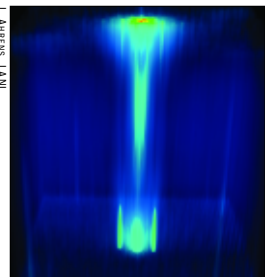


# Research Centers for

Almost 50 years ago at a Caltech lecture, physicist Richard Feynman provided a succinct definition of what has come to be known as nanoscience: "...the problem of manipulating and controlling things on a small scale."



J. ANDREWS, LANL

Advances during the ensuing years have refined the definition, and "small scale" now denotes dimensions less than 100 nm and "things" may include objects from electronic devices, catalysts, and thin film conductors to biological materials, such as proteins and DNA.

Controlling and developing these tiny structures involves manipulation on a molecular and, at least theoretically, atomic scale. Nanoscience must be concerned with scaling issues in order to bridge the gap between size ranges. The physics used to understand the macro-scale does not apply, and nuclear physics does not control the interactions either. For example, gravity plays much less of a role at the nanoscale, while molecular interactions, such as van der Waals attraction and chemical bonds, become much more important.

Nanoscience is a diverse and multidisciplinary field, drawing expertise from chemistry, biology, physics, computing, and others. Nanotechnology relies heavily on computational support; in some cases, physical limitations and challenges bar investigation by all means except simulation. Interestingly, nanoscience holds out the prospect of making revolutionary contributions to computing. New devices and hardware architectures may one day trigger the breakthrough to exascale computing.

The exciting computational nanoscience research conducted at the five U.S. Department of Energy (DOE) Nanoscale Science Research Centers (NSRCs) is the focus of this issue. NSRC research highlights the significant role simulation and theory have in nanotechnology development, and this issue's articles reflect these areas of interest.

The five NSRCs are scientific user facilities managed by the Office of Basic Energy Sciences and collectively are part of the DOE's contribution to the multi-agency National Nanotechnology Initiative. The centers, which opened between 2005 and 2008, have produced significant and exciting research, especially in the DOE's primary nanoscience interests—addressing growing global energy needs and improving the efficiency

of energy production and utilization. These NSRCs will further nanoscience research and application, a key element to America's continued global competitiveness.

- The **Center for Nanophase Materials Sciences (CNMS)** at Oak Ridge National Laboratory (ORNL) integrates nanoscale science research with neutron science, synthesis science, and theory/modeling/simulation. Collocated with the Spallation Neutron Source (SNS) complex, the facility's major scientific thrusts are nanodimensioned soft materials, complex nanophase materials systems, and the crosscutting areas of interfaces and reduced dimensionality that become scientifically critical on the nanoscale. CNMS will exploit two unique ORNL capabilities: (1) neutron scattering at the SNS, and (2) computational leadership at the National Center for Computational Sciences. The CNMS article (p14) highlights research advances in nanomagnetism, yttrium silicide nanowires, nanoparticle growth, and nanostructured thermoelectrics. ORNL's computational end station will play a significant role by supplying codes and methods to users seeking to advance nanoscience.

- The **Molecular Foundry** at Lawrence Berkeley National Laboratory (LBNL) uses six established facilities, including the Advanced Light Source, the National Center for Electron Microscopy, and the National Energy Research Scientific Computing Center, to assist assembly of complex structures from soft, biological, polymeric units and hard, inorganic, microfabricated units. This issue presents studies from the Foundry's Theory Facility (p22), where computation and theory researchers are investigating areas including electrical transport in nanoscale junctions, self-assembly of biological nanostructures, and the development of new methods and algorithms for understanding the spectral fingerprints of such nanomaterials.

- The **Center for Integrated Nanotechnologies (CINT)**, jointly administered by Los Alamos National Laboratory (LANL) and Sandia National Laboratories, focuses on such areas as nanophotonics and nanoelectronics, complex functional nanomaterials, nanomechanics, and the nanoscale/bio/microscale interfaces. This

Nanoscience holds out the prospect of making revolutionary contributions to computing. New devices and hardware architectures may one day trigger the breakthrough to exascale computing.

# NANOSCALE Science

center makes use of a wide range of specialized facilities, including the Los Alamos Neutron Science Center and the National High Magnetic Field Laboratory. The “integrated nanotechnologies” in the center’s name emphasizes the exploration from initial scientific discovery to integration of the nanostructures into the micro- and macro-worlds, and the experimentation and theory along the way. Understanding new performance regimes and concepts, testing designs, and integrating nanoscale materials and structures complete this path. The CINT article (p32) details the contributions from visualization on the understanding of nanoscience and nanoscale effects that control materials properties.

● The focus of the newly operating **Center for Functional Nanomaterials (CFN)** at Brookhaven National Laboratory is to better understand the chemical and physical response of nanomaterials, especially as applicable to sensors, activators, and energy-conversion devices. At CFN, two groups, Electron Microscopy and the Theory and Computation Group, investigate three areas: Interface Science and Catalysis, Electronic Nanomaterials, and Soft and Biological Nanomaterials. Existing facilities, such as the National Synchrotron Light Source and the Laser Electron Accelerator, are also available to CFN researchers. Discussed in the article (p38) are CFN’s efforts to extend computations to the nanoscale, including hydrogen storage in aluminum compounds doped with titanium, new gold-containing catalysts for removing carbon monoxide impurities from hydrogen gas, water-splitting on gallium nitride films, and the geometrical structure of small gold particles.

● Research at Argonne National Laboratory’s **Center for Nanoscale Materials** focuses on advanced magnetic materials, complex oxides, nanophotonics, and bio-inorganic hybrids. Characterization of extremely small structures benefits from the presence of Argonne’s Advanced Photon Source, through a nanoprobe beam line of hard X-rays. The center also uses the Intense Pulsed Neutron Source and the Electron Microscopy Center. This issue presents an overview of computational catalysis (p48), which represents one area of the center’s research.

## NANOSCIENCE CONTENT

**Science at the Nanoscale** p8

INTERVIEW: STANLEY WILLIAMS  
HEWLETT-PACKARD LABORATORIES

**The Computational Materials End Station at the Center for Nanophase Materials Sciences** p14

CENTER FOR NANOPHASE MATERIALS SCIENCES (CNMS)  
OAK RIDGE NATIONAL LABORATORY

**Understanding Nanoscale Systems at the Molecular Foundry** p22

MOLECULAR FOUNDRY  
LAWRENCE BERKELEY NATIONAL LABORATORY

**To See is to Know: Visualization** p32

CENTER FOR INTEGRATED NANOTECHNOLOGIES (CINT)  
LOS ALAMOS AND SANDIA NATIONAL LABORATORIES

**Computational Energy Research at CFN** p38

CENTER FOR FUNCTIONAL NANOMATERIALS (CFN)  
BROOKHAVEN NATIONAL LABORATORY

**Recent Trends in Computational Catalysis** p48

CENTER FOR NANOSCALE MATERIALS  
ARGONNE NATIONAL LABORATORY

**Cortical Computing with Memristive Nanodevices** p58

NEUROMORPHIC COMPUTING  
HEWLETT-PACKARD LABORATORIES

Along with the NSRC articles, read our interview with Stan Williams (p8), a Senior Fellow at Hewlett-Packard Laboratories and the Director of the InformatFion and Quantum Systems Laboratory. From the viewpoint of an industry pioneer, Williams gives a broad overview of nanoscience issues and implications, as well as the future of computing.

Finally, Greg Snider, also of Hewlett-Packard Laboratories, presents a potential new computing paradigm—neuromorphic computing—made possible by the nanotechnological breakthrough of memristors, a new circuit element (p58). Neuromorphic computing not only mimics the neural structure and behavior of the human brain but also solves the same fuzzy, analog problems people face daily, problems yet to be addressed by traditional computers. ●

**Contributor:** Dr. Jeff Nichols, ORNL