

## Nanoscale Science Research Centers

### Portfolio Description

The Nanoscale Science Research Centers (NSRCs) are DOE's premier user facilities for interdisciplinary research to understand and control matter at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. NSRCs provide critical infrastructure to support the national nanoscience research effort in energy and are the single largest investment of the National Nanotechnology Initiative. Each center has particular expertise and capabilities in selected theme areas such as electronic and photonic nanomaterials synthesis, electron microscopy, quantum structures, nanostructure characterization, catalysis, theory/modeling/simulation, soft and biological materials, imaging and spectroscopy, nanofabrication, and nanoscale integration. The centers are housed in custom-designed laboratory buildings located near major BES facilities for x-ray or neutron scattering, which complement and leverage the capabilities of the NSRCs. These laboratories contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other world-class instruments not generally available except at major user facilities. NSRCs are knowledge-based facilities which, in addition to instrumentation capabilities, offer optional collaborative research with expert scientists in their fields. These facilities are routinely made available on a scientific-merit basis to the broad research community. The five NSRCs are:

- Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory
- Center for Integrated Nanotechnologies (CINT) at Los Alamos National Laboratory and Sandia National Laboratories
- Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory
- Center for Nanoscale Materials (CNM) at Argonne National Laboratory
- The Molecular Foundry (TMF) at Lawrence Berkeley National Laboratory

### 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 21<sup>st</sup> 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 develop experimental characterization techniques and theory/modeling/simulation tools necessary to drive the nanoscale revolution; and (4) to take full advantage of synergies with other existing major user facilities.

There are a large number of specific scientific challenges, many of which benefit from the co-location of disparate disciplines in order to fabricate, assemble, and manipulate nanosized components into complex macroscopic 3D structures having functionality at nanoscale dimensions. One of the most challenging scientific problems is interfacing hard and soft matter, e.g., 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, compatibility, performance, and integration of materials at such interfaces towards realizing systems that benefit society. These facilities must be kept in optimal operation to serve the ever-increasing number of users.

## **Projected Evolution**

The NSRCs have established significant major capabilities and scientific leadership in several areas of nanoscience and work effectively with the large user community and their co-located facilities. The NSRC Triennial Reviews in CY 2016 showed that they have very high scientific productivity and serving a record 3,200 Users. The number of user proposals has steadily increased and acceptance rates have begun to decrease, indicating that the Centers are at capacity. Publication productivity in high-impact journals and the increasing user demand are signs that the NSRCs have been effectively assimilated into the national scientific infrastructure. The NSRCs are expected to perform as world-leading institutions, excelling both in scientific impact and productivity and in working with users. As they evolve, they will continue to develop new and unique world-leading capabilities in nanomaterials synthesis, characterization, nanofabrication, theory, and computation to serve the scientific community. Scientific themes are evolving synergistically into the physical biosciences and chemistry disciplines. With comprehensive capabilities and a collaborative research model, NSRCs accelerate the best research with users in a cost-effective way and assist in the translation of basic science with industry users in the area of manufacturing science.

## **Significant Accomplishments**

All five NSRC facilities entered full user operations between FY 2006 and FY 2008. In the operations phase of the NSRCs, user activity has increased substantially from four operational centers with nearly 800 unique users in FY 2007 to the present five operating centers serving over 3,200 users in FY 2016. In FY 2015, the Electron Beam Microcharacterization Centers were merged with their co-located NSRCs, increasing the world-class capabilities available to NSRC users. Since their inception the NSRCs have served over 27,000 users, and they are essentially at capacity. Many new and exciting capabilities and scientific discoveries have emerged in a wide range of nanoscience areas. Research highlights include:

- The electron-beam-directed assembly of polymers with features relevant to terabit-per-square inch magnetic storage media was achieved.
- Novel metamaterials for next-generation terahertz flat optics were developed.
- World record atomic-scale electron tomography measurement capability was developed to determine positions of atoms (22 picometer accuracy).
- Unprecedented-spatial-resolution hard x-ray optics for nanotomography implemented.
- Precision polymer deuteration chemical processes were developed for enhancing neutron-beam probing of soft-material folding behavior.
- Lubricants composed of nanodiamonds and graphene that exhibit near-zero friction were invented.
- A new spectroscopic optical scanning probe for characterizing surface chemistry at the nanoscale was invented and is being commercialized.
- The first 3D crystalline nanoparticle superlattice assembly using a novel solution-based self-assembly approach was achieved.
- Successful synthesis of new 2D materials for quantum sensing and computing was demonstrated.
- New atmospheric pressure *in operando* x-ray characterization capabilities established for catalysis studies.

## **Unique Aspects**

NSRCs are unique in that they provide capabilities and expert resources to the scientific user community to discover, understand, and synthesize nanomaterials and nanostructures, and facilitate access to other co-located major facilities including synchrotron radiation light sources,

neutron scattering centers, high-performance computing, and microfabrication facilities. The NSRC model accelerates cycles of learning and leverages investments in university, government and industry research projects. The NSRCs offer a broad range of capabilities and are accessible without usage fees for non-proprietary work, with instrument time and staff support allocated on the basis of peer-reviewed proposals. The purposes of the NSRCs are as follows:

- Advance the fundamental understanding and control of phenomena and materials at the nanoscale regime.
- Provide an environment to support interdisciplinary 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 unique and state-of-the-art tools to university, laboratory, and industry researchers and leverage the capabilities of other national user facilities for materials characterization employing 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.

### **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* ([report link](#)) 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 ([report link](#)), solar energy utilization ([report link](#)), and solid-state lighting ([report link](#)). The most recent BES Advisory Committee (BESAC) report *Challenges and Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science* ([report link](#)) further emphasizes the importance of nanoscience to achieving breakthroughs at these frontiers. In addition, BES and the National Science and Technology Council co-sponsored a major workshop and report on *Nanoscience Research for Energy Needs* ([report link](#)) 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."

### **Relationship to Other Programs**

- The fundamental science being carried out at the NSRCs is closely related to BES programmatic research spanning nanometer through mesoscales at universities, national laboratories and companies. Over 30% of BES-supported principal investigators are NSRC users. NSRCs strongly support the DOE Energy Innovation Hubs and Energy Frontier Research Centers.
- Researchers supported by other parts of the Office of Science, other parts of DOE, and other federal agencies are part of the overall NSRC user community.
- BES coordinates nanoscience activities with other federal agencies through the National Science and Technology Council (NSTC) Nanoscale Science, Engineering, and Technology (NSET) subcommittee, which leads the National Nanotechnology Initiative.