Research Activity:

Division: Primary Contact(s): Division Director:

Nanoscale Science Research Centers

Scientific User Facilities Altaf (Tof) Carim (carim@science.doe.gov; 301-903-4895) Pedro A. Montano

Portfolio Description:

This activity supports the operation of five Nanoscale Science Research Centers (NSRCs) at Department of Energy (DOE) national laboratories. These are: the Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL); the Molecular Foundry at Lawrence Berkeley National Laboratory (LBNL); the Center for Integrated Nanotechnologies (CINT) at Sandia National Laboratories (SNL) and Los Alamos National Laboratory (LANL); the Center for Nanoscale Materials (CNM) at Argonne National Laboratory (ANL); and the Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory (BNL). The major projects to construct, establish, and equip the NSRCs are now complete, with the last one finished in FY 2008; all five facilities are in full operations serving the user community. All encompass state-of-the-art instrumentation and expert staff to support the synthesis, processing, fabrication, analysis, simulation, and characterization of materials at the nanoscale. The NSRCs are major user facilities serving researchers from academia, national laboratories, and industry and already serve nearly 800 users annually.

Unique Aspects:

Nanotechnology is the understanding and control of matter at dimensions of roughly 1 to 100 nanometers, where unique phenomena enable novel applications. With a nanometer corresponding to one billionth of a meter, nanoscale phenomena occur at the level of small numbers of atoms, molecules, and supramolecular structures. The NSRCs make sophisticated research tools for nanoscience and nanotechnology available to the broad scientific community, and facilitate access to other collocated major facilities including synchrotron radiation light sources, neutron scattering centers, and electron beam microcharacterization facilities. The NSRCs are the DOE signature activity in nanoscale research and constitute the nation's largest scientific infrastructure investment under the National Nanotechnology Initiative (NNI).

NSRCs provide unique scientific and engineering capabilities not available in any of the parallel programs sponsored by other entities. For example, other federal agencies sponsor research in nanoscience at universities, but such programs are generally limited in scope and size, centered on specific research issues or topical areas, and primarily involve researchers of the host institution and a limited number of partners. The NSRCs are larger-scale facilities with a broad remit and range of capabilities and are broadly accessible without usage fees for non-proprietary work, with instrument time and staff support allocated on the basis of peer-review of proposals. The purposes of the NSRCs are as follows:

- Advance the fundamental understanding and control of materials at the nanoscale regime
- Provide an environment to support research of a scope, complexity, and disciplinary breadth not possible under traditional individual investigator or small group efforts
- Provide the foundation for the development of nanotechnologies important to DOE
- Provide state-of-the-art equipment to in-house laboratory, university, and industry researchers and leverage the capabilities of national user facilities for materials characterization employing electrons, photons, and neutrons
- Provide a formal mechanism for both short- and long-term collaborations and partnerships among DOE laboratory, academic, and industrial researchers
- Provide training for graduate students and postdoctoral associates in interdisciplinary nanoscale science, engineering, and technology research

Relationship to Other Programs:

The fundamental science being carried out at the NSRCs is closely related to BES programmatic research on the nanometer scale at both universities and national laboratories. Researchers supported by BES, by other parts of the Office of Science, by other parts of DOE, and by other federal agencies participate in the overall NSRC user community. While not a requirement, a major benefit is the opportunity for users to collaborate with the NSRC scientists. In addition, the NSRCs are collocated with, and serve as access points to, existing major BES user facilities for x-ray, neutron, and electron scattering. The DOE nanoscience activities as a whole are coordinated with other agencies through the Nanoscale Science, Engineering, and Technology (NSET) Subcommittee of the

National Science and Technology Council (NSTC); this Subcommittee is responsible for the federal NNI program and is currently co-chaired by representatives from BES and the Office of Science and Technology Policy.

Significant Accomplishments:

Physical construction of six new buildings has been completed for the five NSRCs, the initial complement of technical equipment has been successfully installed and commissioned, and all five facilities entered full user operations between FY 2006 and FY 2008. All five had robust pre-operations "jump-start" user programs in which existing capabilities of the host laboratories were made available to outside users as a prelude to operations of the NSRCs themselves. Hundreds of user proposals were accommodated during this period, leading to substantial advances in a number of areas; a few examples include the development and application of methods for the controlled synthesis of hollow or filled nanospheres; new insights on charge transport within two-dimensional and quasi-one-dimensional nanocrystal arrays; and the development of modular microlaboratories that facilitate sophisticated, reproducible measurement of the behavior and properties of nanomaterials. In the operations phase of the NSRCs, user activity has picked up accordingly, with nearly 800 unique users in FY 2007 for the four centers that had operations funding that year. Research highlights include the DNA-mediated crystallization of nanoparticle arrays into three-dimensional ordered structures, the production of hollow protein nanotubes by self-assembly of surface-modified hexameric ring structures, and the deposition of metallic nanoparticles on a preapplied film of carbon nanotubes on plastic to create flexible hydrogen sensors.

Mission Relevance:

A part of the mission of the Office of Science is to "deliver the premier tools of science to our Nation's research enterprise." The NSRCs join the suite of major DOE user facilities that fulfill this objective. A seminal DOE-BES workshop and subsequent report on *Basic Research Needs to Assure a Secure Energy Future* cited nanoscience as a critical cross-cutting theme, and this has been reiterated in numerous follow-up reports on Basic Research Needs for specific focused aspects of energy research, such as the hydrogen economy, solar energy utilization, and solid-state lighting. In addition, BES and the NSTC cosponsored a major workshop and report on *Nanoscience Research for Energy Needs* that identified key research targets and foundational themes for energy-related nanoscience. As stated in the Executive Summary of that report, "At the root of the opportunities provided by nanoscience to enhance our energy security is the fact that all of the elementary steps of energy conversion (e.g., charge transfer, molecular rearrangement, chemical reactions, etc.) take place on the nanoscale."

Scientific Challenges:

Strategic investments in scientific areas of opportunity are necessary to help our nation develop a balanced research and development infrastructure, advance critical research areas, and nurture the scientific and technical workforce of the 21st century. Nanotechnology R&D is a top federal priority with broad potential implications for the nation's competitiveness. DOE's participation in this effort includes the development and operation of the NSRCs, whose goals include: (1) to attain a fundamental scientific understanding of nanoscale phenomena, particularly collective phenomena; (2) to achieve the ability to design and synthesize materials at the atomic level to produce materials with desired properties and functions; (3) to take full advantage of other existing major user facilities, and (4) to develop experimental characterization techniques and theory/modeling/simulation tools necessary to drive the nanoscale revolution.

There are a large number of specific scientific challenges, many of which benefit from the collocation of disparate disciplines in order to fabricate, assemble, and otherwise manipulate nanosized components. One of the most challenging scientific problems is interfacing hard and soft matter, i.e., the world of electronic and structural materials with the world of biomaterials. These centers employ advanced experimental and theoretical tools to tailor and control the functionality (e.g., detection ability and sensitivity), compatibility, performance, and integration of materials at such interfaces.

Funding Summary:

	<u>FY 2007</u>	<u>FY 2008</u>	<u>FY 2009</u> <u>Request</u>
Construction:			
The Molecular Foundry, LBNL	257	0	0
Center for Integrated Nanotechnologies, SNL/LANL	247	0	0
Center for Functional Nanomaterials, BNL	18,864	363	0
Other Project Costs - CFN	500	0	0
Operation:			
Center for Nanoscale Materials, ANL	18,019	18,526	20,857
Center for Nanophase Materials Sciences, ORNL	18,115	18,000	19,975
The Molecular Foundry, LBNL	19,056	18,250	20,150
Center for Integrated Nanotechnologies, SNL/LANL	17,864	18,100	20,100
Center for Functional Nanomaterials, BNL	<u>0</u>	<u>18,250</u>	20,150
TOTAL	92,922	91,489	101,232

Projected Program Evolution:

The NSRCs are completing the transition to standard user operations within the new facilities and with their initial suite of specialized technical equipment. This process is bringing major new resources on-line for users, including nanoprobe beamlines at synchrotron radiation sources, extensive cleanroom facilities, nanoscale electron beam writers, and extensive nanomaterials synthesis and assembly capabilities. User programs are already adapting to respond to the needs of the community, with targeted acquisitions of new capital equipment and allocation of staff and accompanying resources to those areas that are most in demand. While a substantial user base is established already, the NSRCs are still being assimilated into the national scientific infrastructure; there will continue to be an increase in submitted proposals with a corresponding increase in users and/or corresponding decrease in the proposal approval rate, until a steady state is reached. The NSRCs are expected to perform as world-leading institutions, excelling both in scientific impact and productivity and in working with users. These are the fundamental criteria for evaluation of the NSRC facilities; each has undergone an initial (baseline) operations review and subsequent reviews will follow triennially.

Dollars in Thousands