support instrumentation. These capabilities are currently being set up within the Physics, Chemistry, Materials Science, and Instrumentation buildings. The NSLS endstations will be specialized for microimaging and small-angle scattering.

As part of the CFN, BNL also offers access to other key national facilities for studying the properties of nanomaterials, including the NSLS, the Laser-Electron Accelerator Facility (LEAF), and a transmission electron microscope facility, and to the scientific staff and collaborating university scientists associated with them. Each of these facilities offers unique and important advantages. For example, the NSLS offers a complete set of scattering, spectroscopy, and imaging capabilities in the hard X-ray, soft X-ray, and infrared wavelength ranges. LEAF is the fastest facility in the country for studying the kinetics of radiation-induced reactions, also called pulse radiolysis, making it ideal for studying charge injection into and charge transport between molecules.

Before the CFN becomes fully operational, users will have access to all existing nanoscience facilities in the developing Laboratory Clusters, the Theory and Computation Center, LEAF, and the NSLS beamlines. An initial Call for Proposals will be issued in March 2003 (see www.bnl.gov/CFN/ for details).

Contact:
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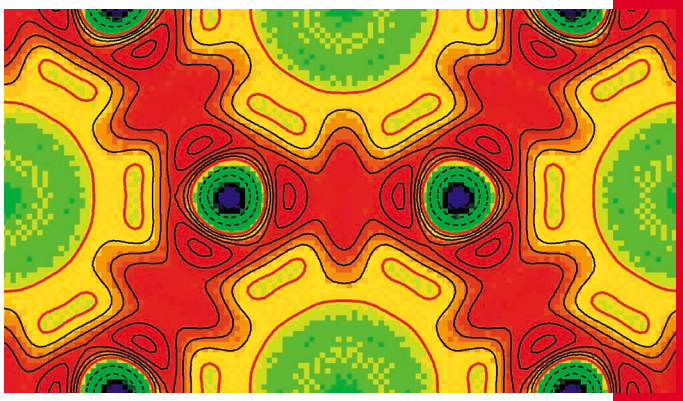
Fax: (631) 344-7206
E-mail: cfnuser@bnl.gov

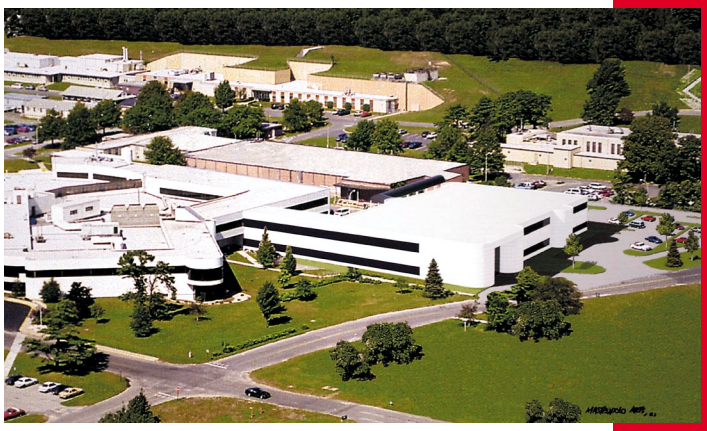
On the Web:
www.bnl.gov/CFN/



Two-dimensional contours of valence electron distribution in the superconducting material magnesium diboride.

User Program

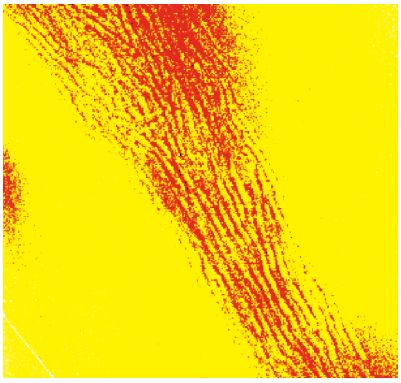
The CFN will be operated as a national user facility, accessible to researchers at universities, industrial laboratories, and national laboratories through peer-reviewed proposals. The user program will provide access to the Laboratory Clusters and related facilities staffed by laboratory scientists, postdoctoral appointees, and technical support personnel who are active in nanoscience research. The number of users will grow from modest levels in the first year, following the initial Call for Proposals in March 2003, as the new facilities are constructed and commissioned in the succeeding years. We invite proposals from external scientific and industrial researchers that involve a broad spectrum of activities ranging from short-term capability access to long-term joint research programs.



The Center for Functional Nanomaterials (right) will be adjacent to the National Synchrotron Light Source (front, left) and the Instrumentation Building (rear, left).

Center for Integrated Nanotechnologies

The Center for Integrated Nanotechnologies (CINT) is devoted to establishing the scientific principles that govern the design, performance, and integration of nanoscale materials. Through its core facility in Albuquerque, New Mexico, and its gateways to both Sandia National Laboratories and Los Alamos National Laboratory, CINT will provide access to tools and expertise to explore the continuum from scientific discovery to the integration of nanostructures into the microworld and the macroworld.

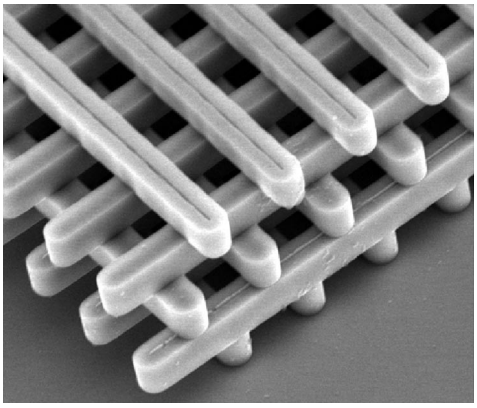


Nanostructuring of conjugated polymers may allow control of charge and energy transfer.

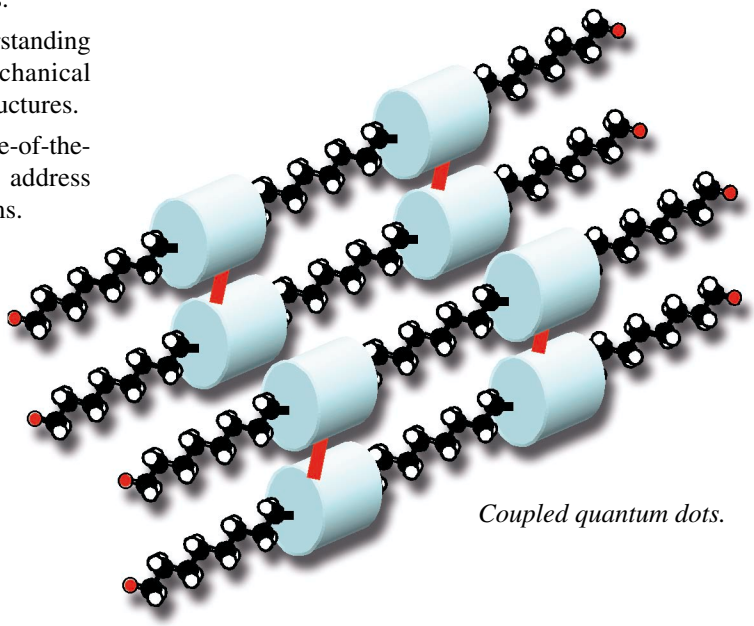
Scientific Themes

To address the national grand challenges of nanoscience and technology, CINT supports five scientific thrusts that serve as integrated synergistic building blocks for the user community.

- **Nano-Bio-Micro-Interfaces:** Importing biological principles and functions into artificial biomimetic nanosystems and microsystems.
- **Nanophotonics and Nanoelectronics:** Developing novel and unique properties necessary for the precise control of electronic and photonic wave functions.
- **Complex Functional Nanomaterials:** Promoting complex and collective interactions between individual components in materials to yield emergent properties and functions.
- **Nanomechanics:** Increasing our understanding of the underlying mechanisms of mechanical behavior of nanoscale materials and structures.
- **Theory and Simulation:** Providing state-of-the-art computational resources needed to address complex, multiple-length-scale problems.



Photonic lattice constructed of 1.2-mm-wide silicon "logs."



Coupled quantum dots.

Facilities and Capabilities

The CINT community will have access to dedicated research capabilities in a new 90,000-ft^2 core facility in Albuquerque, the new CINT Gateway to Los Alamos, and the existing CINT Gateway to Sandia. Together, these three facilities will provide laboratory and office space for researchers to synthesize and characterize nanostructured materials, theoretically model and simulate their performance, and integrate nanoscale materials into larger-scale systems in a flexible, clean-room environment.

CINT researchers will also have streamlined access to user facilities at both locations, including the Los Alamos Neutron Science Center and the National High Magnetic Field Laboratory. Through the CINT Gateways, researchers will be able to access leveraged Los Alamos and Sandia capabilities in biosciences, microelectronics, nanofabrication, and computing.

User Program

CINT operates as a national user facility devoted to establishing the scientific principles that govern the design, performance, and integration of nanoscale materials. The user program provides access to state-of-the-art facilities staffed by laboratory scientists, post-doctoral fellows, and technical support personnel who are leaders in the CINT scientific thrust areas. Access is via peer-reviewed technical proposals for independent or collaborative research. Proposal submission information is available on the CINT Web site.

Contact:
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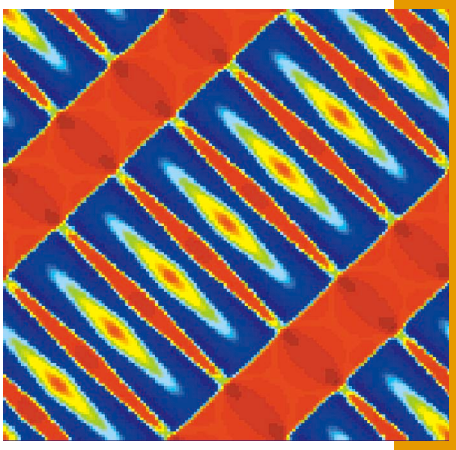
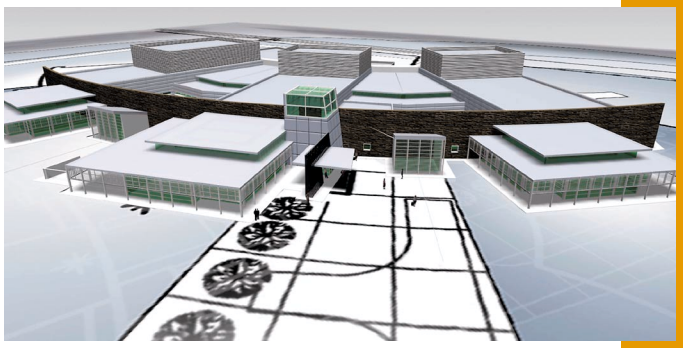
cint.lanl.gov



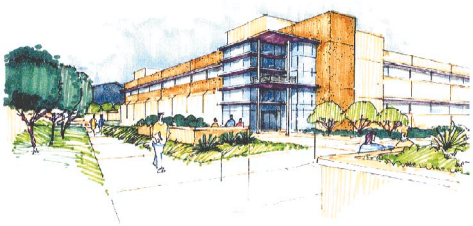
Simulation of pressure-induced nanoscale twins in an elastic material.

"One scientific community focused on nanoscience integration"

The CINT Gateway to Sandia will focus on nanomaterials and microfabrication, leveraging the existing Integrated Materials Research Laboratory.



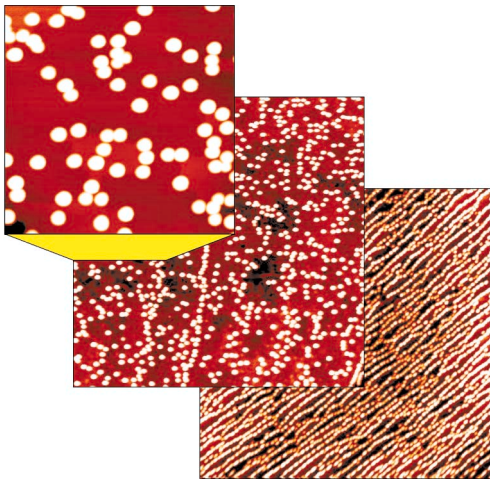
The CINT Core Facility in Albuquerque will provide an interdisciplinary environment for the research community.



The CINT Gateway to Los Alamos will focus on biosciences and nanomaterials.

Center for Nanophase Materials Sciences

The Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL) will integrate nanoscale science with neutron science, synthesis science, and with theory, modeling, and simulation. Operating as a national user facility, the CNMS will create unique opportunities to understand nanoscale materials and phenomena in a highly collaborative and multidisciplinary environment. It will provide a broad community of scientists, engineers, and students from throughout the nation, but particularly the southeastern United States, with readily accessible resources for research focusing on the controlled synthesis and directed assembly of functional nanomaterials and on the integration of soft (polymeric, biological) and hard materials.

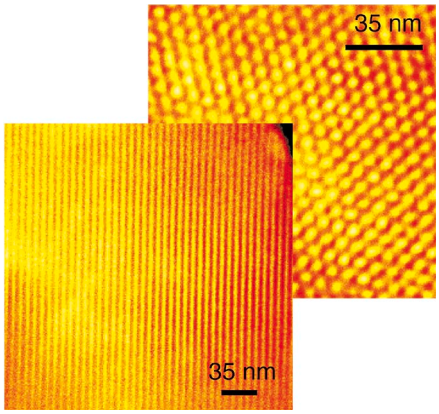


AFM images of Fe nanodots and nanowires on flat and stepped NaCl surfaces (edge length 750 nm).

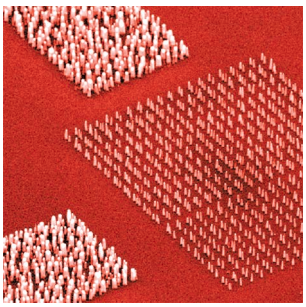
Scientific Themes

Research will be organized under five related scientific thrusts, selected to address grand challenges to scientific understanding and nanotechnology needs.

- **Soft and Hybrid Materials:** Novel synthesis and characterization of organic, hybrid, and interfacial nanophases, including polymers, biologically derived systems, carbon nanotubes and related structures, nanostructured catalysts, nanoconfined fluids, and nanoscale mechanics.
- **Complex Hard Materials:** Synthesis and characterization of nanofunctional materials, addressing opportunities in nanoscale magnetism, manipulation of collective behavior, effects of reduced dimensionality, quantum transport, structural nanocomposites, and nano-interface science.
- **Nanofabrication:** Facilities and techniques for controlled synthesis and directed assembly, to link nanoscale phenomena to the macroscale and to functionally integrate soft and hard materials, including nanostructures for sensing and electronics.
- **Theory, Modeling, and Simulation:** Computational nanoscience (multiscale modeling, nanomaterials design, and virtual synthesis) using terascale computing capabilities, developed through the Nanomaterials Theory Institute.



Ordered nanoporous silica synthesized using an organic template.



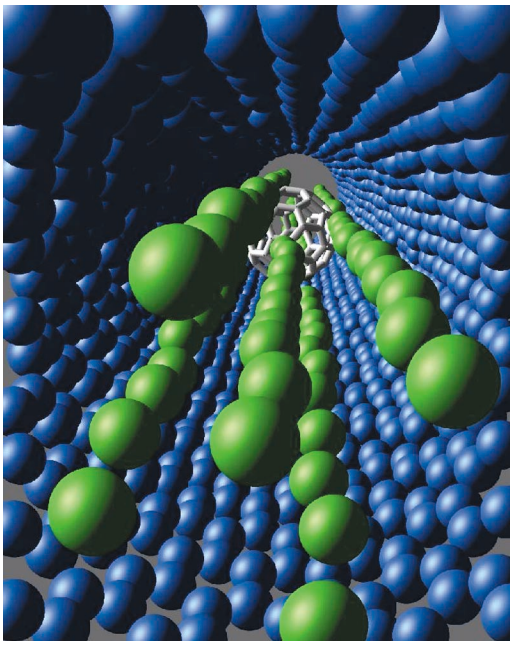
Random and ordered arrays of vertically aligned carbon nanofibers, useful for electron field emission and probing into living cells.

- **Nanoscale Imaging and Characterization:** New methods to manipulate nanostructures for properties measurements using neutron scattering, or combining electron microscopy with scanning probe and environmental techniques.

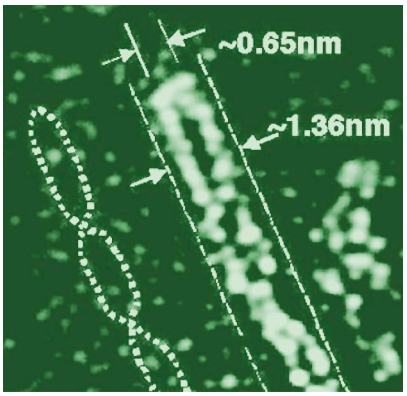
Facilities and Capabilities

The CNMS will be housed in a new 80,000-ft^2 building on Chestnut Ridge, near the Spallation Neutron Source (SNS). Construction of the CNMS facility will begin in 2003. The four-level main building comprises wet and dry laboratories, office space, and common areas to promote interaction among staff, long-term research guests, and users. It will be equipped with a wide range of specialized tools for synthesis, characterization, and integration of hard and soft materials. The 10,000-ft^2 Nanofabrication Research Laboratory, housed in a one-level wing of the building, includes clean rooms and an area designed to meet the requirements of electron-beam imaging and writing instruments (low electromagnetic field, low vibration, low acoustic noise). The Nanomaterials Theory Institute will provide collaborative workspaces, visualization equipment, and high-speed connections to the terascale computing facilities of ORNL's Center for Computational Sciences.

The intense neutron beams from the SNS (which is scheduled to begin operation in 2006) and from the recently upgraded High Flux Isotope Reactor afford unique opportunities for fundamental studies of the structure and dynamics of nanomaterials. The CNMS will provide a gateway to these and other ORNL user facilities, including electron microscopy in the Shared Research Equipment and High Temperature Materials Laboratory user programs, for users whose research can benefit from access to multiple facilities.



Computer simulation of a fullerene molecule (white) moving a helium-atom fluid (green) through a carbon nanotube (blue).



Electron microscopy reveals a double helix chain of iodine atoms inside a carbon nanotube.

User Program

The CNMS user program will provide access to state-of-the-art equipment for nanoscale research and engineering. Users will join a vibrant research community that brings together ORNL research staff, technical support staff, students, postdoctoral scholars, and collaborating guest scientists. The program will accommodate both short-term and long-term collaborative research partners. Access will be through brief peer-reviewed proposals. User activities prior to completion of the CNMS facility will draw on ORNL's existing nanoscience capabilities and staff.

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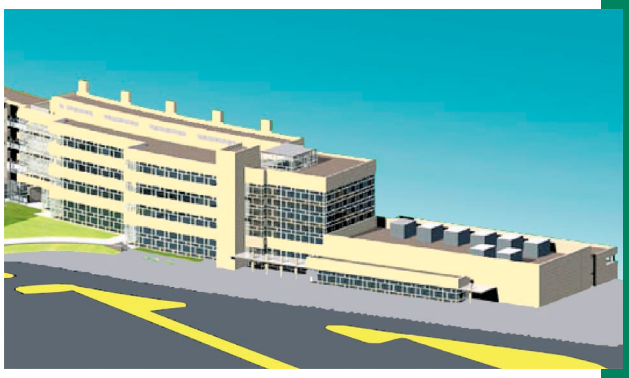


The Center for Nanophase Materials Sciences will be connected to the Central Laboratory and Office Building of the Spallation Neutron Source.

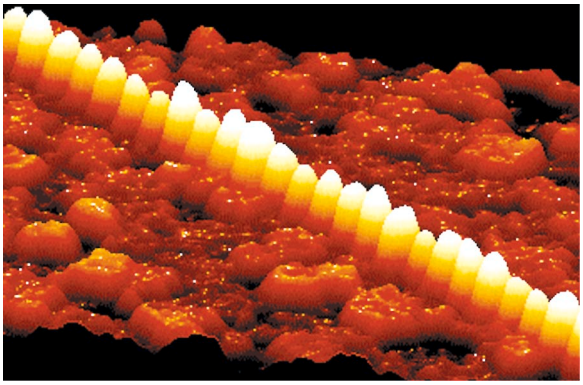
Center for Nanoscale Materials

The Center for Nanoscale Materials (CNM) at Argonne National Laboratory will provide capabilities explicitly tailored to the creation and characterization of new functional materials on the nanoscale. New technologies and new industries can be expected to emerge from CNM's basic explorations.

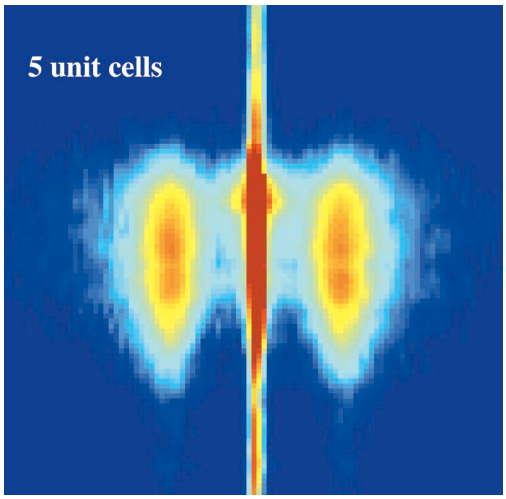
Scientific Themes

The CNM will focus on forging new methods for self-assembly of nanostructures, exploring the nanoscale physics and chemistry of nontraditional electronic materials, and creating new probes for exploring nanoscale phenomena. To address these grand challenges of nanoscience and nanotechnology both experimentally and theoretically, the CNM is organized around five scientific themes:

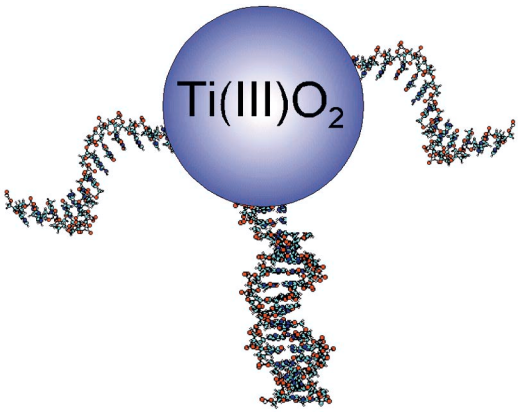
- **Nanomagnetism:** Creating new functionality by nanostructuring magnetic materials. The new physics of nanocomposite magnets will enable a revolution in magnetic-based electronics and ultrastrong permanent magnets.
- **Bio-Inorganics:** Bridging the interface between soft matter (complex organic and biological molecules) and hard matter (inorganic nano-particles and patterned systems) to generate hybrids that exploit the best properties of each type of building block.
- **Nanocrystalline Diamond:** Use of Argonne's nanocrystalline diamond films to develop nanodevices that are 1,000 times as wear-resistant as those made of silicon.
- **Complex Oxides:** Exploration of novel methods for fabricating, understanding, and controlling the synthesis of nanoferroelectrics, spin-polarized oxides, and multiferroics.
- **Nanophotonics:** Creation of a new generation of miniature optical (photonic) devices that process light without being physically limited by the fundamental length scales corresponding to the light's wavelength. This approach will enable control and manipulation of light at the nanoscale.



An array of 100-nm-diameter silver particles allows photon propagation at the nanoscale.



X-ray scattering confirms that ferroelectric properties are retained in a complex oxide film only 1.6 nm thick.



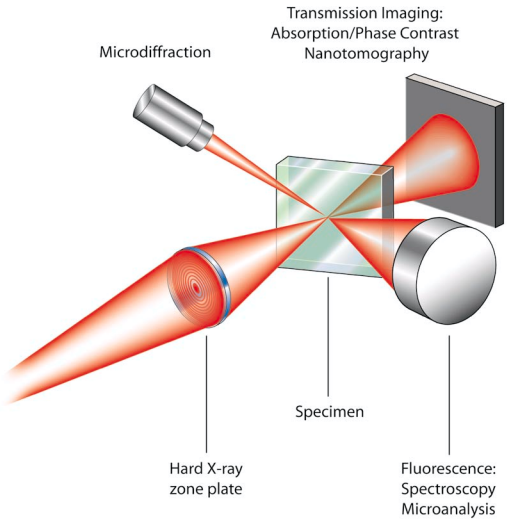
Useful new nanoscale chemical properties emerge when titanium dioxide nanoparticles are fused to DNA.

Facilities and Capabilities

The CNM will develop new structures using molecular self-assembly ("bottom-up" fabrication) guided by the way biological systems organize hierarchically. Nanolithography ("top-down" fabrication) based on electron-beam and focused-ion-beam techniques will be used to create low-dimensional structures and provide templates to assist in creating ordered arrays via self-assembly. We will develop new instruments for nanofabrication based on, for instance, scanning probes, and create novel tools for nanocharacterization to enable visualization of nanostructures. the CNM will also provide a "virtual fab lab" for theoretical analysis and computational simulations of nanoscale phenomena.

The CNM will be closely linked to Argonne's existing user facilities, including the Advanced Photon Source, the Intense Pulsed Neutron Source, and the Electron Microscopy Center. To maximize this synergy, the new building that will house the CNM will adjoin the Advanced Photon Source, and the CNM will construct a state-of-the-art, hard X-ray nanoprobe beamline there. This new beamline will focus hard (i.e., 10-keV) X rays down to a 30-nm spot size; research now under way is aimed at approaching a spot size of 1 nm. The nanoprobe will enable a variety of imaging, spectroscopic, and diffraction studies that cannot be performed elsewhere.

The CNM building, funded by the State of Illinois, is in the design/construction phase and will be completed in 2005. It will house 10,000 ft^2 of clean room space and 10,000 ft^2 of conventional laboratory space for characterization and support. Office space is designed to accommodate CNM staff and users.



The CNM's nanoprobe beamline at the Advanced Photon Source will focus hard X rays down to a spot size of 30 nm or smaller.

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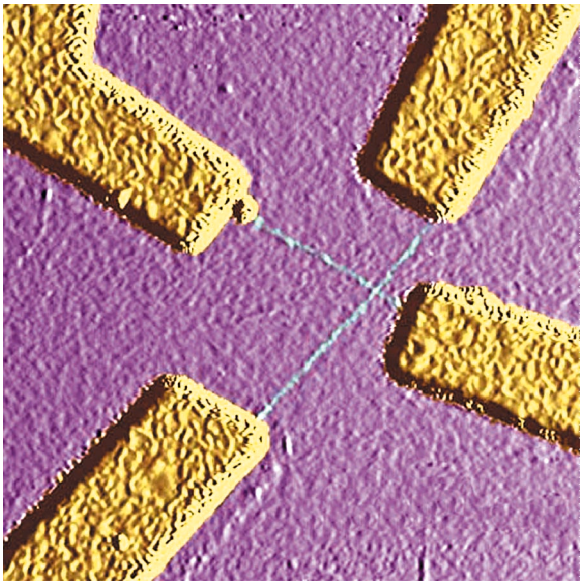
User Program

The CNM will be accessible to users from academia, industry, and other government laboratories through peer-reviewed proposals. Its user program will enable independent investigators to make use of state-of-the-art equipment and collaborate with a world-class scientific staff in a dynamic environment. The CNM will energize new partnerships that will strengthen the nanoscience community nationwide, especially in the Midwest. As the CNM ramps up to full operation, we invite proposals to make use of established Argonne facilities for nanoscience and nanocharacterization. These facilities include the Advanced Photon Source, the Intense Pulsed Neutron Source, and the Electron Microscopy Center.

The Center for Nanoscale Materials facility, shown in the foreground, will be adjacent to the Advanced Photon Source, which is seen in the background.

The Molecular Foundry

The Molecular Foundry at the Lawrence Berkeley National Laboratory (Berkeley Lab) will provide unprecedented opportunities for studying the synthesis, characterization, and theory of nanoscale materials. Its focus will be on the development and understanding of both "soft" (biological and polymer) and "hard" (inorganic and microfabricated) nanostructured building blocks and the integration of these building blocks into complex functional assemblies. Research will be accomplished through multidisciplinary collaborations with users from around the world.



Atomic force microscope image showing two single-walled nanotubes spanning gold contacts. These structures form the basis of the first nanoscale electronic devices.

Scientific Themes

The Molecular Foundry will house six facilities available to users.

Inorganic Nanostructures: Comprehensive study of the science of optimally preparing metal, carbon, and semiconductor nanostructures. The program will encompass the design and synthesis of precursors, the study of microscopic elementary processes in nanostructure nucleation and growth, and the modeling of growth processes. It will also explore the use of robotics in these studies.

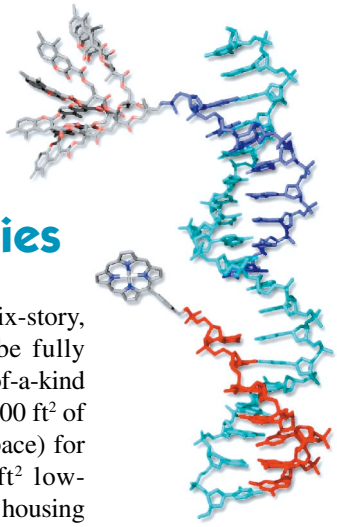
Nanofabrication: State-of-the-art lithographic and thin-film processing. The emphasis will be on processes and techniques for integrating advanced semiconductor nanofabrication technologies with chemical and biological nanosystems.

Organic, Polymer/Biopolymer Synthesis: Resources for studying "soft" materials: organic molecules and macromolecules and their assemblies, including access to component synthesis, libraries, functional assemblies, hybrid materials, organic/polymer characterization, synthesis, and molecular assembly and characterization.

Biological Nanostructures: Materials and training for users pursuing integration of biological components into materials. Techniques will include production of biological macromolecules, protein expression and purification, cell culture, and characterization, with services spanning microbial, plant, and mammalian cell culture and preparation of cellular components and products for construction of bio/inorganic assemblies.

Imaging and Manipulation: Design, development, and maintenance of instruments for the characterization and manipulation of a variety of nanostructures, from hard to very soft matter: electron microscopes equipped with *in situ* manipulators and electrical probes, ultrahigh-vacuum scanning tunneling microscopy and atomic force microscopy (AFM) laboratories, advanced optical systems, and optical tweezers and AFM facilities for structural and functional analysis.

Theory: Theoretical support to explain specific experiments, guide the development of new principles that unify disparate observations, and predict possible new behavior and applications. It will offer expertise in a variety of methods, including electronic structure, *ab initio* and classical molecular dynamics, and quantum and classical Monte Carlo approaches.



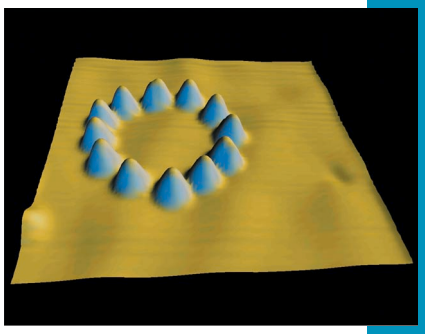
Double-stranded DNA of defined sequence, designed and synthesized to align photosynthetic-like light-harvesting structures in precise three-dimensional arrangements.

Facilities and Capabilities

The Molecular Foundry Laboratory will be a six-story, 94,500-ft^2 structure. Its six facilities will be fully equipped with state-of-the-art, sometimes one-of-a-kind instruments. It will have two clean rooms (4,000 ft^2 of Class 1000 space and 725 ft^2 of Class 100 space) for nanofabrication/lithography and a 5,500-ft^2 low-vibration, low-electromagnetic-field laboratory housing state-of-the-art imaging and manipulation tools. A considerable amount of space will be dedicated to offices and laboratories for the visiting scientists and resident technical support staff.

The Molecular Foundry will also provide nanoscience researchers with a portal to Berkeley Lab's established major user facilities, giving them unparalleled nanoscience research capabilities. These facilities include

- the Advanced Light Source, one of the world's brightest sources of ultraviolet and soft X-ray beams,
- the National Center for Electron Microscopy, housing several of the world's most advanced microscopes and microcharacterization tools,
- the National Energy Research Scientific Computing Center, which provides high-performance computing tools and expertise, and
- the Berkeley Lab Nanowriter, an ultrahigh-resolution electron-beam lithography system, which can generate an electron beam with a diameter of 5 nm and write highly accurate patterns over an area some 150 mm wide.



Quantum corral of 12 sodium atoms, constructed using the tip of a scanning tunneling microscope.

User Program

Investigators from academic, government, and industrial laboratories will be invited to submit proposals for research in one or more of the Foundry facilities. A review panel will select those that are of the highest scientific merit and that make the best use of the unique, multidisciplinary capabilities of the Foundry. Both short-term and long-term visitors are expected.

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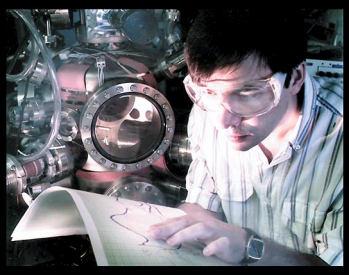
The Molecular Foundry Laboratory will provide its users with access to Berkeley Lab's facilities for microscopy, synchrotron radiation, and computation.



About DOE

The U.S. Department of Energy (DOE) has four major program lines in keeping with its missions in energy, national security, environment, and science. The energy programs promote new approaches to energy production and use. The national security programs ensure the integrity of the Nation's nuclear weapons and advance nuclear safety and nonproliferation. The environmental programs address the legacies of the Cold War and the disposal of the Nation's radioactive wastes. The science programs, which are contained within DOE's Office of Science, support fundamental research to address current and future challenges in all of these mission areas.

With a budget of more than $3 billion, DOE's Office of Science leads the Nation in supporting basic research in the physical sciences and makes significant contributions in other major scientific fields, including advanced computing and life sciences. Researchers funded by these programs have explored some of the major scientific questions of our time, performing the basic research that is helping us to understand the origins and fate of the universe, the complexity of chemical reactivity, the challenge of making new materials, the diversity of life on the planet, and anthropogenic changes in our global climate. DOE's contributions in science, along with those of its predecessor agencies, are partially reflected through its support to 70 Nobel Laureates. The Office of Science is also responsible for planning, constructing, and operating the world's most advanced scientific user facilities, which attract more than 18,000 researchers annually.

Within the Office of Science, the Office of Basic Energy Sciences (BES) supports fundamental research in materials sciences and engineering, chemistry, geosciences, and molecular biosciences. In 2001, BES funded research at more than 150 academic institutions in 48 states and at 13 DOE laboratories in 9 states. The BES program also supports four synchrotron radiation light sources, three neutron scattering facilities, and four electron-beam microcharacterization centers, which together host more than 8,000 researchers annually. The five Nanoscale Science Research Centers described in this booklet will soon take their place alongside these highly successful user facilities and research programs.

Users of the Nanoscale Science Research Centers will join more than 8,000 researchers who perform experiments at existing BES user facilities each year.

The BES Nanoscale Science Research Centers are located near major scientific facilities

Argonne National Laboratory

Center for Nanoscale Materials
Advanced Photon Source
Intense Pulsed Neutron Source
Electron Microscopy Center for Materials Research

Lawrence Berkeley National Laboratory

Molecular Foundry
Advanced Light Source
National Center for Electron Microscopy
National Energy Research
Scientific Computing Center
Nanowriter

Brookhaven National Laboratory

Center for Functional Nanomaterials
National Synchrotron Light Source
Laser-Electron Accelerator Facility
Electron Microscopy Facility

Sandia National Laboratories and Los Alamos National Laboratory

Center for Integrated Nanotechnologies
Compound Semiconductor Research Laboratory
Microelectronics Development Laboratory
Combustion Research Facility
Los Alamos Neutron Science Center
National High Magnetic Field Laboratory
High-Performance Computing

Oak Ridge National Laboratory

Center for Nanophase Materials Sciences
Spallation Neutron Source
High Flux Isotope Reactor
Center for Computational Sciences
High Temperature Materials Laboratory
Shared Research Equipment Program

This booklet was prepared at Oak Ridge National Laboratory (ORNL) for the Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy. We thank the staff of the Nanoscale Science Research Centers for supplying information, graphics, and reviews, and we gratefully acknowledge the contributions of Bonnie Nestor and Jamie Payne of ORNL for their assistance in editing and design.

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Contact Information for DOE's Nanoscale Science Research Centers

Center for Functional Nanomaterials, Brookhaven National Laboratory • www.bnl.gov/CFN/

Center for Integrated Nanotechnology, Sandia National Laboratories and Los Alamos National Laboratory • cint.sandia.gov • cint.lanl.gov

Center for Nanophase Materials Sciences, Oak Ridge National Laboratory • www.cnms.ornl.gov

Center for Nanoscale Materials, Argonne National Laboratory • nano.anl.gov

Molecular Foundry, Lawrence Berkeley National Laboratory • www.foundry.lbl.gov

National Nanotechnology Initiative

On the Web: www.nano.gov

February 2003