SAND2008-1858P

Potential Contributions of the DOE Nanoscale Science Research Centers to Solid-State Lighting

Prepared for:

Lighting Research and Development
Building Technologies Program
Office of Energy Efficiency and Renewable Energy
U. S. Department of Energy

Prepared by:

National Center for Solid-State Lighting R&D
Center for Integrated Nanotechnologies
Sandia National Laboratories and
Los Alamos National Laboratory

March
2008

Potential Contributions of the DOE Nanoscale Science Research Centers to Solid-State Lighting

Prepared for:

Lighting Research and Development
Building Technologies Program
Office of Energy Efficiency and Renewable Energy
U. S. Department of Energy

Prepared by:

National Center for Solid-State Lighting R&D
Center for Integrated Nanotechnologies
Sandia National Laboratories and
Los Alamos National Laboratory

March
2008

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

ACKNOWLEDGMENTS

We gratefully acknowledge support of the research by the Department of Energy's Office of Energy Efficiency and Renewable Energy's Building Technologies Program administered by the National Energy Technology Laboratory. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

Table of Contents

Executive Summary **7**
1.0 Nanoscale Science and Solid-State Lighting **7**
1.1 The National Center for Solid-State Lighting R&D 7
1.2 DOE Solid-State Lighting Portfolio Strategy 8
1.3 Critical R&D Priorities 10
1.4 Basic Research Needs for Solid-State Lighting 15
1.5 Nanoscale Science Research Centers (NSRCs) 19
1.6 NSRC Common Capabilities Relevant to SSL 21
2.0 Center for Functional Nanomaterials **25**
2.1 General Information 25
2.2 CFN Scientific Themes 25
2.3 Center for Functional Nanomaterials Facilities 28
2.4 National Synchrotron Light Source 30
2.5 CFN Interactions with Users 31
2.6 CFN Contact Information 31
2.7 List of Capabilities 32
3.0 Center for Integrated Nanotechnologies **33**
3.1 General Information 33
3.2 CINT Research Thrusts 33
3.3 Grand Challenges 36
3.4 Discovery Platforms 37
3.5 Facilities 38
3.6 Interactions with Users 38
3.7 CINT Contact Information 39
3.8 List of Capabilities 39
4.0 Center for Nanophase Materials Sciences **42**
4.1 General Information 42
4.2 CNMS Scientific Themes 42
4.3 CNMS Research Capabilities 43
4.4 Facilities 47
4.5 Associated Major User Facilities at Oak Ridge National Lab 47
4.6 Interactions with Users 48
4.7 CNMS Contact Information 48
4.8 List of Capabilites 49
5.0 Center for Nanoscale Materials **52**
5.1 General Information 52
5.2 CNM Scientific Themes 52
5.3 Center for Nanoscale Materials Facilities 56
5.4 Associated Major User Facilities at Argonne National Laboratory 57
5.5 CNM Interactions with Users 58
5.6 CNM Contact Information 59
5.7 List of Capabilities 59
6.0 Molecular Foundry **62**
6.1 General Information 62

6.2 Molecular Foundry Research Themes 62
6.3 Molecular Foundry Research Facilities 63
6.4 Molecular Foundry Laboratory Building... 65
6.5 Associated Major User Facilities at Berkeley Lab 65
6.6 Interactions with Users 66
6.7 Molecular Foundry Contact Information... 68
6.8 List of Capabilities.. 68

Executive Summary

The Department of Energy has made a long-term commitment to advance the development and introduction of energy-efficient Solid-State Lighting (SSL) for general illumination. The Office of Energy Efficiency and Renewable Energy (through the Building Technologies Program) has outlined the most important research and development priorities for addressing SSL technology hurdles. At the same time, the Office of Science has established five Nanoscale Science Research Centers (NSRCs) with unparalleled capabilities to advance the new field of nanoscience. Nanomaterials offer different chemical and physical properties than bulk materials, and understanding these properties may allow researchers to design materials with properties tailored to specific needs. Because many important energy transformation and transport processes occur at the nanoscale, nanoscience may ultimately make important contributions to the solutions of various SSL technology challenges. This report outlines the potential contributions that nanoscience, through the DOE Nanoscale Science Research Centers, could make to solid-state lighting technology. Some of the common NSRC capabilities that could be especially important in addressing fundamental nanoscale aspects of SSL include: nanostructure materials synthesis, nanofabrication, nanophotonics, nanoelectronics, materials structure and characterization, and theory / modeling.

1.0 Nanoscale Science and Solid-State Lighting

1.1 The National Center for Solid-State Lighting R&D

The National Center for Solid-State Lighting Research and Development (NCSSL) was created in 2006 to support research in the emerging field of nanotechnology that could be applied to Solid-State Lighting (SSL) Core technology. SSL Core nanotechnology research includes scientific efforts that seek to gain more comprehensive knowledge or understanding of nanometer scale phenomena for the specific application of SSL.

The NCSSL was formed as a virtual, multi-lab center to maximize: the flexibility of time-appropriate research topics; the unique capabilities of the National Laboratories to contribute to this work; and the results and rate of production. The five Department of Energy (DOE) Office of Science (SC) Nanoscale Science Research Centers (NSRCs) were eligible to compete for initial funding administered by the National Energy Technology Laboratory (NETL), on behalf of the Office of Energy Efficiency and Renewable Energy's (EERE) Building Technologies Program (BT). A total of $5M in research grants of up to 18 months duration were awarded for seven technical projects at the NSRCs. (Specific results from those projects are not the covered in this document.) The Center for Integrated Nanotechnologies (CINT), jointly operated by Sandia National Laboratories and Los Alamos National Laboratory, was selected as the lead center for the NCSSL.

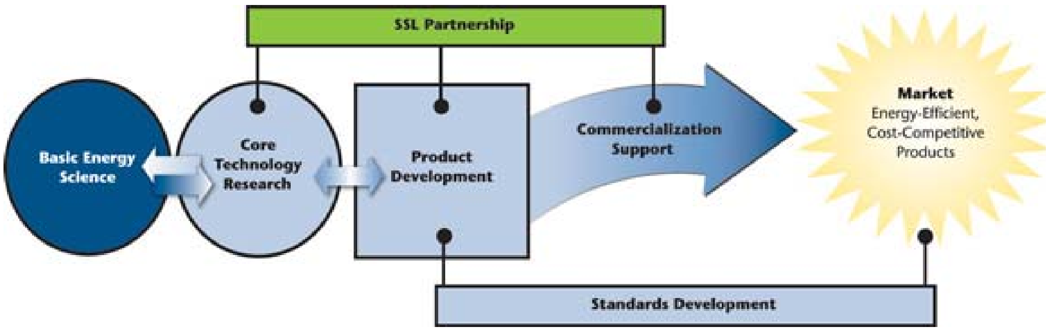

Figure 1. Department of Energy Solid-State Lighting Portfolio Strategy.

This report was commissioned by the NCSSL to summarize areas in which nanoscience, and specifically the five DOE / Office of Science Nanocenters, could impact Solid-State Lighting research and development.

1.2 DOE Solid-State Lighting Portfolio Strategy

The Department of Energy has made a long-term commitment to advance the development and market introduction of energy-efficient white-light sources for general illumination. Solid-state lighting differs fundamentally from today's lighting technologies, and its unique attributes drive the need for a coordinated approach that guides technology advances from laboratory to marketplace. The DOE program in Solid-State Lighting is coordinated by the Office of Energy Efficiency and Renewable Energy through the Building Technologies Program. The official government SSL web site is maintained at http://www.netl.doe.gov/ssl/ .

The DOE goal of the SSL portfolio is:

> *By 2025, develop advanced solid state lighting technologies that, compared to conventional lighting technologies, are much more energy efficient, longer lasting, and cost-competitive by targeting a product system efficiency of 50 percent with lighting that accurately reproduces sunlight spectrum.*

DOE has developed a comprehensive national strategy that encompasses Basic Energy Science, Core Technology Research, Product Development, Commercialization Support, Standards Development, and an SSL Partnership. The definitive description of the DOE Solid-State Lighting strategy is given in the "Multi-Year Program Plan: FY08-FY13," available on the web at http://www.netl.doe.gov/ssl/PDFs/SSLMYPP2007_web.pdf (along with a supplement / update published in early 2008 with revisions to Section 4, available at http://www.netl.doe.gov/ssl/PDFs/Materials_2008/SSL-MYPP2008.pdf).

Basic Energy Science

The Basic Energy Sciences Program within DOE's Office of Science conducts basic research to advance our fundamental understanding of materials behavior, with the goal of impacting future directions in applied research and technology development. Project results often have multiple applications, which could include SSL. For additional information, visit the BES web site at http://www.sc.doe.gov/bes/ .

Core Technology Research

Through a series of ongoing, interactive workshops, DOE and its SSL partners have refined an extensive R&D agenda to ensure that DOE funds the appropriate research topics that will improve efficiency and speed SSL technologies to market. Core Technology Research – conducted primarily by academia, national laboratories, and research institutions – involves applied research efforts to seek more comprehensive knowledge about a technology area such as Solid-State Lighitng. These projects fill technology gaps, provide enabling knowledge or data, and represent a significant advance in our knowledge base.

Product Development

Conducted primarily by industry, Product Development is the systematic use of knowledge gained from basic or applied research to develop or improve commercially viable materials, devices, or systems for Solid-State Lighitng. Laboratory testing is conducted on prototypes, and feedback is used to improve prototype design. In addition to technical activities, market and fiscal studies are performed to ensure a successful transition to the marketplace.

Commercialization Support

To ensure that DOE investments in Core Technology Research and Product Development lead to SSL technology commercialization, DOE has developed a national strategy to guide market introduction of SSL for general illumination. This strategy draws on DOE's involvement in virtually every aspect of SSL R&D and the Department's ongoing relationships with the SSL industry, research community, standards setting groups, and energy efficiency organizations.

Standards Development

The development of national standards and rating systems for new products enables consumers to compare products made by different manufacturers, since all companies must test their products and apply the rating in the same way. DOE works closely with industry and standards setting organizations, providing leadership and support to accelerate the standards development process and technical assistance in the development of new standards.

SSL Partnership

Supporting DOE SSL portfolio activities is the SSL Partnership. DOE's Memorandum of Agreement with the Next Generation Lighting Industry Alliance, signed in February 2005, details a strategy to enhance the manufacturing and commercialization focus of the DOE SSL portfolio by utilizing the expertise of an organization of SSL manufacturers. The Partnership provides significant input to shape DOE research priorities and, at DOE's discretion, provides technical expertise for proposal and project reviews.

1.3 Critical R&D Priorities

The Solid-State Lighting Research and Development "Multi-Year Program Plan FY08-FY13" lists SSL Priority Tasks, with task metrics, current status, and 2015 program targets. The original task structure and initial priorities were defined at a workshop in San Diego in February, 2005. These research priorities were updated in 2006 and again in the most recent Multi-Year Plan. These tasks and priorities are the result of considerable input and discussion amongst industrial, academic, and national laboratory experts in the lighting field. The Multi-Year Plan containing a complete list of the prioritized Tasks can be found at: http://www.netl.doe.gov/ssl/PDFs/SSLMYPP2007_web.pdf (along with a 2008 update at http://www.netl.doe.gov/ssl/PDFs/Materials_2008/SSL-MYPP2008.pdf).

The EERE / NETL Solid-State Lighting program relies upon these prioritized SSL task lists as a basis for target areas in Calls for Proposals and in evaluating research proposals. A partial list of tasks from the 2008 updates, including the designated Task number (e.g., 1.3.2), title, and a short description (in parentheses), is given next. The highest priority tasks are designated as "2008 Priority Tasks." Additional "Later Priority" and "Long-Term Priority" tasks may ultimately need attention to achieve the overall SSL goals.

The EERE priority tasks listed next are areas that could potentially benefit from fundamental nanoscience research using capabilities at the DOE NSRCs. Section 1.4 of this report contains a list of basic research needs in solid-state lighting that was compiled at a workshop sponsored by the Office of Basic Energy Sciences (see more details in that section). The designators in square brackets listed below, e.g., [PRD4], provide a mapping of basic research areas onto the EERE priority tasks; a complete description of these basic research areas is given in Section 1.4. A complete list of the overlap between the BES basic research recommendations and the EERE priority tasks is presented in Table 1.

LED Core Technology Research Tasks (2008 Priority Tasks)

- 1.1.2: High-efficiency semiconductor materials (Improve IQE across the visible spectrum and in the near UV, down to 360 nm); [GC1, GC2, PRD1, PRD2, PRD3, PRD4, CCRD3, CCRD5]
- 1.3.1: Phosphors and conversion materials (High-efficiency wavelength conversion materials for improved quantum yield, optical efficiency, color stability); [PRD2, CCRD5]

LED Core Technology Research Tasks (Later Priority Tasks)

- 1.2.1: Device approaches, structures and systems (Alternative emitter geometries and emission mechanisms, i.e., lasing, surface plasmon enhanced emission); [GC1, CCRD1, CCRD2, CCRD3]
- 1.2.2: Strategies for improved light extraction / manipulation (Improved chip level light extraction / LED system efficiency; phosphor scattering / encapsulation); [GC1, CCRD2, CCRD3]

LED Core Technology Research Tasks (Long-Term Priority Tasks)

- 1.1.3: Reliability and defect physics for improved emitter lifetime and efficiency (Dopant and defect physics; device characterization and modeling; investigation of droop, i.e., reduced efficiency at high temperature and current density); [GC2, PRD4, CCRD5]

LED Product Development Tasks (Later Priority Tasks)

- 2.1.2: High-efficiency semiconductor materials (Improve IQE across the visible spectrum and in the near UV, down to 360 nm); [GC1, GC2, PRD1, PRD4, CCRD5]
- 2.1.3: Implementing strategies for improved light extraction and manipulation (Develop high refractive index encapsulants for improved light extraction and large-area light extraction and current injection); [CCRD2]

OLED Core Technology Research Tasks (2008 Priority Tasks)

- 3.1.2, 3.2.2: Novel materials and device architectures (Single and multi-layered device structures to increase IQE, reduce voltage, and improve device lifetime); [PRD5, PRD6, PRD7, CCRD5]

OLED Core Technology Research Tasks (Long-Term Priority Tasks)

- 3.3.1: Down conversion materials; [PRD2]
- 3.4.1: Physical, chemical and optical modeling for fabrication of OLED devices; [GC1, CCRD4]

OLED Product Development Research Tasks (Later Priority Tasks)

- 4.2.3: Demonstrate device architectures: e.g., white-light engines, multi-color versus single emission (Includes demonstrating a device that is scalable); [CCRD4]

OLED Product Development Research Tasks (Long-Term Priority Tasks)

- 4.3.2: Simulation tools for modeling OLED devices; [GC1, CCRD4]

Thus, fundamental nanoscale *science* can clearly impact the important *technology* areas identified by EERE program (although the timescale for this pay-off will be longer term).

Table 1. Overlap between the EERE Priority Task Lists and BES Workshop "Basic Research Needs for SSL" Recommendations

Type of R&D	Priority	Task	Task Title	GC1 Rational Design of SSL Structures	GC2 Controlling Losses in the Light-Emission Process	PRD1 Unconventional Light-Emitting Semiconductors	PRD2 Photon Conversion Materials	PRD3 Polar Materials and Heterostructures	PRD4 Luminescence Efficiency of InGaN Structures	PRD5 Managing and Exploiting Disorder in Organic Films	PRD6 Understanding Purity and Degradation in OLEDs	PRD7 Integrated Approach to OLED Design	CCRD1 New Functionalities through Heterogeneous Nanostructures	CCRD2 Innovative Photon Management	CCRD3 Enhanced Light-Matter Interactions	CCRD4 Multiscale modeling for Solid-State Lighting	CCRD5 Precision Nanoscale Characterization
LED Core Tech.	2008	1.1.2	High-efficiency semiconductor materials	x	x	x	x	x	x						x		x
LED Core Tech.	2008	1.3.1	Phosphors and conversion materials				x										x
LED Core Tech.	2008	1.3.2	Encapsulants and packaging materials														
LED Core Tech.	2008	1.4.x	Inorganic growth and fabrication processes and manufacturing research.														
LED Core Tech.	Later	1.2.1	Device approaches, structures and systems	x									x	x	x		
LED Core Tech.	Later	1.2.2	Strategies for improved light extraction and manipulation	x										x	x		
LED Core Tech.	Later	1.3.4	Measurement metrics and color perception														
LED Core Tech.	Long Term	1.1.1	Large-area substrates, buffer layers, and wafer research														
LED Core Tech.	Long Term	1.1.3	Reliability and defect physics for improved emitter lifetime and efficiency		x				x								x

Table 1 (continued)

Type of R&D	Priority	Task	Task Title	GC1	GC2	PRD1	PRD2	PRD3	PRD4	PRD5	PRD6	PRD7	CCRD1	CCRD2	CCRD3	CCRD4	CCRD5
LED Core Tech.	Long Term	1.3.3	Electrodes and interconnects														
LED Prod. Devel.	2008	2.2.1	Manufactured materials														
LED Prod. Devel.	2008	2.2.2	LED packages and packaging materials														
LED Prod. Devel.	2008	2.3.1	Optical coupling and modeling														
LED Prod. Devel.	2008	2.3.4	Thermal design														
LED Prod. Devel.	2008	2.3.6	Evaluate luminaire lifetime and performance characteristics														
LED Prod. Devel.	2008	2.3.3	Power Electronics Development														
LED Prod. Devel.	Later	2.1.2	High-efficiency semiconductor materials	x	x	x			x								x
LED Prod. Devel.	Later	2.1.3	Implementing strategies for improved light extraction and manipulation											x			
LED Prod. Devel.	Later	2.2.3	Modeling, distribution, and coupling issues														
LED Prod. Devel.	Later	2.4.1	Incorporate proven in-situ diagnostic tools into existing equipment.														
LED Prod. Devel.	Later	2.4.2	Develop low-cost, high-efficiency reactor designs														
LED Prod. Devel.	Later	2.4.3	Develop techniques for die separation, chip shaping, and wafer bonding														
LED Prod. Devel.	Long Term	2.1.1	Substrate, buffer layer and wafer engineering and development														
LED Prod. Devel.	Long Term	2.1.4	Device architectures with high power-conversion efficiencies														
LED Prod. Devel.	Long Term	2.2.4	Evaluate component lifetime and performance characteristics														
LED Prod. Devel.	Long Term	2.3.2	Mechanical design														
LED Prod. Devel.	Long Term	2.3.5	Evaluate human factors and metrics														
OLED Core Tech.	2008	3.1.2, 3.2.2	Novel materials and device architectures.							x	x	x					x
OLED Core Tech.	2008	3.2.1	Novel strategies for improved light extraction														
OLED Core Tech.	2008	3.2.3	Research on low-cost transparent electrodes														
OLED Core Tech.	2008	3.4.2	Investigation of low-cost fabrication and patterning techniques and tools														

Table 1 (continued)

Type of R&D	Priority	Task	Task Title	GC1	GC2	PRD1	PRD2	PRD3	PRD4	PRD5	PRD6	PRD7	CCRD1	CCRD2	CCRD3	CCRD4	CCRD5
OLED Core Tech.	2008	3.3.2	Encapsulation and packaging technology														
OLED Core Tech.	Later	3.1.1	Substrate materials for electro-active organic devices														
OLED Core Tech.	Later	3.1.3	Improved contact materials, surface modification techniques to improve charge injection														
OLED Core Tech.	Later	3.1.4	Applied Research in OLED devices														
OLED Core Tech.	Later	3.3.1	Down conversion materials				x										
OLED Core Tech.	Later	3.3.3	Electrodes and interconnects														
OLED Core Tech.	Later	3.3.4	Measurement metrics and human factors														
OLED Core Tech.	Later	3.4.1	Physical, chemical and optical modeling for fabrication	x												x	
OLED Prod. Devel.	2008	4.1.1	Low-cost substrates														
OLED Prod. Devel.	2008	4.1.2, 4.2.2	Practical implementation of materials and device architectures.														
OLED Prod. Devel.	2008	4.2.1	Practical application of light extraction technology.														
OLED Prod. Devel.	2008	4.4.1	Module and process optimization and manufacturing														
OLED Prod. Devel.	2008	4.3.1	OLED encapsulation packaging for lighting applications														
OLED Prod. Devel.	Later	4.1.3	Improved contact materials and surface modification techniques to improve charge injection														
OLED Prod. Devel.	Later	4.2.3	Demonstrate device architectures: e.g., white-light engines (multi-color versus single emission)													x	
OLED Prod. Devel.	Long Term	4.3.2	Simulation tools for modeling OLED devices	x												x	
OLED Prod. Devel.	Long Term	4.3.3	Voltage conversion, current density and power distribution and driver electronics														
OLED Prod. Devel.	Long Term	4.3.4	Luminaire design, engineered applications, field tests and demonstrations														
OLED Prod. Devel.	Long Term	4.4.2	Synthesis manufacturing scale-up of active OLED materials														
OLED Prod. Devel.	Long Term	4.4.3	Tools for manufacturing the lighting module														

1.4 Basic Research Needs for Solid-State Lighting

To accelerate the laying of the scientific foundation that would enable technology breakthroughs in Solid-State Lighting, the Office of Basic Energy Sciences of the DOE convened the Workshop on Basic Energy Needs for Solid-State Lighting in 2006. A copy of the final workshop report is available on the web at: http://www.sc.doe.gov/bes/reports/files/SSL_rpt.pdf .

The charge to the workshop was to examine the gap separating current state-of-the-art SSL technology from an energy efficient, high-quality, and economical SSL technology suitable for general illumination; and to identify the most significant fundamental scientific challenges and research directions that would enable that gap to be bridged. Many of the SSL challenges identified in the workshop involve phenomena at the nanometer scale. Thus, researchers from academia, industry, and national labs (including the NSRCs) are well-suited to make significant contributions to these SSL fundamental research needs.

SSL Grand Challenges. The DOE / BES Workshop participants identified two Grand Challenges (GCs) – science questions so broad and fundamental that any significant progress towards their understanding and solution would be foundational to any future SSL technology. The following short descriptions of the GCs are summaries from the workshop report, cited above. In square brackets, e.g., [2.1.2], we also list the EERE Critical R&D priorities from Section 1.3 that could be impacted by each GC.

(GC1) Rational Design of SSL Structures: The goal of this Grand Challenge is holistic design of new light-emitting architectures and materials. Current designs consist of many interconnected components to manage the transport of charge carriers, photons, and heat. Individual components and materials are often chosen for their specific performance characteristics and then integrated into devices. The net light-emission efficiency is limited not only by the performance of each component, but also can be significantly limited by compatibility issues and interface losses in the integrated device architecture. Moreover, most new materials incorporated into light-emitting devices are "discovered" rather than rationally designed and then synthesized anew with their specific performance characteristics in mind. To approach 100% efficiency, fundamental building blocks should be designed so they work together seamlessly, but such a design process will require much greater insight than we currently possess. Hence, the aim of this Grand Challenge is to understand light-emitting organic and inorganic (and hybrid) materials and nanostructures at a fundamental level to enable the rational design of low-cost, high-color-quality, near-100% efficient SSL structures from the ground up. [EERE priority areas impacted: 1.1.2, 1.2.2, 1.2.1, 2.1.2, 3.4.1, 4.3.2]

(GC2) Controlling Losses in the Light-Emission Process: To achieve the highest-possible efficiency in light emission every electron and hole injected into the device must combine to emit a photon but no heat. However, there are many decay pathways that compete with the desired light production. Thus, the aim of this Grand Challenge is to discover and control the materials and nanostructure properties that mediate the competing conversion of electrons to light and heat, enabling the conversion of every injected electron into useful photons. Success in this Grand Challenge will produce ultra-high-efficiency light-emitting materials and nanostructures for SSL. In addition, the resulting scientific understanding of how light interacts with matter would have broader impact on science and other technology areas. [EERE priority areas impacted: 1.1.3, 1.1.2, 2.1.2]

SSL Priority and Cross-Cutting Research Directions. The BES Workshop participants identified a number of Priority Research Directions (PRDs) that would specifically impact inorganic-based (LED) or organic-based (OLED) Solid-State Lighting and several Cross-Cutting Research Directions (CCRDs) that could potentially impact both LEDs and OLEDs. The PRDs and CCRDs are areas for fundamental scientific inquiry. They are not as overarching as the Grand Challenges, but are more focused on a particular approach to SSL, or a particular scientific challenge. The following short descriptions of the PRDs and CCRDs are summaries from the workshop report, cited above. In square brackets, e.g., [2.1.2], we also list the EERE Critical R&D priorities from Section 1.3 that could be impacted by each PRD and CCRD.

(PRD1) Unconventional Light-Emitting Semiconductors: This PRD seeks to design and create unconventional light-emitting materials using advanced tools from computational modeling and theory and thin-film / bulk synthesis. Success would result in creation of materials with hybridized band structure, exciton states, transport properties, and doping properties for specific light-creation characteristics. Achieving this goal will require a fundamental understanding of how structure and solid-state chemistry dictate electroluminescent properties. [EERE priority areas impacted: 1.1.2, 2.1.2]

(PRD2) Photon Conversion Materials: Most of today's solid-state lighting approaches involve converting emission from a wide-bandgap semiconductor to longer wavelength photons by a phosphor material. Scientific research and development of photon conversion materials for SSL are at an early stage. Two areas of science are the focus of this PRD: the first area is discovery of new classes of phosphor materials; the second is design and synthesis of new classes of binder matrices that contain and protect phosphor grains. [EERE priority areas impacted: 1.3.1, 3.3.1]

(PRD3) Polar Materials and Heterostructures: Most of the known inorganic semiconductors with bandgaps wide enough to emit light in the ultraviolet and visible are polar materials. This PRD proposes a concerted effort aimed at manipulating and understanding the electronic and optoelectronic properties of polar materials and heterostructures. For example, in a polar material strain-induced piezoelectric fields cause separation of electrons and holes within quantum wells, which decreases radiative recombination rates and, thus, overall efficiency. In addition, polarization discontinuities at heterointerfaces can lead to high densities of interfacial charge, which can significantly affect charge injection and transport. Materials of interest in this PRD include those based on III-Nitrides, as well as other wide-bandgap polar semiconductors such as those based on ZnO. [EERE priority area impacted: 1.1.2]

(PRD4) Luminescence Efficiency of InGaN Structures: Presently the most promising approaches to inorganic solid-state lighting are based on InGaN alloys. However, InGaN materials that emit light efficiently at the high electron-hole injection densities critical to white-light illumination, and at the green-yellow wavelengths critical to human visual perception, have proven elusive. These limitations is not well understood, but are thought to arise from the complex interplay of a range of materials properties including compositional disorder, high defect densities and the presence of strong piezoelectric fields. This PRD calls for a deeper scientific understanding of luminescence mechanisms and limitations in InGaN alloys. [EERE priority area impacted: 1.1.2, 1.1.3, 2.1.2]

(PRD5) Managing and Exploiting Disorder in Organic Films: The influence of molecular scale order on properties of organic light-emitting devices is poorly understood, and our ability to control it is primitive. It is known, however, that disorder can either improve or degrade device performance, depending on its location within the thin film structure. One consequence of structural disorder is that electronic excitations and charges are spatially localized in organic thin films. Since charge transport takes place via hopping between localized states, the mobility is related to transfer mechanisms that depend sensitively on positional and orientational disorder between neighboring molecules. The goal of this PRD is to develop the fundamental science needed to understand, quantify, and control ordering in molecular thin films. [EERE priority areas impacted: 3.1.2, 3.2.2]

(PRD6) Understanding Purity and Degradation in OLEDs: This PRD seeks a fundamental understanding of degradation in organic light-emitting diodes. It appears that the purity of starting components, as well as degradation mechanisms that occur during device operation, seriously limit OLED device efficiency and lifetime. The ability to identify and quantify starting-reagent impurities and degradation byproducts will require major advances in analytical chemistry. New synthesis and purification techniques will be required to eliminate defects in the organic starting materials well beyond the requirements in most other organic chemistry applications, e.g., the chemicals industry. To prevent the formation of defects during device operation, a comprehensive approach that relates the degradation mechanisms to materials properties will be required to design materials that ultimately avoid these detrimental pathways. [EERE priority areas impacted: 3.1.2, 3.2.2]

(PRD7) Integrated Approach to OLED Design: The PRD seeks to move beyond an empirical Edisonian approach to a predictive science-based approach to OLED design, with the goal of higher efficiency, longer operating lifetime, and lower costs. To maximize efficiency, it is necessary to ensure that (1) essentially all electrons and holes injected into the structure form excitons, (2) the excitons recombine radiatively with high probability, (3) the light from these recombinations is efficiently coupled out of the device, (4) the drive voltage required to establish a given current density in the device is minimized, and (5) the material and device are stable under continuous operation. It has proven difficult to satisfy all the requirements simultaneously and there is a critical need for basic scientific research on the fundamental physical properties of organic electronic materials in realistic device structures. [EERE priority areas impacted: 3.1.2, 3.2.2]

(CCRD1) New Functionalities through Heterogeneous Nanostructures: Materials can exhibit unique and controllable size-dependent properties at the nanometer scale, leading to new degrees of freedom that can be exploited to control the fundamental physical and optoelectronic processes important for solid-state lighting. Electronic and optical properties of nanostructures depend strongly on their size, so light emission wavelength and efficiency can be tuned by the size of the nanostructure. Such size-tunable properties occur in all dimensions: 1-D confinement in semiconductor quantum wells, 2-D confinement in quantum wires, and 3-D confinement in quantum dots. This CCRD addresses science questions and opportunities that are key to developing new SSL functionalities through heterogeneous nanostructures. The important challenges are broadly divided into three areas: synthesis and self-assembly issues, understanding and control of radiative and nonradiative processes, and integration into SSL structures. The advanced functionality needed for SSL might require the precision alignment of nanomaterials, and thus advances in the science of synthesis and assembly are expected to have great impact. It is important to optimize the radiative processes relative to the nonradiative channels within such nanostructures, so fundamental science issues related to coupling of excitations in complex heterostructures and optical mode control must be addressed. A final challenge is to integrate the carefully designed, synthesized, and assembled heterogeneous nanostructures with optimized radiative efficiency into SSL structures. This gives rise to a need to understand the properties of the interface to heterogeneous nanostructures. [EERE priority area impacted:1.2.1]

(CCRD2) Innovative Photon Management: A key to the success of solid-state-lighting is ultra high-efficiency light extraction. Basic research is needed to investigate fundamental photon modes that directly influence the brightness, directionality, polarization, and efficiency of emitted light. Recent advances in nanotechnology, particularly in creating photonic/plasmonic structures, present an unprecedented opportunity to explore strong photon-structure interaction and to manipulate photon modes. Such innovative photon management is a new frontier in optical science. Success in this CCRD will lead to new designs and paradigms in light extraction, and will help enable ultra-efficient solid-state lighting. [EERE priority areas impacted:1.2.2, 1.2.1, 2.1.3]

(CCRD3) Enhanced Light-Matter Interactions: Traditionally, the operation of an LED or OLED is viewed as the sequential processes of internal generation of photons by electronic excitations in a semiconductor followed by extraction of those photons to the device surroundings. These individual processes are optimized for high-efficiency SSL device development. This CCRD focuses on the fundamentals of light-matter interactions with the goal of discovering and implementing approaches by which the sequential processes involving conversion of electronic energy to light become intimately integrated. Basic research is needed to identify material and device configurations in which the distinction between internal end external quantum efficiency merges to a unitary figure of merit. This new strategy will rely on discovering and designing nanoscale optical materials and structures wherein the resonant interaction between the electronic and photonic degrees of freedom is significantly stronger than the perturbation interaction regime typical of today’s light-emitting devices. [EERE priority areas impacted: 1.1.2, 1.2.2, 1.2.1]

(CCRD4) Multiscale modeling for Solid-State Lighting: Developing and implementing hierarchical multi-scale modeling and establishing global optimization schemes are the focus of this CCRD. Models must accurately describe the physical processes that determine behavior at vastly different length- and time-scales. Quantum mechanical models, used to describe fundamental processes on an atomic scale, must be interfaced with semi-empirical mesoscale models, which must in turn connect to classical continuum models that describe behavior at the device scale. Special research challenges include developing a correct description of interactions between the different length scales in the set of models. [EERE priority areas impacted: 3.4.1, 4.2.3, 4.3.2]

(CCRD5) Precision Nanoscale Characterization: SSL structures rely now, and are expected to rely in the future, on complex organic and inorganic material nanostructures within which a variety of complex phenomena (charge transport, recombination pathways, and photon extraction) occur. Understanding these nanostructures and phenomena necessitates precise characterization at levels beyond those currently possible. A key catalyst for advances in SSL is therefore the development of new, structurally sensitive tools. These measurements need resolutions spanning the entire range of relevant length scales from individual molecules or dopant atoms to integrated heterostructures and functional devices. New tools developed within this CCRD will enable determination of local nanoscale properties under conditions relevant to understanding the basic phenomena behind electroluminescence. Novel *in situ* techniques for monitoring materials synthesis will also drive improvements in materials properties. [EERE priority areas impacted: 1.1.2, 1.3.1, 1.1.3, 2.1.1, 3.1.2, 3.2.2]

1.5 Nanoscale Science Research Centers (NSRCs)

The National Nanotechnology Initiative (NNI) is a federal R&D program established to coordinate the multi-agency efforts in nanoscale science, engineering, and technology. Because of the promise of nanotechnology to improve lives and to contribute to economic growth, the U.S. Government, through the NNI, is supporting research in nanotechnology. For additional information about the NNI, visit their web site at http://www.nano.gov.

A major portion of the DOE's participation in the NNI is through five Office of Science Nanoscale Science Research Centers located at National Laboratories across the country:

- Center for Functional Nanomaterials (Brookhaven National Laboratory)
- Center for Integrated Nanotechnologies (Los Alamos and Sandia National Labs)
- Center for Nanophase Materials Sciences (Oak Ridge National Laboratory)
- Center for Nanoscale Materials (Argonne National Laboratory)
- Molecular Foundry (Lawrence Berkeley National Laboratory)

Detailed descriptions of the research thrusts, facilities, and contact information for the five NSRCs comprise Sections 2 - 6 of this report.

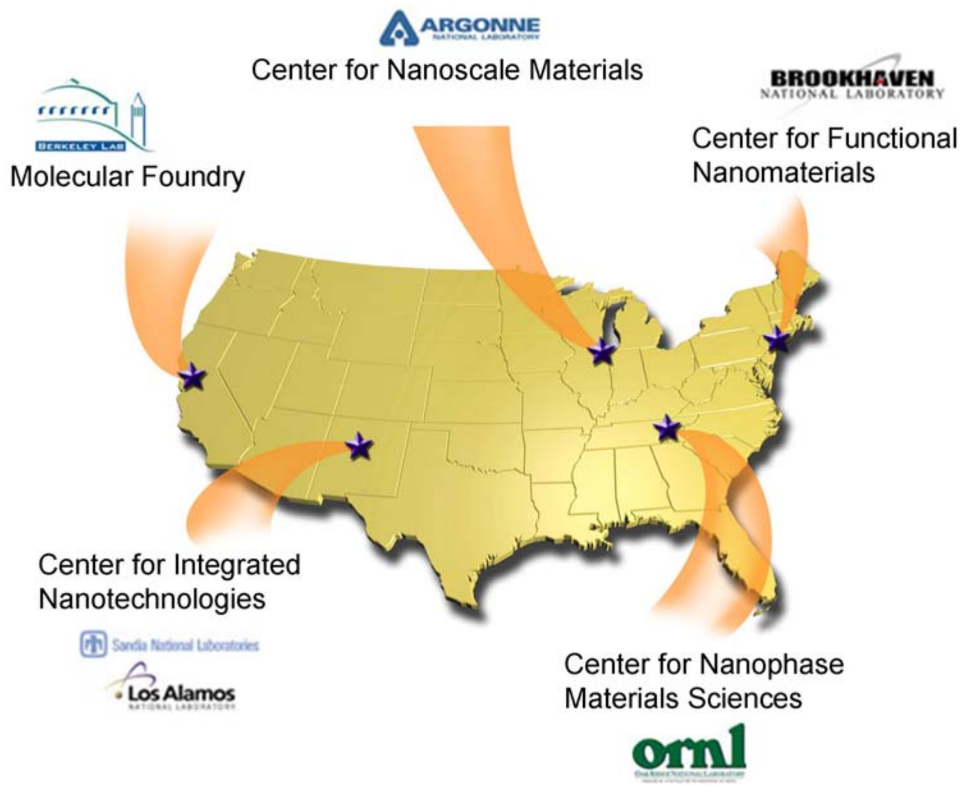

Figure 2. The five Department of Energy Nanoscale Science Research Centers are located at National Laboratories distributed across the country.

Each of the five NSRCs has identified certain research thrusts in nanoscience for concentration; there are also many areas of expertise and capabilities that are common across the NSRCs. As such, each of these five premier Office of Science user facilities is positioned to make important contributions to Solid-State Lighting. There are two primary mechanisms by which research at the NSRCs could impact Solid-State Lighting:

SSL Research at NSRC Facilities by Outside Users. Staff scientists at the NSRCs are available to collaborate and assist outside users from academia, government, and industry. Generally, access to NSRC staff and facilities is granted to users on the basis of competitive research proposals.

If the nature of the joint work is basic research, the results of which will be published in the open scientific literature, this access is available at no additional cost to the user. Funding for the outside user's time and materials comes from their home institution and the user's funding agency for their project, for example, from the DOE / EERE Core Technology Calls for proposals, or through the DOE Office of Basic Energy Sciences funding opportunities. Most of the NSRCs can undertake proprietary research with industry, with appropriate Intellectual Property agreements in place, on a full-cost-recovery basis.

Thus, external researchers from the U.S., as well as internationally, can utilize the state-of-the-art facilities and collaborate with experts at the NSCRs to study nanoscale phenomena in areas that could yield breakthroughs in Solid-State Lighting.

SSL Research Projects Initiated by NSRC Scientists. Many of the scientific staff members at the NSRCs also conduct their own research programs, funded by a variety of sources. The Office of Science funds extensive programs of research supporting DOE missions in science, energy, national security, and the environment. The NSRCs are expected to make major contributions to meeting DOE mission needs.

Solid-State Lighting falls squarely within the scientific and applied DOE mission space for which the NSRCs were created. Each of the NSRCs has identified different aspects of nanoscience upon which to focus their efforts, and SSL-related activities may have more natural synergy at some of the nanocenters than at others. However, the nanoscale basic research challenges for SSL (discussed in the next section) are so broad that each of the NSRCs and their premier research scientists could make substantial contributions to SSL, based on staff interests and institutional priorities.

Funding vehicles for direct support of SSL research originating at the NSRCs include Calls for Proposals from the DOE / EERE Core Technology Program (which also included a Call for Proposals specifically targeted at the NSRCs in 2006), possible future targeted SSL Calls for Proposals from DOE Basic Energy Sciences, proposals to the DOE / BES core research programs that support fundamental research at each of the associated National Laboratories, and other federal agencies.

Staff members at the National Center for Solid-State Lighting R&D housed at Sandia and Los Alamos National Laboratories have broad experience in SSL and nanoscale research needs. They would be glad to assist NSRC staff scientists and management in discussing potential areas in which the NSRCs could contribute to SSL.

1.6 NSRC Common Capabilities Relevant to SSL

Each of the five Nanoscale Science Research Centers has chosen specific aspects of nanoscience for special emphasis. Summaries of the specific capabilities of the five NSRCs are given in Sections 2 through 6 of this report.

In addition to the unique research areas of concentration at the NSRCs, there are also many capabilities and strengths common across most of these facilities. In order for these premier centers to have the flexibility to address a broad range of nanoscience issues, some common core capabilities are present in most of the NSRCs. Some of the common capabilities that could be especially important in addressing fundamental nanoscale aspects of SSL include: nanostructure materials synthesis, nanofabrication, nanophotonics, nanoelectronics, materials structure and characterization, and theory / modeling.

Synthesis

Many of present limitations to ultra-efficient solid-state lighting are due to materials issues. Unprecedented control of materials structures, defects, unique new architectures and functionalities will be enabled by nanoscale synthesis approaches. Researchers at the NSRCs are developing new synthesis techniques for organic molecules, macromolecules and their assemblies. Scientists are investigating new routes to self-assembly, combinatorial synthesis, and polymerizations for organic-based materials, with direct application to developing new OLED designs.

Much work at the NSRCs is aimed at controlled synthesis of low-dimensional nanostructures, for example, 0-D quantum dots, 1-D nanowires and nanotubes, as well as 2-D quantum wells. Such low-dimensional nanostructures can have unique optical and electronic properties that will enable unimagined mechanisms for creation, control, and extraction of light.

Scientists at the NSRCs are working to synthesize new hybrid materials and interfaces, for example integrating “soft materials” (such as organics or biological materials) with “hard materials (such as inorganic semiconductors and metals). Long-range examples in lighting materials might include new LED architectures, especially in OLEDs, or incorporating biological materials with exceptional light-manipulation capabilities and efficiencies into inorganic semiconductor active regions.

Basic Research Needs for SSL that could be impacted by the controlled synthesis of new nanostructures using NSRC capabilities (using the numbering scheme in Section 1.5) include: GC1, PRD1, PRD2, PRD3, PRD5, PRD7, and CCRD1.

The later Sections of this report list specific examples, approaches, and capabilities of research into nanoscale synthesis at the five NSRCs.

Nanofabrication

The NSRC facilities all include dedicated clean room space and specialized tools for lithographic patterning, etching, deposition and the like. Users and staff can fabricate complete prototype optical and electronic devices at each of the nanocenters. Such devices can be used to understand new nanoscale phenomena and to test unique architectures in nanofunctional materials. Research into new nanophotonic and nanoelectronic designs and phenomena will be enabled by these nanofabrication capabilities.

Basic Research Needs for SSL that could be impacted by the nanofabrication tools at the NSRCs include: GC1, PRD1, PRD2, PRD3, PRD5, PRD5, PRD7, CCRD1, CCRD2, and CCRD3.

The specific nanofabrication tools available vary across the NSRCs. Please see the individual descriptions and capabilities lists for each of the nanocenters in Sections 2-6 of this report.

Nanophotonics and Nanoelectronics

Fundamentally new ways of generating and harvesting light are at the heart of the potential impact of nanoscience research on solid-state lighting. It is possible to confine EM fields within low-dimensional nanostructures creating extraordinarily strong "near-fields" of evanescent fields due to this localization. The photochemical and photophysical response of materials to these confined EM fields is often non-linear, producing phenomenal new effects and sensitivities. Optical oscillator strengths can be manipulated by tailoring the electronic properties of such low-dimensional nanostructures to accelerate radiative processes and to control spectral properties. Nanoscale optical enclosures such as photonic crystals or resonant cavity emitters patterned at sub-wavelength dimensions can dramatically alter and enhance emission properties and could lead to novel LED and OLED designs.

Basic Research Needs for SSL that could be impacted by research in nanophotonics and nanoelectronics at the NSRCs include: GC1, GC2, PRD1, PRD2, PRD3, PRD4, PRD7, CCRD1, CCRD2, and CCRD3.

Materials Structure and Characterization

The NSRCs provide access to an astounding array of tools for structural analysis and characterization of nanoscale materials. Most of the NSRCs are co-located with DOE flagship user facilities providing access to high-intensity particle scattering and light sources at national laboratories. Neutron scattering capabilities are available through the High-Flux Isotope Reactor and Spallation Neutron Source at Oak Ridge National Laboratory. Ultraviolet and soft X-ray beams are provided by the Advanced Light Source and access to the National Center for Electron Microscopy is available at Lawrence Berkeley National Laboratory. The National Synchrotron Light Source is a high intensity source of UV, visible, infrared light and X-rays at Brookhaven National Laboratory. The Advanced Photon Source for brilliant X-ray beams and the Electron Microscopy Center are available to users at Argonne National Laboratory. In addition most of the NSRCs provide access to scanning probes such as AFM, STM, SEM, scanning Auger, NSOM, LEEM, PEEM and to various optical spectroscopies.

Every one of the Basic Research Needs for SSL GCs, PRDs, and CCRDs listed in Section 1.5 could be impacted by the materials structure and characterization tools available at the NSRCs.

The specific analytical facilities available vary across the NSRCs. Please see the individual descriptions and capabilities lists for each of the nanocenters in Sections 2-6 of this report.

Theory and Modeling

Each of the NSRCs has a significant research thrust in theory and modeling of nanoscale phenomena. Staff scientists at the NSRCs are available for theoretical collaboration with and support of experimental projects and visiting users. A broad suite of codes and capabilities are available to enable theoretical prediction of nanoscale behaviors and interpretation of laboratory measurements. Theoretical methods available at the NSRCs include: electronic structure, *ab initio* and classical molecular dynamics, quantum and classical Monte Carlo, many-particle Green's functions, time-dependent density functional theory, force fields and molecular mechanics, quantum dynamics, transition-state theory, electrodynamics simulations; atomistic, mesoscale, and continuum methods.

The NSRCs also provide access (or gateways) to significant computational resources, either through in-house computer clusters or through corollary access to national super computer facilities such as the National Energy Research Supercomputer Center and the National Center for Computer Sciences

Every one of the Basic Research Needs for SSL GCs, PRDs, and CCRDs listed in Section 1.5 could be impacted by the theory and modeling capabilities available at the NSRCs.

2.0 Center for Functional Nanomaterials

2.1 General Information

The Center for Functional Nanomaterials (CFN) NSRC is located at Brookhaven National Laboratory. An overarching goal at CFN is to create "functional nanomaterials" whose response to external stimuli can be tailored to perform unique, specific, and useful functions. Such functional nanomaterials will have properties and applications far different from bulk materials that are possible only at the nanometer scale.

Special focus at CFN is to apply nanotechnologies to create alternate, more efficient energy technologies. Example applications include new materials that enable more efficient solar energy or utilization and employing hydrogen as a next-generation fuel.

The following sections summarize CFN research focus areas, facilities, capabilities, and user's program. Additional information is available from the CFN web site at http://www.bnl.gov/cfn/ .

2.2 CFN Scientific Themes

Center for Functional Nanomaterials has identified four scientific themes in nanoscience to focus its research activities.

- Nanocatalysis
- Biological and Soft Nanomaterials
- Electronic Nanomaterials
- Theory and Computation

Within each of the scientific theme areas are particular sub-topics upon which CFN research is concentrating.

Figure 3. Center for Functional Nanomaterials at Brookhaven National Laboratory. (Photo courtesy of BNL.)

Nanocatalysis

Group Leader: Jan Hrbek

Catalysts are widely used in the chemicals industry for synthesis of new chemicals and materials, in petroleum refining for efficient cracking of hydrocarbons, in environmental protection to reduce emission of pollutants from automotive exhaust or from factory smoke stacks. Although extraordinarily useful, the mechanisms and performance of most catalytic systems are poorly understood. Finding appropriate and effective catalysts for new applications can be very time-consuming and inefficient.

Because of their high surface-to-volume ratios and unique interactions with light and electromagnetic fields, nanoscale materials can have tremendous catalytic activities. The CFN Nanocatalysis scientific theme area focuses on rational design of new nanometer-scale catalysts. Research includes: fundamental understanding of nanocatalyst reaction mechanisms; synthesis, processing, and testing of new catalytic systems.

Several prototype nanocatalytic systems are being addressed at CFN. Scientists are designing and studying gold nanoparticles, which are found to be very effective catalysts for removal of sulfur dioxide, an environmental pollutant. Nanostructured Pt / Ru catalysts are being tested as PEM fuel cell applications, with the potential for lower cost and longer lasting operation. New Ru / C nanoscale catalysts are being developed with applications to ammonia synthesis, which could enable lower-temperature processes (energy savings) with higher reactivity than current industry approaches.

Biological and Soft Nanomaterials

Group Leader: Oleg Gang

Biological systems exhibit unique and phenomenal abilities for self-assembly, self-directed healing of defects, and integration of functionality across disparate length scales. This scientific theme area seeks to understand, utilize, and mimic mechanisms found in biological systems to create new nanoscale materials with specific and useful functions. A second focus of this theme area is understanding interfaces between biological and inorganic materials.

Within this area of research, three subthemes have been identified. First is the study of functional hybrid nanomaterials with specialized properties, synthesized from simpler biological and organic building blocks. A second subtheme is self-assembly and programmable assembly. This work attempts to utilize the instruction encoding and specificity of biological molecules as a means to synthesizing new materials with specialized properties and functionality. The third subtheme is a fundamental understanding of the unique ways in which nanoscale particles interact with biological systems.

Electronic Nanomaterials

Group Leader: Jim Misewich

The Electronic Nanomaterials scientific theme studies the unique interactions that occur between electromagnetic fields and nanoparticles. When the size of the particles is smaller than or comparable to the wavelength of the electromagnetic field, enhanced non-linear interactions can be produced. These effects could lead to new technologies in energy storage and ultra-fast / ultra-small electronic circuits and computer memory.

Three subthemes have been identified within the Electronic Nanomaterials area. The first subtheme is heterogeneous nanomaterials, which endeavors to create new functionalities by combining different type of materials (for example BN nanotubes filled with C_{60} molecules), or combining nanostructures of different dimensionalities (for example, 0D quantum dots, 1-D quantum wires, or 2-D quantum wells). A second subtheme is to understand correlations on the nanoscale; examples include studying 2-D correlated systems in 1-D, and transport in low-dimensional systems such as nanowires. The subtheme on multiscale magnetism studies properties of magnetic behavior at the nanometer scale and emergent magnetic behavior.

Theory and Computation

Group Leader: Mark Hybertsen

The Theory and Computation theme supports the three scientific themes discussed above. This effort provides access to software tools and computational facilities, enabling the prediction of fundamental properties and behaviors at the nanometer scale and interpretation of experimental data. Close collaboration between experimentalists and theorists is an emphasis of the Theory and Computation thrust area. Staff scientists can also provide support and guidance to experimentalists and other users wishing to learn these modeling techniques.

2.3 Center for Functional Nanomaterials Facilities

The CFN facility consists 94,000 square feet of offices and laboratories located next to the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory. The facility is organized around several state-of-the-art groups of laboratories called Laboratory Facilities, a Theory and Computational Center, and advanced end-stations on beamlines at the NSLS. The CFN building includes capabilities in materials synthesis, nanopatterning, proximal probes, electron microscopy, and ultrafast laser sources. The CNF includes Class 1000 clean rooms and access to the Laser Electron Accelerator Facility (LEAF).

Materials Synthesis

Leader: Arnold Moodenbaugh

The Materials Synthesis facility provides a wide range of state-of-the-art synthesis capabilities for functional nanomaterials and bulk materials. Characterization capabilities include X-ray diffraction, MPMS, DTA/TGA, and optical microscopy. Wet chemical synthesis techniques available at CFN include: sol get, micelle, hydrothermal, spin coating, and a SILAR robot. Thin film deposition tools include: PLD, an e-beam evaporator, and surface profiling.

Nanopatterning

Leaders: John Warren, Chris Jacobson

The nanopatterning facility provides state-of-the-art electron and ion beam patterning, as well as bulk patterning methods such as deep reactive ion etching. Processing technologies available to users include optical lithography, reactive-ion etching, resist processing, e-beam patterning, mask alignment, oxidation furnace, vacuum evaporation and sputtering, and analytical scanning electron microscopy.

Proximal Probes

Leader: Peter Sutter

This facility provides state-of-the-art real-time imaging by low-energy electron microscopy (LEEM) and synchrotron-based photoelectron microscopy (PEEM). Other probes available to users include variable temperature UHV scanning tunneling microscopy (STM), atomic force microscopy, optical confocal microscopy, and near-field microscopy. Also available are fluid and environmentally controlled STM, electrochemistry, and eight dual-processor clustered workstations.

Theory & Computation

Leader: James Davenport

The Theory and Computation Laboratory offers state-of-the-art hardware and software support for nanoscience researchers at the CFN. Applications for modeling and simulation include: analysis of experimental results in comparison with theory, advanced visualization and other data analysis, or using first-principles (or other approaches) to predict nanoscale properties or to design structures of specific functionality.

Theory and computational capabilities available to users include: density functional codes for crystals and crystalline surfaces; ab initio and density functional quantum chemistry codes for molecules and small clusters; molecular dynamics codes for biosystems and self assembly; Monte Carlo codes for thermal effects in magnetic systems; TEM and X-ray analysis codes; visualization and graphics software; molecular mechanics.

Electron Microscopy

Leader: Yimei Zhu

Advanced Transmission Electron Microscopy (TEM) capabilities in the CFM Electron Microscopy facility allow image resolution better than 0.1 nm and spectroscopic resolution better than 1 eV. Instruments can operate under a range of environmental conditions. Applications range from in situ nanoscale fabrication to structural and property characterization. TEM capabilities include high-resolution imaging, electron diffraction, energy dispersive X-ray analysis, and electron energy loss spectroscopy. SEM capabilitiesinclude imaging, image analysis, and both quantitative and qualitative X-ray analysis. Scanning Auger capability is available for surface analysis, imaging, and depth profiling

Ultrafast Lasers

Leader: Alex Harris

The Ultrafast Lasers facility provides a range of techniques to probe the structure and dynamics of nanostructured systems on femtosecond time scales. Example applications include measurement of the growth kinetics, reaction kinetics and surface molecular dynamics of nanostructured systems under well-controlled ambients ranging from ultrahigh vacuum (UHV) to the solution phase. Techniques include terahertz spectroscopy, novel single shot measurement techniques, ultrafast near field microscopy,

Figure 4. National Synchrotron Light Source, Brookhaven National Laboratory. (Photo courtesy of BNL.)

and ultrafast short wavelength sources. The CFN Nonlinear Optical Surface Probe Facility supports synthesis and *in situ* characterization of supported nanoparticles. Also available is an ultrafast laser-driven X-ray source permitting pump-probe experiments with X-rays and ultrafast optical sources.

National Synchrotron Light Source (NSLS) End Station

Leader: Ronald Pindak

The CFN offers two specialized capabilities associated with the NSLS. The first capability is small-angle X-ray scattering (SAXS) and grazing-incidence small-angle x-ray scattering (GISAXS) measurements. The second capability combines low-energy electron microscopy and synchrotron-based photoelectron microscopy (LEEM-PEEM) measurements.

2.4 National Synchrotron Light Source

In addition to the core CFN facility, users also can have access to the National Synchrotron Light Source (NSLS) housed at Brookhaven National Laboratory.

The NSLS is divided into two storage rings. The smaller of the two is called the VUV (vacuum ultra-violet) ring, with approximately 25 beamlines. This ring produces mostly UV, visible, and infrared light, although some X-rays are produced. The larger X-ray storage ring has approximately 60 beamlines, and produces more of the higher energy x-rays than the VUV ring.
The NSLS operates 24 hours a day and different experiments can be performed on most of the 80 beamlines simultaneously. Each year over 2,000 scientists visit the NSLS to perform experiments. More information about the National Synchrotron Light Source is available at the NSLS web site: http://www.nsls.bnl.gov/ .

2.5 CFN Interactions with Users

The Center for Functional Nanomaterials is a national user facility, accessible to researchers at universities, industrial laboratories and national laboratories through peer-reviewed proposals. The User Program provides access to CFN facilities staffed by laboratory scientists, postdocs and technical support personnel who are active in nanoscience research. Proposals are encouraged from external scientific and industrial communities that involve a broad spectrum of activities ranging from short-term capability access to long-term joint research programs.

Proposals are reviewed and rated by the Proposal Review Panel (PRP) and facility equipment time allocations are made by the CFN Allocation Committee. Prospective users are encouraged to contact the appropriate CFN facility leader early in the proposal development process for assistance in developing their proposal prior to submission.

Proposal deadlines are: September 30 (January - April cycle); January 31 (May - August cycle); May 31 (September - December cycle). Send proposals by email (preferred), mail, or fax to:

CFN User Administration
Brookhaven National Laboratory
P.O. Box 5000, Bldg. 555
Upton, NY 11973
Email: cfnuser@bnl.gov
Fax: 631-344-3093

More information about the User Program is available at the CFN web site: http://www.nsls.bnl.gov/cfn/user/proposal.asp.

2.6 CFN Contact Information

Emilio Mendez
CFN Director

Michael Schaeffer
CFN Deputy Project Director
631.344.7941

Judith Thompson
CFN Administrative Assistant
631.344.4176
FAX 631.344.3093

Grace Webster
User Admin. Program & Outreach Coord.
631.344.6266
FAX: 631.344.3093

Michael Harrison
CFN Project Director
631.344.7173

Steven Hoey
ES&H Coordinator
631.344.6266

2.7 List of Capabilities

In addition to the synchrotron characterization techniques available through the CFN Contributing User programs, there are a number of nanoscience characterization techniques available on NSLS Facility Beamlines. Proposals for beam time to use these synchrotron characterization techniques should be submitted through the NSLS PASS system. See the NSLS web site for more details: http://www.nsls.bnl.gov/ . The available techniques, their associated beamlines and local contacts are:

Technique	Beamline	Local Contact
Angle-resolved Ultraviolet photoelectron spectroscopy (UPS), spin-resolved	U5UA	Elio Vescovo
Infrared micro-spectroscopy	U10B	Randy Smith
Infrared transmission and reflection spectroscopy	U12IR	Randy Smith
X-ray scattering, resonant magnetic circular dichroism	X13A	Cecilia Sanchez Hanke
Micro-diffraction Imaging	X13B	Kenneth Evans-Lutterodt
X-ray absorption spectroscopy, extended fine structure, near edge, and near edge fine structure	X18B	Syed Khalid
X-ray scattering, resonant X-ray absorption spectroscopy; extended fine structure, near edge, and near edge fine structure	X19A	Syed Khalid
Single crystal X-ray diffraction; X-ray scattering (magnetic, resonant, small angle)	X21	Christie Nelson
X-ray microprobe	X27A	James Ablett

3.0 Center for Integrated Nanotechnologies

3.1 General Information

The Center for Integrated Nanotechnologies (CINT) NSRC is jointly operated by Sandia National Laboratories and Los Alamos National Laboratory. The unifying research theme at CINT is taking nanoscale discoveries and integrating them into larger systems to make real-world discoveries. The CINT core facility is located in Albuquerque, NM with a gateway facility in Los Alamos.

At Sandia the emphasis is on integrating nano- and micro-scale technologies, taking advantage of Sandia's strengths in microelectronic and microelectromechanical system (MEMS). They are developing modular microlabs on a chip to enable nanoscale synthesis and characterization. At Los Alamos they are exploring the connection between nanotechnology and biology and developing new concepts in nanophotonics.

The following sections summarize CINT research thrusts, facilities, capabilities, and user's program. Additional information is available from the CINT web sites at http://cint.lanl.gov/ or http://cint.sandia.gov/ .

3.2 CINT Research Thrusts

CINT has identified four scientific thrust areas in which to concentrate its research activities. These science thrusts were identified through discussions, surveys, and workshops involving potential users, the CINT Science Advisory Committee, and Sandia and Los Alamos staff.

The CINT Scientific Trusts are:

- Nanoscale Electronics, Mechanics, and Systems
- Nanophotonics and Optical Nanomaterials
- Soft, Biological and Composite Nanomaterials
- Theory and Simulation of Nanoscale Phenomena

Figure 5. Center for Integrated Nanotechnologies core facility located adjacent to Sandia National Laboratories in Albuquerque, NM. (Photo courtesy of SNL.)

Nanoscale Electronics, Mechanics, and Systems

Thrust Leaders: Mike Lilly (SNL) and Mike Nastasi (LANL)

This thrust emphasizes study of the electrical and mechanical properties of nanosystems. Particular areas of interest include: charge carrier transport and interactions in low-dimensional system; materials interface properties; and electrical and mechanical properties of nanostructures, e.g., nanowires. Research includes inorganic nanostructures, as well as biological systems.

Research topics include: control of electronic transport and wave functions using nanostructured materials; mechanical properties and coupling of nanostructured materials; and exploring new ways to integrate diverse classes of functional materials on the nanoscale.

The work on transport in low-dimensional systems is enabled by world-class molecular beam epitaxy (MBE) synthesis of ultra-low defect material, ion implantation. Scanning probes such as *in situ* STM / TEM are also heavily employed.

This thrust is developing two of the Discovery Platforms™ (discussed in a subsequent section), the Cantilever Array Platform to measure mechanical properties in nanostructured films, and the Electrical Transport and Optical Spectroscopy Platform.

Nanophotonics and Optical Nanomaterials

Thrust Leaders: Victor Klimov (LANL) and Igal Brener (SNL)

Research in this thrust area includes understanding and controlling fundamental photonic, electronic, and magnetic interactions in nanoscale optical materials, and study of interfaces between disparate materials types, e.g., semiconductors and metals, organics and inorganics. Work in this thrust is addressing multi-function materials with unique magneto-optical, electro-optical, or multi-ferroic properties. Workers also seek to explore energy transformations on the nanoscale, including energy and charge transfer, and electronic relaxation across multiple length-, time-, and energy scales. Collective and

Figure 6. Center for Integrated Nanotechnologies gateway facility located at Los Alamos National Laboratory. (Photo courtesy of LANL.)

emergent electromagnetic phenomena (plasmonics, metamaterials, photonic lattices, solitons) are also focus areas of this scientific thrust.

Research includes synthesis of nanostructures and modification of properties by manipulating their size, shape, and / or surface functionalization. Synthesis techniques employed include: colloidal lithography, self-assembly, atomic-layer deposition, polymer assisted film growth, pulsed-laser deposition, molecular beam epitaxy, VLS (vapor-liquid-solid growth mechanism).

Specialized capabilities being employed include: ultrafast and single-nanostructure spectroscopies.

This thrust area makes use of the Electrical Transport and Optical Spectroscopy Discovery Platform™ for measurement of nanostructured materials properties, and Microfluidics Synthesis Discovery Platform™ for controlled nanostructure synthesis and diagnostics of growth.

Soft, Biological and Composite Nanomaterials

Thrust Leaders: Andrew Shreve (LANL) and Bruce Bunker (SNL)

Work in this thrust lies at the intersection of materials science and biology. Research in this thrust includes synthesis, assembly, and characterization of soft or biological materials. Of particular interest is understanding and exploiting the interface between inorganic and biological materials. A goal is integrating these materials across multiple length scales to create new, functional structures.

Research topics include developing transduction schemes for coupling molecular-scale events; chemical and biomolecular functionalization of interfaces to control assembly of material; assembly of complex nanomaterials with complex or emergent behaviors; molecular and biological recognition.

Staff in this thrust are active in the design and optimization of the Microfluidics Synthesis Discovery Platform™ for nanostructure synthesis. Significant experimental capabilities include: cell-culturing and biomolecular engineering, self-assembled material and thin-film preparation, chemical synthesis, scanning probe microscopies, optical microscopy and spectroscopy, Langmuir-Blodgett troughs, interfacial force measurements, and spectroscopic or imaging ellipsometry.

Theory and Simulation of Nanoscale Phenomena

Thrust Leaders: Mark Stevens (SNL) and Alexander Balatsky (LANL)

The theory and simulation effort is a cross-cutting thrust that impacts and interacts closely with the other three scientific thrusts, discussed above. Large scale classical and quantum mechanical calculations are brought to bear to simulate active and passive nanostructure synthesis, materials properties, interfacial interactions, and emergent behavior.

Current research topics include: theoretical spectroscopy and nonlinear optical response, energy transfer and charge transport, DNA nanoelectronics, local defects, optical and tunneling probes, and mechanical properties of nanocomposites. Capabilities and expertise include molecular theory methods, atomistic and coarse-grained molecular dynamics simulations, static and time dependent density functional theory, and many body quantum methods.

3.3 Grand Challenges

Two Grand Challenges in nanoscience integration have been identified as CINT research themes that will have broad and significant impact:

Energy Transfer

Some of the important issues that will impact all of nanotechnology are understanding processes such as: energy transfer at the nanoscale; energy transfer across widely disparate length scales; efficient energy transduction from one form of energy to another. Examples include highly efficient transfer of solar energy into chemical or electrical energy, or the complementary process of converting electrical energy into light for solid-state lighting applications.

Emergent Behavior

Emergent behavior is that which emerges from collections of smaller components that cannot be predicted solely based on the properties / behaviors of the individual constituents. Some characteristics of emergent behavior include complex patterns, self-organization, and cooperation among dissimilar parts. Examples are very common in biological systems, but also occur in other systems of nature, such as hurricanes. It is a grand and unifying challenge in nanoscience to understand such emergent behavior. An equally important grand challenge in nanotechnology is to learn how to exploit and direct emergent behavior for designed purposes.

3.4 Discovery Platforms

A Discovery Platform™ is essentially a specialized lab on a chip designed to integrate nanoscale phenomena with microelectronic (microscale) infrastructure for control and analysis. The Discovery Platforms™ allow connection to other laboratory-scale synthesis components (e.g., gas or liquid reagent sources, carrier gas, etc.), specialized diagnostics (e.g., laser-based or scanning probe analysis), and interface to computer-based control and data collection. The Discovery Platforms™ will provide a set of standard capabilities to enable the nanoscience community to reproducibly compare (and share) experimental results. There are currently two Discovery Platforms™ under development:

Cantilever Array Discovery Platform

The Cantilever Array is a multipurpose platform, with applications in nanomechanics, chemical and biological sensing, magnetization, and coupled oscillators. For example, one could deposit a film of a newly synthesized nanomaterial or biological specimen on the cantilever arrays to measure the material's modulus, *in situ* film stress, and internal energy dissipation. In addition, certain of the cantilevers are accessible for additional processing or diagnostics such as: metal lines for resistive heating; thin film resistor thermometry; scanning electrical conduction measurements; magnetic force sensing.

Electrical Transport and Optical Spectroscopy Discovery Platform

The Electrical Transport and Optical Spectroscopy Discovery Platform™ is designed for a variety of optical, electronic, and transport measurements on molecules, nanowires, and composite nanostructures (e.g., semiconductor or metal nanoparticle arrays). The user can deposit nanomaterials of interest on top of gates provided on the platform for making electrical contacts. Electrical active regions consist of gates separated from the Si-doped active regions by silicon nitride and silicon oxide insulators. The platform is compatible with other measurement techniques including scanning probes such as AFM, STM, NSOM, TEM and SEM, cryostats and magnetic fields. The platform is designed to accommodate a great deal of additional user-specified microcircuitry for specialized electrical and transport experiments.

Discovery Platform Hybrid Integration Tools

The Discovery Platform™ Hybrid Integration tool is a computer module (i.e., PC board) designed to allow the user to drop-in one of the platforms described above to perform the computer-based command and control and data acquisition to actually perform the experiments. The Hybrid Integration tool also supports access by other diagnostic tools, e.g., scanning probe, electrical, optical, or magnetic measurements, etc.

3.5 Facilities

CINT's core facility in Albuquerque consists of 96,000 square feet of laboratory and office space. It includes low-vibration characterization laboratories, chemical / biological synthesis laboratories, and a Class 1000 clean room.

The CINT gateway facility in Los Alamos is also open. It features specialized laboratory space and equipment for bioscience and nanomaterial research. More detailed information about CINT facilities and capabilities is given in the accompanying List of Capabilities at the end of this Section.

3.6 Interactions with Users

CINT provides access to its unique nanoscience experimental and computational facilities to outside users from universities, industry, other federal laboratories, and in the international science community. Equally important is the opportunity to work collaboratively with CINT scientific staff, if the user desires. User access to CINT is based on a competitive research proposal process, based on scientific proposal quality.

Currently CINT issues Calls for Proposals twice per year. In addition, there is a special "rapid access" procedure that is available in special cases that arise between the normal funding cycles. This special program provides only bridging access until a regular proposal can be evaluated through normal channels in the semiannual schedule.

Access to CINT is available on a no-cost basis. CINT operating funds pay for staff and facility costs. Users are required to pay for their own salaries and expenses from their own research grants, for example external NSF, DOE, and NIH programs.

Proprietary work can also be performed at CINT. In this case, approval must go through the regular proposal process and is based on scientific quality. However, such work must be done on a full cost-recovery basis, as required by DOE.

Proposal Review Panels are composed of external scientists who serve on three-year rotating appointments. These panels are charged with evaluating the technical quality of user proposals. Each panel consists of 4-6 members and is led by a chair.
Current panels are:

- Chemical Synthesis & Properties
  Electronics/Magnetics Synthesis & Properties
  Electronics & Micro-Nanofabrication
  Mechanics, Fabrication, Characterization & Properties
  Bio-Nano Materials
  Photonics, Spectroscopy & Microscopy

3.7 CINT Contact Information

Robert Hwang, CINT Co-Director
Sandia National Laboratories
P. O. Box 5800
Albuquerque, NM 87185-1427
505.844.1071
FAX 505.844.6098
jmphill@sandia.gov

Toni Taylor, CINT Co-Director
Los Alamos National Laboratory
P. O. Box 1663, MS G756
Los Alamos, NM 87545
505.665.0030
FAX: 505.665.9030
ttaylor@lanl.gov

Neal Shinn, User Program Manager
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185-1415
505.844.5457
FAX: 505.844.1197
ndshinn@sandia.gov

Tom Picraux, CINT Chief Scientist
Los Alamos National Laboratory
MST-CINT, MS G756
Los Alamos, NM 87545
505.665.8554
FAX: 505.665.9030
picraux@lanl.gov

3.8 List of Capabilities

The following sections list CINT experimental capabilities, baseline equipment available in the CINT core and gateway facilities, and CINT theory and simulation capabilities.

The information in this list was obtained from the CINT web site http://cint.lanl.gov/ or http://cint.sandia.gov/ .

CINT Core Facility

Synthesis Tools **:**

- Molecular Beam Epitaxy (MBE)
- Pulsed Laser Deposition System (PLD)

Characterization Tools**:**

- Transmission Electron Microscope (TEM)
- Atomic Force Microscope (AFM)
- Fourier Transform Infrared Spectrometer (FTIR)
- Spectroscopic Ellipsometer
- Ultraviolet/Visible Spectrometer

- Nano-Indenter
- Field-Emission Scanning Electron Microscope (FE-SEM)
- Top Loading Dilution Refrigerator
- Superconducting Magnet
- Ultrafast Laser System
- Femtosecond Oscillator Pump Laser
- CW Laser System for Raman Spectroscopy
- Scientific Grade CCD Detector Array
- Time Correlated Single Photon Counting System

***Integration Lab Tools*:**

- Electron Beam Writer
- Photolithography Mask Aligner
- Reactive Ion Etch tool
- Electron Beam Evaporator tool
- Inductively Coupled Plasma Chemical Vapor Deposition (ICP-CVD)
- Rapid Thermal Annealer
- Profilometer
- Wafer Processing Tools
- Clean Room Benches (Solvent, Acid, Base)
- Inductively Coupled Plasma Reactive Ion Etch (ICP-RIE)

***Characterization Tools*:**

- Atomic Force Microscope (AFM)
- Interfacial Force Microscope (IFM)
- Scanning Electron Microscope (SEM)
- Transmission Electron Microscope (TEM)

CINT Gateway to Los Alamos Facility

***Synthesis Tools*:**

- Langmuir-Blodgett Trough
- Magnetron sputtering chamber
- E-beam evaporator
- Vacuum annealing furnaces

***Characterization Tools*:**

- Near-Field Optical Microscope (NSOM)
- Spectroscopic Ellipsometer
- Ultraviolet/Visible Spectrometer
- Environmental Scanning Electron Microscope (SEM)

- Atomic Force Microscope (AFM)
- Nano-Indenter
- Ultrafast Laser
- Oscillator Pump
- High Cycle Fatigue Tester
- Laser Strain Measurement
- Tribometer
- Profilometer

Other

- Computational Cluster

CINT Gateway to Sandia Facility

***Synthesis Tools*:**

- Molecular Beam Epitaxy (MBE) – Metals

***Characterization Tools*:**

- Atomic Force Microscope (AFM)
- Low Energy Electron Microscope (LEEM)
- Interfacial Force Microscope (IFM)

4.0 Center for Nanophase Materials Sciences

4.1 General Information

The Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL) integrates nanoscale science with neutron science; synthesis science; and theory, modeling, and simulation. Operating as a national user facility, the CNMS has a highly collaborative and multidisciplinary environment for research to understand nanoscale materials and phenomena.

The following sections summarize the CNMS's research thrusts, facilities, capabilities, and user's program. Additional information is available from the Center for Nanophase Materials Sciences web site at http://www.cnms.ornl.gov/ .

4.2 CNMS Scientific Themes

Research at the Center for Nanophase Materials Sciences focuses on understanding, designing and controlling the dynamics, spatial chemistry, and functionality of nanoscale materials and architectures. To achieve these goals the CNMS has identified three overarching scientific themes:

- Imaging Nanoscale Functionality
- Synthesis and Dynamics of Nanostructured Polymeric and Hybrid Materials
- Emergent Behavior in Nanoscale Systems

Imaging Nanoscale Functionality

This scientific theme develops techniques to image functionality of materials at the nanometer scale. CNMS researchers seek to understand the new chemical and physical phenomena that can be exploited in nanoscale materials. The theme uses a variety of techniques including scanning probes, neutron scattering, electron microscopy, and related techniques.

Figure 7. Center for Nanophase Materials Science, Oak Ridge National Laboratory. (Photo courtesy of ORNL.)

Synthesis and Dynamics of Nanostructured Polymeric and Hybrid Materials

This theme area concentrates on synthesis and processing of a nanostructured polymers. Scientists seek to understand and control the structure and properties of classes of materials such as bio-inspired and hybrid polymers.

Emergent Behavior in Nanoscale Systems

This theme area focuses on understanding the emergence of collective behavior across length scales in complex systems. Examples include systems of bio-inspired and oxide nanostructured materials. This are includes a strong theoretical component, in close cooperation with the Nanomaterials Theory Institute.

4.3 CNMS Research Capabilities

In support of these scientific themes, the CNMS offers the following major research capabilities:

- Macromolecular Nanomaterials
- Catalytic Nanosystems
- Functional Hybrid Nanomaterials
- Scanning Probes and Nanoscale Physics
- Electron Microscopy, Neutron and X-Ray Scattering
- Nanomaterials Theory Institute
- Nanofabrication Research Laboratory
- General Characterization Facilities

Macromolecular Nanomaterials

Principal Contacts: Phil Britt, and Jimmy Mays

The Macromolecular Nanomaterials laboratories include a wide range of polymer synthesis capabilities, including ionic polymerizations, controlled radical polymerizations, polymer composites, novel architectures, and deuterated monomers and polymers. A wide range of characterization tools are available to users, such as determination of macromolecular molecular weight and size, thermal analysis, optical and spectroscopic analysis, imaging and structural characterization, scanning probes, and electron microscopy.

See the List of Capabilities for details of the specialized equipment associated with the Macromolecular Nanomaterials capability.

Catalytic Nanosystems

Principal Contact: Steve Overbury, Viviane Schwartz, and Sheng Dai

Three labs with the CNMS are available for catalyst preparation using a wide variety of synthesis methods, including template-assisted synthesis of mesoporous oxides and carbon catalysts, metal oxide nanoparticles, functionalization of porous supports, and solvothermal synthesis of materials. CNMS staff scientists collaborate with users on synthesis and characterization of these nanomaterials.

See the List of Capabilities for details of the specialized equipment associated with the Catalytic Nanosystems capability.

Functional Hybrid Nanomaterials

Principal Contacts: Dave Geohegan and Hans Christen

CNMS capabilities include synthesis, processing, and characterization of functional hybrid nanomaterials. Synthesis techniques include: pulsed laser vaporization, thermal chemical vapor deposition (CVD), and molecular beam epitaxy (MBE). Expertise includes growth of single-walled nanotubes, nanowires, nanoparticles, and complex oxide heterostructures. Processing capabilities include: photolithography, e-beam lithography, focused-ion beam patterning / wiring of nanomaterials for devices, SWNT purification and functionalization, and electrospinning.

Capabilities include: UV-VIS-NIR absorption spectroscopy, fluorometry, ultra-fast spectroscopy, Raman spectroscopy, and a variety of other femtosecond and nanosecond laser techniques, and spectroelectrochemical characterization.

See the List of Capabilities for details of the specialized equipment associated with the Functional Hybrid Nanomaterials capability.

Scanning Probes and Nanoscale Physics

Principal Contacts: John Wendelken, Ward Plummer, Art Baddorf, and Jian Shen

Advanced scanning probes and analytical tools are offered to users at the CNMS. A UHV variable-temperature Atomic Force Microscopy (AFM) is available that includes *in situ* pulsed-laser deposition growth capability, high-pressure RHEED, MBE growth, AES / XPS electron spectroscopies, and LEED. An ambient AFM can be used for topography and force characterization in air and liquid environments, and an ambient Scanning Probe Microscope (SPM) can be used for electrical characterization. Also under development is a high-field, low temperature Scanning Tunneling Microscope (STM). Other capabilities include a UHV 4-probe STM with 10-nm resolution SEM and SAM analyzer and an SEM equipped with Polarization Analysis for nanomagnetism studies.

See the List of Capabilities for details of the specialized equipment associated with the Scanning Probes and Nanoscale Physics capability.

Electron Microscopy, Neutron and X-Ray Scattering

Principal Contact: Mike Somonson

Aside from equipment located in the CNMS facility itself, users have access to other SEM, TEM, and STEM equipment at Oak Ridge National Laboratory. Access to these capabilities is through the ORNL Shared Research Equipment (SHaRE) program and the High-Temperature Materials Laboratory (HTML). The advanced capabilities of these tools include atomic-resolution imaging, high spatial resolution microanalysis (EDS and EELS), and electron holography using TEM/STEM instruments; a Scanning Auger Microprobe for nanometer-scale surface microanalysis and depth profiling; a fully automated electron microprobe for trace element determinations; and a variable pressure SEM incorporating EDS and XRF analysis for the study of polymeric and nano-bio samples.

CNMS users also have access to the neutron scattering facilities at ORNL's High-Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS). Capabilities include small-angle scattering and reflectometry instruments on the HFIR cold source, HFIR thermal neutron diffraction and spectroscopy capabilities, and a backscattering spectrometer and liquid / magnetism reflectometers at the SNS.

See the List of Capabilities for details of the specialized equipment associated with the Electron Microscopy, Neutron and X-Ray Scattering capability.

Nanomaterials Theory Institute

Principal Contacts: Peter Cummings, Thomas Schulthess, and Malcolm Stocks

The Nanomaterials Theory Institute (NTI) offers users access to significant computational, theory, and modeling capabilities. The NTI has a 5 teraflop Beowulf cluster, as well as a high-performance parallel visualization capability to view simulation results for analysis and to develop understanding of calculated properties. The NTI has a significant allocation of computer time on the National Energy Research Supercomputing Center (NERSC) at Lawrence Berkeley National Laboratory. NTI staff also compete for large allocations of time on the supercomputers of the National Center for Computational Sciences. NTI staff can provide theoretical support to experimental user projects through collaborative efforts. Staff are also available to assist experimentalist who wish to learn to run many of the state-of-the-art computational tools used within the NTI.

See the List of Capabilities for details of the specialized equipment associated with the Nanomaterials Theory Institute.

Nanofabrication Research Laboratory

Principal Contact: Mike Simpson

Capabilities in the Nanofabrication Research Laboratory center on patterning materials with varied biological, chemical and physical functionality. Staff scientists are developing techniques for modifying the functionality at the nanoscale, which will be a key component in understanding and directing weak interactions, nanoscale assembly, and hybrid system interactions. Other areas of concentration include deposition of materials on two and three-dimensional structures, particularly nanoscale components and products of unique nanomaterials synthesis, and development of new etch chemistries and techniques that enable the patterning and spatial organization of unique materials.

See the List of Capabilities for details of the specialized equipment associated with the Nanofabrication Research Laboratory.

General Characterization Facilities

A cooperative arrangement with the ORNL SHaRE User Program (mentioned earlier) provides access to other advance analytical tools not available within the CNMS. Examples include: advanced SEM, TEM, STEM; bolometric X-ray detector; scanning Auger microprobe for nanometer-scale surface microanalysis and depth profiling; electron holography; a fully automated electron microprobe for trace element determinations; and a variable pressure SEM incorporating EDS and XRF analysis for the study of polymeric and nano-bio samples.

Note: SHaRE and the High Temperature Materials Laboratory each operate their own user program. Users needing only the capabilities of one of these facilities and no other CNMS resources should apply directly to the facility concerned rather than the CNMS.

See the List of Capabilities for details of the specialized equipment associated with the General Characterization Facilities.

4.4 Facilities

The CNMS is located at Oak Ridge National Laboratory adjacent to the Spallation Neutron Source. The 80,000 sq. ft. facility houses a total of 32 laboratories, and approximately 10,000 ft^2 of clean room space. The building contains office space for up to 190 people, including CNMS staff, visiting senior staff, postdocs, graduate students, and other users.

CNMS has established partnerships with other ORNL user programs. The CNMS Nanomaterials Theory Institute provides collaborative workspaces, visualization equipment, and high-speed connections to the terascale computing facilities of ORNL's National Center for Computational Sciences. The CNMS also provides a gateway to electron microscopy, atom probe, nanoindentation and other capabilities in the Shared Research Equipment (www.ms.ornl/share/index.shtml) and High Temperature Materials Laboratory (www.ms.ornl.gov/htmlhome/) user programs.

4.5 Associated Major User Facilities at Oak Ridge National Lab

In addition to the core Center for Nanophase Materials Sciences facility, users also can have access to other major user facilities at Oak Ridge National Laboratory.

CNMS users are encouraged to take advantage of the world-class neutron scattering facilities that are available at ORNL's High-Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS). Beamlines of particular relevance to CNMS Scientific Themes include the small-angle scattering and reflectometry instruments on the HFIR cold source, HFIR thermal neutron diffraction and spectroscopy capabilities, and early-availability instruments at SNS including the backscattering spectrometer and the liquids and magnetism reflectometers.

CNMS users who may be interested in neutron scattering opportunities are encouraged to indicate their interest in the designated box on the CNMS proposal form. The CNMS will assist its users to identify the appropriate neutron scattering resources, develop competitive beamtime proposals, or collaborate with arrangements for potential access as initial users as additional instruments are commissioned.

Figure 8. Spallation Neutron Source, Oak Ridge National Laboratory. (Photo courtesy of ORNL.)

4.6 Interactions with Users

The CNMS user program provides access to equipment and technical expertise for nanoscale research that defines the state of the art. The program is open to users from academia, business and industry, and research institutes worldwide. Users join a vibrant research community that brings together ORNL research staff, technical support staff, students, postdoctoral scholars, and collaborating guest scientists. The program accommodates both short-term and long-term collaborative research partners. Access is through a brief peer-reviewed proposal and there is no charge for users who intend to publish their results. Access is also available on a cost-recovery basis for research that is not intended to be published. Prospective users are encouraged to consult CNMS staff members to learn more about the center's science and capabilities.

4.7 CNMS Contact Information

Linda Horton
CNMS Director
865.574.5081
FAX: 865.574.1753
hortonll@ornl.gov

Peter Cummings
Principal Scientist
865.241.4779
FAX: 865.574.1753
cummingspt@ornl.gov

Tony Haynes
User Coordinator
865.576.2858
FAX: 865.574.1753
hayneste@ornl.gov

Randy Ogle
Operations Manager
865.574.5744
FAX: 865.574.1753
oglerb@ornl.gov

4.8 List of Capabilites

The information in this list was obtained from the CNMS web site at http://www.cnms.ornl.gov/ .

CNMS Specialized Equipment and Instrumentation

Macromolecular Nanomaterials:

- Nuclear Magnetic Resonance Spectroscopy (NMR)
- Organic and aqueous Gel Permeation Chromatography (GPC)
- High-Temperature GPC
- Membrane and Vapor-Phase Osmometer systems (MO)
- Multi-angle Laser Light Scattering (18 angles) (MALLS)
- Absolute and differential refractive index detector (DNDC)
- Simultaneous Static and Dynamic Light Scattering
- Rheometer
- Dynamic Mechanical Analyzer
- GC / GC-MS
- Fluorescence Spectrometer (Spex Fluorolog 2)
- Matrix Assisted Laser Desorption Ionization- Time-of-Flight Mass Spectrometer
- Thermogravimetric Analyzer Differential Scanning Calorimeter
- UV-Visible-NIR
- Fourier Transform Infrared Spectrometer (FTIR)
- Spectroscopic Ellipsometer
- *In Situ* Fourier Transform Infrared Spectrometer (*In-situ IR*)

Catalytic Nanomaterials:

- Thermal gravimetric analyzer and differential scanning analysis
- Nanozetameter with high-temperature capability
- Volumetric gas adsorption
- Raman spectroscopy
- ICP for composition analysis
- Pulsed and Plug-flow gas phase catalytic reactors; high-pressure flow reactor
- Temperature programmed transformations
- Pulsed chemisorption
- Automated potentiometric surface acid/base titration
- Electrocatalysis
- High-Pressure Flow Reactor, Benchtop Flow Reactor, and Ex-Situ Reactor
- 500 MHz Liquid/Solid NMR Spectroscopy
- θ -2θ X-ray powder diffraction
- First principles computational catalysis

Functional Hybrid Nanomaterials:

- Robotically-scanned 600W Nd:YAG laser system
- Gated Intensified CCD imaging and spectroscopy
- CVD system in a 3"-i.d. tube furnace (1200°C) with pressures down to ~ 1 torr
- Molecular Beam Growth of Carbon nanotubes on substrates
- Time-resolved reflectivity
- Rapid thermal laser-CVD growth and processing facility with X-Y-Z control
- Complex oxide heterostructure Pulsed-Laser Deposition
- Oxide Target Synthesis
- Photo- and e-beam lithography
- Laser/nanomaterial interactions and X-Y-Z processing
- Chemical purification and functionalization of carbon nanotubes
- Thermal diffusivity measurements
- Electrospinning of nanocomposite fibers
- Semiconductor parameter analyzer
- Cryogenic probe station
- AC impedance spectroscopy system
- Zahner controlled intensity modulated photospectroscopy
- UV-VIS-NIR Characterization of SWNTs, etc. by Absorption Spectroscopy
- UV-VIS-NIR Fluorometry with remote fiber probing of liquids/surfaces
- Ultrafast laser spectroscopy of nanomaterials and composites
- Raman characterization of carbon nanotubes, oxides, polymers
- Tunable Raman (micro/macro) spectroscopy (0.25 – 1.6 µm)
- In situ Raman spectroscopy at <1500°C: CVD, annealing, electrochemistry
- Tunable (0.25 – 1.6 µm) fs/ps laser system (nJ @ 80 MHz)
- Tunable (0.3 – 2.6 µm) High energy, fs laser system (2.5 mJ @ 1 kz, 40 fs)
- Tunable (0.22 – 1.8 µm) ns laser system (mJ @ 10Hz)
- Spectroelectrochemical characterization of nanomaterials and composites

Scanning Probes and Nanoscale Physics:

- *In Situ* MBE in UHV chambers attached to SEMPA, 4-probe STM, UHV MOKE
- *In Situ* laser MBE with RHEED, AFM/STM, surface characterization
- *In Situ* PLD with high pressure RHEED for monitored growth of metals, oxides
- Low Energy Electron Diffraction (LEED)
- Auger Electron Spectroscopy (AES)
- X-ray Photoelectron Spectroscopy (XPS)
- Scanning Electron Microscopy with Polarization Analysis (SEMPA)
- Ultra-high Vacuum Cryo 4-probe STM
- Ultra-high Vacuum Variable Temperature AFM/STM with *in situ* growth
- Atomic Force Microscopy
- Ambient Scanning Probe Microscopy for air or liquid environments

Electron Microscopy, Neutron and X-Ray Scattering:

- Advanced Scanning Electron Microscopy and Spectroscopy
- Z-Contrast Scanning Transmission Electron Microscopy
- X-ray Diffraction (2-circle and 4-circle XRD)
- X-ray Fluorescence
- Shared Research Equipment
- Neutron Scattering

Nanomaterials Theory Institute:

- NTI Beowulf cluster (~5 TFlops)
- National Energy Research Supercomputing Center computing allocation
- National Leadership Computing Facility (NLCF) allocation
- 16-screen video wall
- 16-quad-processor-node visualization cluster/data storage to drive video wall
- Visualization workstations

Nanofabrication Research Laboratory:

- JEOL JBX-9300–100 kV e-beam lithography for high resolution nanopatterning
- FEI Nova 600 SEM/focused ion beam system for micro- and nanofabrication.
- Optical Lithography with broadband (405–365 nm) exposure optics
- JEOL JSM-7400 field-emission scanning electron microscope.
- Oxford 100 DRIE/RIE system
- Thermal Oxidation Furnace
- Low pressure CVD of SiO_2, Si_3N_4 (low stress), and poly-Si (doped and undoped).
- Low temperature plasma enhanced CVD of SiO_2, Si_3N_4 and silicon oxy-nitrides
- E-beam evaporation, thermal evaporation, and sputter deposition of metals, semiconductors, and dielectrics
- Technics Reactive Ion Etching system for dry etching dielectric, polymer material
- Spectroscopic Reflectometry
- Surface Profilometry
- Electrical Properties Measurements (DC to 6 GHZ)

General Characterization Facilities:

- X-ray Diffraction and Fluorescence
- Hitachi HD2000 STEM and Hitachi S4700 FEG-SEM at the CNMS
- Ambient AFM and SPM
- Differential Scanning Calorimeter, temperature range -180–730°C
- UV-Visible-NIR spectroscopy
- Fluorescence spectroscopy
- Spectroscopic Ellipsometer
- Nanoindentation and Atom Probe Field Ion Microscopes (SHaRE Program)

5.0 Center for Nanoscale Materials

5.1 General Information

The Center for Nanoscale Materials (CNM) NSRC is located at Argonne National Laboratory. CNM provides state-of-the-art tools, facilities, and expertise to partner with users from across the U.S. and worldwide nanoscience research. The nanocenter is collocated with major Argonne National Laboratory (ANL) user facilities, i.e., the Advanced Photon Source and Electron Microscopy Center. Users of CNM can obtain access to these facilities for specialized diagnostics and materials analysis of extremely small structures.

The Center for Nanoscale Materials builds on Argonne's long history and culture of open and collaborative research with the broad scientific community, both academic and industrial. CNM is able to host visiting scientists as independent investigators or as collaborative partners.

The following sections summarize CNM research focus areas, facilities, capabilities, and user's program. Additional information is available from the CNM web site at http://nano.anl.gov/ .

5.2 CNM Scientific Themes

Center for Nanoscale Materials has identified six scientific themes in nanoscience to focus its research activities.

- Electronic and Magnetic Materials & Devices
- Nano-Bio Interfaces
- Nanofabrication
- Nanophotonics
- Theory and Modeling
- X-Ray Imaging

Figure 9. Center for Nanoscale Materials, Argonne National Laboratory. (Photo courtesy of ANL.)

Electronic and Magnetic Materials & Devices

Group Leader: Matthias Bode

The goal of this scientific research theme is understanding and control of electronic and magnetic behavior of materials at the nanometer scale. Unique and non-linear electronic / magnetic interactions between electromagnetic fields and matter emerge when nanostructure dimensions become comparable to, or less than, radiation wavelengths. In addition, the EM properties and response can often be tailored with nanostructure size.

Synthesis and processing of these nanomaterials includes hierarchical assembly via polymeric and bio-templating, colloidal synthesis of core-shell structures, and nano-photolithographic patterning. Materials of interest span metallic, semiconductor, superconductor, oxide, and hybrid systems. Research includes experiment, theory, and modeling.

Some possible applications of research in this theme area include: creation of ultra-strong permanent magnets for energy-efficient motors; advanced information storage technologies; spin-related quantum computing; new medical therapies; and biomedical diagnostics.

Nano-Bio Interfaces

Acting Group Leader: Tijana Rajh

The Nano-Bio Interfaces scientific theme area is focusing on the design, synthesis, and characterization unique interfaces between biological and inorganic materials. Such biological (“soft”) and inorganic (“hard”) materials can have dramatically different properties and functionality. Thus, hybrids between these material types could enable new and important functional materials. One example might be combining the established technologies and infrastructure from inorganic electronic materials with the responsiveness, sensitivity, and molecular specificity of biological structures.

Research in this area includes X-ray, electron, neutron, and photonic characterization. Theory and modeling play an important role in the nano-bio interface design and prediction of performance.

Possible applications are far reaching. New chemical catalysts could be created combining robustness and reactivity of inorganic nanoparticles with the specificity of biological molecules. Artificial vision may be possible by joining biological photoreceptors with inorganic semiconductor based microelectronics. Similarly, biological material could be used for energy harvesting, storage, and transduction coupled with inorganic structures for energy transfer to the macroscopic regime.

Nanofabrication

Acting Group Leader: Derrick Mancini

Research in the Nanofabrication scientific theme is exploring new synthesis techniques for fabrication of nanostructures. Research goals include pushing the state-of-the-art in nanofabrication to 10-nm regime, and combining self-assembly and lithographic patterning approaches to produce unique structures.

The nanofabrication activity also provides support to all areas of CNM nanoscale research. This support entails collaborative with users to develop new nanomaterials, as well as training users in these techniques.

Techniques and capabilities of the group include electron and focused ion beam nanopatterning, nanoimprinting, optical lithography, and advanced pattern transfer and thin-film deposition and synthesis capabilities. Argonne operates a 30-kV Raith 150 e-beam lithography tool, and a 100-kV e-beam lithography tool that will be installed in the CNM. There will also be clean room space dedicated to metrology, electrochemistry, wet etching, and biosynthesis.

Argonne currently operates a 30-kV Raith 150 e-beam lithography tool, and a 100-kV e-beam lithography tool will ultimately be installed in the CNM. Other capabilities include an optical ultraviolet mask aligner, optical microscopes, profilometer, photoresist spinner and developing stations, plasma etchers, ovens and hotplates, and facilities for wet etching and electroplating.

Nanophotonics

Acting Group Leader: Gary Wiederrecht

The goal of the Nanophotonics scientific theme is a fundamental understanding of photon creation and control at the nanometer scale.

The smallest feature- that can be resolved by light is normally a size on the order of the wavelength of the light, i.e., the diffraction limit. However, it is possible to confine electromagnetic (EM) fields on the surfaces of nanoparticles, creating extraordinarily strong "near-fields" or evanescent fields due to this localization. The photochemical and photophysical response of materials to EM fields is often non-linear. Thus, the combination of nanoparticle-confined near fields and non-linear response can lead to incredible effects only possible at the nanometer scale.

The Nanophotonics group relies heavily on recent advances in near-field scanning optical microscopy (NSOM) to probe, understand, and control these largely unexplored phenomena. The ultra-high resolution NSOM diagnostic is being combined with time-resolved spectroscopy to study photo-initiated processes. Research in the group also includes a theory component for a first-principles understanding of these enhanced light-matter interactions.

Possible applications of research in Nanophotonics could be optical integrated circuits, nanolasers, optical computing, light harvesting, and nano-sized optical interconnects for telecommunications, surface plasmon-assisted reactive chemistry (SPARC); and metamaterials (i.e., negative index materials).

Theory and Modeling

Acting Group Leader: Larry Curtiss

The Theory and Modeling group will work closely with the experimental efforts in the other CNM scientific theme areas. The goal of this group is to use theory and multiscale computer simulations to help guide and interpret laboratory investigations and create new nanoscale functional systems. A long-term vision is to create a "Virtual Fab Lab" to guide design, fabrication, and testing of nanoscale materials.

Computational capabilities of the group include: *ab initio* quantum chemistry; density functional theory; quantum dynamics; transition-state theory; electrodynamics simulations; atomistic, mesoscale, and continuum methods. Activities in this group include interactions with, assisting, and instructing users (both theorists and experimentalists) in applying these techniques. Researchers in the group are also involved in computational method development and implementing new parallel computing algorithms. Nanoscale processes to be addressed by the Theory and Modeling group include self-assembly, nanocatalysis, nanophotonics, and charge transfer at the bio-inorganic interface.

X-Ray Imaging

Acting Group Leader: Jorg Maser

The X-Ray Imaging project will provide a hard X-ray microscopy beamline with the highest spatial resolution in the world. This capability will provide for fluorescence, diffraction, and transmission imaging with hard X-rays at a spatial resolution of 30 nm or better. The nanoprobe will cover the spectral range of 3-30 keV; the working distance between the focusing optics and the sample will be in the range of 10-20 mm.

This X-ray Imaging facility will be a unique, enabling capability for CNM nanoscale research and the broader nanoscience community in studying nanomaterials and nanostructures, particularly for embedded structures.

The X-Ray Imaging tool can be applied in a number of different operational modes to provide complementary sample information. *Transmission* can be used to map the sample's density, spatial location of elemental constituents, and internal structure. *Diffraction* mode can provide structural information, such as crystallographic phase, strain, and texture. *Fluorescence* mode can reveal spatial distribution of individual elements in a sample, including quantitative trace element analysis, important for understanding material properties such as second-phase particles, defects, and interfacial segregation. In *spectroscopy* mode, the primary X-ray beam's energy is scanned across the absorption edge of an element, providing information on its chemical state (XANES) or its local environment (EXAFS). In *tomography*, the above modes can be combined with sample rotation to produce two-dimensional projection images, to be used for reconstructing the sample's internal three-dimensional structure.

5.3 Center for Nanoscale Materials Facilities

The CNM is housed in a two-story, 83,000 square foot building at Argonne National Laboratories, completed in April, 2006. The facility is located on the west side of ANL's Advanced Photo Source, and CNM will have a dedicated beamline for study of materials properties at the nanoscale.

CNM has facilities for synthesis, fabrication, and characterization of nanoscale materials, dedicated laboratories for interactions, training, and collaborative research with visiting users, and office space for CNM staff, administration, and visitors. Areas in both the clean room and conventional laboratories will allow research using biological materials with Biosafety Level 2 protocols.

More detailed information about CNM facilities and capabilities is given in the accompanying List of Capabilities at the end of this Section.

Figure 10. Advanced Photon Source, Argonne National Laboratory. (Photo courtesy of ANL.)

5.4 Associated Major User Facilities at Argonne National Laboratory

In addition to the core CNM facility, users also can have access to three major user facilities at Argonne National Laboratory.

Advanced Photon Source

The Advanced Photon Source (APS) is a major U.S. scientific resource that provides the most brilliant x-ray beams in this hemisphere. These x-rays allow visiting scientists to probe the structure and properties of a wide range of materials for research in materials science, biology, chemistry, and physics. At the periphery of the accelerator's storage ring is the Experimental Hall, consisting of 35 sectors with access to the x-ray beamlines, allowing users to set-up their individual experiments.

More information about the Advanced Photon Source is available at its web site: http://www.aps.anl.gov/About/APS_Overview/index.html .

Electron Microscopy Center

The Electron Microscopy Center (EMC) is a User Facility for electron-beam characterization of materials. The EMC staff works with researchers from across Argonne National Laboratory, as well as visitors from universities and other laboratories worldwide. Research by EMC personnel includes microscopy based studies in high Tc superconducting materials, irradiation effects in metals and semiconductors, phase transformations, and processing related structure and chemistry of interfaces in thin films.

More information about the Intense Electron Microscopy Center is available at its web site:
http://www.msd.anl.gov/groups/emc/

5.5 CNM Interactions with Users

The purpose of the User Program is to provide access to equipment, facilities, and staff at CNM in support of fundamental research in nanoscience. Access is available to interested users worldwide by means of a competitive research proposal process. Proposals are submitted under the six broad scientific themes described earlier through a web-based system; the group leaders (listed above) of each theme area are available for initial contact and to provide additional information in their area. However, work that spans more than one of the scientific themes is encouraged. Proposed research can range from a single visit for access to specific tools to a series of visits to CNM over an extended period.

Proposals from users are associated with specific CNM personnel and capabilities, ideally, proposals are coordinated with the appropriate CNM staff to assure resources (time and equipment) and mutual scientific interests and goals. The proposed nanoscience research can take advantage of major user facilities at Argonne National Laboratory (the Advanced Photon Source and Electron Microscopy Center).

Proposed work is reviewed by a Proposal Evaluation Board to evaluate its scientific merit, technical feasibility, capability of the experimental group, and availability of required resources.

5.6 CNM Contact Information

Eric Isaacs
CNM Director
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439
630.252.5749
FAX 630.252.6866

Derrick Mancini
CNM Associate Director
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439
630.252.0147
FAX: 630.252.5739

Stephen Streiffer
Associate Division Director for Science
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439
630.252.5832
FAX 630.252.5769

Thomas Burt
Assistant Division Director
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439
630.252.2625
FAX: 630.252.6866

Sam Bader
Chief Scientist
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439
630.252.4960
FAX 630.252.5219

Katie Carrado Gregar
Manager, User & Outreach Programs
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439
630.252.7968
FAX: 630.252.6866

5.7 List of Capabilities

The following information on Center for Nanoscale Materials capabilities and equipment was obtained from the CNM web site at http://nano.anl.gov/ .

Electronic and Magnetic Materials & Devices

- Molecular beam epitaxy
- E-beam evaporation and sputtering
- Powder and high-resolution X-ray diffractometry
- Scanning probe microscopy
- Electrical characterization: impedance analysis, I-V, polarization
- Four-probe ultrahigh-voltage scanning transmission/electron microcopy
- SQUID magnetometry
- Magnetotransport measurements
- Raman spectrometry

NanoBio Interfaces

- Synthesis of nanoparticles and bio-inorganic composites, including diamond films
- Synthesis of surface-modified metal and metal-oxide nanoparticles; quantum dots
- Peptide and molecular synthesis
- Post-self-assembly processing of soft materials
- Chemical vapor deposition
- Photochemical functionalization
- Electrodeposition, electrochemical functionalization
- Access to synchrotron X-ray spectroscopy; scattering, and nanoparticle diffraction
- Thermal and rheological analysis
- Scanning probe microscopy
- Electrochemical analysis
- Laser scanning confocal microscopy
- Optical spectroscopy

Nanofabrication

- Raith 150 30-kV e-beam lithography
- JEOL 9300F 100-kV e-beam lithography
- Focused ion-beam patterning
- Karl Suss MA6 aligner optical lithography
- Oriel exposure system for up to 100-mm-diameter substrates
- Reactive ion etching
- Resist processing: spin coating and bake
- Selective etching of metals and dielectrics
- Silicon anisotropic etching; silicon and silicon nitride membrane fabrication
- Gold, platinum, copper, and nickel electroforming
- Chromatography system
- Scanning vibrating electrode system
- Voltammetry system
- Wafer spin rinse tools (2, 4, and 6 inch)
- Wafer priming oven
- Nanoimprinter
- Spectroscopic ellipsometer
- Surface profilometer

Nanophotonics

- Aperture and apertureless near-field scanning optical microscopy
- Confocal imaging and pump-probe spectroscopy
- Ultrafast transient absorption

- Size-selected clusters and cluster-based nanomaterials for nanophotonics
- Photocatalytic size-selected metal and composite clusters and nanostructures

Theory and Modeling

- Web-based magneto-optic simulation
- Time-domain nanophotonics simulation
- DFT tight-binding electronic structure (clusters, periodic structures, *ab initio* MD)
- MPI-based parallel versions of nanophotonics and tight-binding codes
- 350 Xeon processor Linux cluster at the Laboratory Computing Resource Center

X-Ray Imaging

- Synchrotron microbeam techniques
- Hard X-ray nanoprobe with 30-nm resolution at 10 keV
- Access to the ANL Electron Microscopy Center through the existing EMC proposal mechanism in cases where this would benefit research at the CNM

Nanosynthesis and Characterization

- Confocal Raman Spectrometer
- Luminescence Spectrometer
- UV-Visible-NIR Spectrometer
- Centrifuges
- Solvent Purification System
- Thermogravimetric Analysis and Rheology
- Automated Synthesizer
- Langmuir-Blodgett Trough System
- Laser Scanning Confocal Microscope
- Sputtering System
- Electron-Beam Evaporator
- Oxide MBE System
- Microwave Plasma CVD System
- Magnetometers
- Near-Field Scanning Optical Microscope, Ultrafast Spectroscopy
- Combined Scanning Electron/Scanning Probe Microscope
- Scanning Probe Microscopes
- X-ray Diffractometer
- Optical Microscope
- Electrical Characterization

6.0 Molecular Foundry

6.1 General Information

The Molecular Foundry is located at Lawrence Berkeley National Laboratory (Berkeley Lab). A major research effort at the Molecular Foundry is the synthesis and characterization of unique nanoscale structures and materials. Scientists at the Molecular Foundry seek to understand and develop techniques to use nanostructured "building blocks" to create new, functional nanoscale assemblies. Visiting researchers can utilize the specialized laboratories and characterization tools at Molecular Foundry to further their own nanoscience projects. The Molecular Foundry staff is available to assist and instruct Users, or for longer-term collaborative scientific studies. Access to the Molecular Foundry staff and facilities is gained through a peer-reviewed competitive proposal process.

The following sections summarize the Molecular Foundry's research thrusts, facilities, capabilities, and user's program. Additional information is available from the Molecular Foundry web site at http://foundry.lbl.gov/ .

6.2 Molecular Foundry Research Themes

Nanoscience research at the Molecular Foundry centers around three central themes:

- Characterization and control of the interface between organic and inorganic materials
- Synthesis of supra-molecular assemblies from nano-components
- Patterning of substrates with single digit nanometer resolution

The specialized facilities within the Molecular Foundry support these over-arching research themes.

6.3 Molecular Foundry Research Facilities

The Molecular Foundry houses six facilities focusing on specific aspects of nanoscale science:

- Inorganic Nanostructures
- Nanofabrication
- Organic and Macromolecular Synthesis
- Biological Nanostructures
- Imaging and Manipulation of Nanostructures
- Theory of Nanostructures

Inorganic Nanostructures

Director: A. Paul Alivisatos

The Inorganic Nanostructures facility focuses on metal, carbon, and semiconductor nanostructures. Nanocrystals, nanotubes, and nanowires are synthesized by a variety of techniques, for example chemical vapor deposition and colloidal approaches. Staff scientists are developing growth precursors of nanoscale inorganic materials, studying their growth mechanisms, and functional properties. Experimental work is complimented by fundamental theoretical studies of nanostructure properties.

Example projects in the Inorganic Nanostructures facility include: growth of BN and carbon nanotubes, Si and CaN nanowires, and III-V semiconductor nanowires; synthesis of metallic oxide and semiconducting nanoparticles; and structural, electrical, and optical characterization of these nanostructures.

Nanofabrication

Director: Jeff Bokor

The Nanofabrication facility provides access to high-resolution lithographic and thin-film growth / processing tools for fabrication of nanostructures. These facilities enable integration of chemical and biological nanostructures with advanced semiconductor processing techniques. Within the Class 1000 and Class 100 clean room space this facility offers a wide range of state-of-the-art nanoscale processing tools, including: high-resolution e-beam, focused ion beam, optical, and nanoimprint lithography; plasma etching; focused electron beam and ion beam deposition; resist processing; thin-film deposition, wet chemical processing; and thermal evaporation / sputtering.

Organic and Macromolecular Synthesis

Director: Jean M.J. Frechet

This facility concentrates on synthesis and properties of organic molecules and macromolecules. Organic synthesis capabilities range from single molecules to molecular assemblies, building block libraries, liquid crystals, organic electronic and photonic nanomaterials. The facility offers polymer capabilities such as polymerization reactors, polymers with controlled sequence / architecture, and dendritic materials. Libraries of ligands and catalysts enable combinatorial synthesis of materials. Hybrid materials, for example organic – inorganic or biological – artificial hybrids, are also being synthesized by the facility users and staff.

Biological Nanostructures

Director: Carolyn R. Bertozzi

The Biological Nanostructures effort encompasses a broad range of topics, including systems integration, biomimetic structures, and fundamental understanding of biological systems. One research thrust is to integrate biological components into nanomaterials with unique, designed function or properties. In the biomimetics efforts, scientists are seeking to build nanoscale devices or functions, for example self-assembly or self-repair of materials, whose operating principles / mechanisms mimic those found in nature. Researchers are also using nanotechnology tools as means to study biological mechanisms.

Imaging and Manipulation of Nanostructures

Director: Miquel Salmeron

This facility provides tools and expertise for characterization and manipulation of nanostructures. Imaging probes in the facility include scanning and transmission electron microscopy and spectroscopy, near-field optical scanning microscopy, optical spectro-microscopy, and linear / non-linear spectroscopy with broadly tunable light sources, and Auger XPS. A variety of scanning probe instruments are available for nanostructure characterization. Available techniques include atomic force microscopy (AFM) and scanning tunneling microscopy (STM) in air or liquid environments, electrostatic AFM for liquid films, quantitative AFM for characterization of mechanical properties.

Theory of Nanostructures

Director: Steven G. Louie

The Theory of Nanostructures facility conducts fundamental work to understand and predict behaviors and properties of nanostructures. Scientific staff members work on projects originating within the five experimental facilities within the Molecular Foundry, as well as on their own theoretical investigations. A wide array of theoretical and computational techniques are available to investigate / understand nanostructure electronic, structural, and magnetic properties, spectroscopic signatures, and mechanical behavior. Capabilities and expertise include: molecular dynamics and force-field calculations, quantum and classical Monte Carlo, time-dependent density functional theory, and first-principles transport calculations.

6.4 Molecular Foundry Laboratory Building

The Molecular Foundry is located at Lawrence Berkeley National Laboratory in a new facility near the Advanced Light Source. It is housed with a six-story, 94,500 square-foot facility providing laboratory and office space. The building includes approximately 4,000 square feet of Class 1000 clean room space (and an addition 725 square feet of Class 100 clean room space) for nanofabrication / lithography and clean measurements, and a 5,500 square-foot low vibration, low-electromagnetic-field laboratory housing state-of-the-art imaging and manipulation tools. Offices and laboratories are available for visiting scientists, technical user-support staff, and onsite Users.

Figure 11. Advanced Light Source, Lawrence Berkeley National Laboratory. (Photo courtesy of LBNL.)

6.5 Associated Major User Facilities at Berkeley Lab

In addition to the core Molecular Foundry facility, users also can have access to three major user facilities at Lawrence Berkeley National Laboratory.

<u>Advanced Light Source</u>

The Advanced Light Source (ALS), a division of Berkeley Lab, is a national user facility that generates intense light for scientific and technological research. As one of the world's brightest sources of ultraviolet and soft x-ray beams--and the world's first third-generation synchrotron light source in its energy range--the ALS makes previously impossible studies possible. The facility welcomes researchers from universities, industries, and government laboratories around the world. It is funded by the U.S. Department of Energy's Office of Basic Energy Sciences. For more information, see the ALS web site at http://www.als.lbl.gov/ .

National Center for Electron Microscopy

The National Center for Electron Microscopy (NCEM) is a national user facility for electron microscopy and micro-characterization. The NCEM features several unique instruments, complemented by strong expertise in computer image simulation and analysis. The NCEM also maintains one-of-a-kind instruments for imaging of magnetic materials, and develops techniques and instrumentation for dynamic *in-situ* experimentation. Visiting researchers and center facilities are supported by resident scientific and technical staff. In addition to providing guidance to visiting researchers, the NCEM's staff scientists conduct their own specialized research. For more information on the NCEM, see their web site at http://ncem.lbl.gov/ .

National Energy Research Scientific Computer Center

The National Energy Research Scientific Computing Center (NERSC) is one of the largest facilities in the world devoted to providing computational resources and expertise for basic scientific research. , NERSC is a world leader in accelerating scientific discovery through computation. More than 2000 computational scientists use the NERSC to perform basic scientific research across a wide range of disciplines, including climate modeling, research into new materials, simulations of the early universe, analysis of data from high energy physics experiments, investigations of protein structure, and a host of other scientific endeavors. For more information about the NERSC, see their web site at http://www.nersc.gov/ .

6.6 Interactions with Users

(The following detailed description of the MF User Program, regulations and procedures are quoted from their web site.)

The Molecular Foundry User Program offers domestic and international researchers (Users) from academia, industry, and government laboratories direct access to the Foundry, other LBNL User facilities and affiliated nanoscience research labs. Access is gained through a peer-reviewed proposal process. User proposals undergo an internal feasibility assessment encompassing technical, Environmental Health and Safety (EHS) and staffing resource considerations, followed by an evaluation by an external Proposal Study Panel (PSP). An average of eight weeks is required from submission to author notification.

Approved, non-proprietary projects receive no-cost access to staff and laboratory facilities. Proprietary users, those wishing to maintain confidential data, pay a fixed rate, currently $15K per month.

A proposal may request the use of a single Foundry facility or several. Multi-facility projects are encouraged and can result in more favorable proposal ratings since they make the best use of the Foundry's unique capabilities.

Standard Projects:

- Synthesis of nanostructures
- Preparation of new nanoscale materials or devices
- Training in new methods
- Development of new methods
- Instruction in the replication of Foundry instruments and techniques
- Pursuit of long term collaborations with Foundry staff

Sample-Only Project:

A request for material regularly synthesized at the Foundry, and thus requiring no dedicated staff (i.e., routinely generated peptoids or quantum dots). Accelerated review for feasibility and merit by the Foundry Directorate without PSP evaluation.

Instrument-Only Project:

A project requiring limited access to a specialized Foundry instrument and little staff time. Accelerated review for feasibility and merit by the Foundry Directorate without PSP evaluation.

Proprietary Project:

Like a standard project, but with the intent to withhold research results from publication for up to 5 years. Although the proposed work may be proprietary, sufficient information must be included in the proposal to permit evaluation of its scientific merit.

More complete information about Molecular Foundry User Program can be found at: http://foundry.lbl.gov/users/access.htm .

6.7 Molecular Foundry Contact Information

Carolyn Bertozzi
MF Director
Lawrence Berkeley National Lab.
1 Cyclotron Road, MS67-R3207
Berkeley, CA 94720
510.643.1682
FAX: 510.486.5846
CRBertozzi@lbl.gov

Mark D. Alper
MF Deputy Director
Lawrence Berkeley National Lab.
1 Cyclotron Road, MS66
Berkeley, CA 94720
510.486.6581
FAX: 510.486.7768
MDAlper@lbl.gov

Jeffrey Bokor
MF Deputy Dir., Scientific Program
Lawrence Berkeley National Lab.
1 Cyclotron Road, MS67-R2206
Berkeley, CA 94720
510.642.4134
FAX: 510.642.2739
JBokor@lbl.gov

James M. Bustillo
MF Deputy Dir., User Program
Lawrence Berkeley National Lab.
1 Cyclotron Road, MS67-R3207
Berkeley, CA 94720
510.486.4574
FAX: 510.486.7424
JMBustillo@lbl.gov

Molecular Foundry
Lawrence Berkeley National Laboratory
1 Cyclotron Road, MS67-R3207
Berkeley, CA 94720
510.486.4574
FAX: 510.486.5846
molecularfoundry@lbl.gov

6.8 List of Capabilities

The following information on the Molecular Foundry specialized equipment and instrumentation was obtained from the MF web site at http://foundry.lbl.gov/ .

Molecular Foundry Specialized Equipment and Instrumentation

Inorganic Nanostructures:

- Bruker AXS D8 Discover GADDS XRD Diffractometer system
- (two) Thomas Swann 3x2 CCS MOCVD reactors
- Yabin Ivon Fluorolog 3 Spectrofluorimeter with PL life-time capability
- Agilent Precision Semiconductor Parameter Analyzer
- Shimadzu UV-near IR Spectrophotometer
- Rucker and Kolls Probe Station
- Low temperature, inert atmosphere probe station

Nanofabrication:

- Vistec (formerly Leica) VB300 Electron Beam Lithography system
- Molecular Imprints Imprio 55 'Step and Flash' Imprint Lithography system
- Zeiss XB 1540 Focused Ion Beam/SEM Etching/Deposition system
- Zeiss Ultra 60 Field Emission SEM/STEM system with multiple detection
- ABM Contact Printer (broadband Hg arc lamp source, 5 micron resolution)

Organic and Macromolecular Synthesis:

- Bruker Biospin Avance II 500 MHz High Performance NMR Spectrometer
- Applied Biosystems TF4800 Maldi-TOF-TOF Spectrometer
- Bruker Daltonics UltroTOF Mass Spectrometer
- Varian 3200 FT-IR
- Viscotek Size Exclusion Chromatograph
- Dionex UltiMate 3000 nanoHPLC
- Agilent GC-MS 6890
- ChemSpeed Multiplant reactors
- Micromeritics ASAP 2020 Surface area and porosity measurement
- Horiba Light Scattering particle size distribution analyzer LA 950
- Biotage Microwave Reactor

Biological Nanostructures:

- Total internal Reflection Microscopy System with Olympus IX-81w/Andor EMCCD camera
- Amersham Biosciences Akta FPLC
- Agilent 1100 series (ion trap) LC-MC-MC Mass spectrometer
- Beckman NXp High Throughput Screening Robot
- Varian analytical and semi-prep HPLCs
- GeneVac Evaporator
- Biotage SP1 Flash Chromatography System
- Custom-built Robotic Combinatorial Synthesizers
- ACT Apex 396 Peptide Synthesizer
- Applied Biosystems 3400 DNA Synthesizer
- Real-time PCR 7000 Sequence Detection System
- Applied Biosystems GeneAmp PCR Thermal Cycler
- Molecular Devices Absorbance and Fluorescence Plate Readers
- Perkin-Elmer Lambda 35 UV-VIS Spectrophotometer
- Cell culture incubators and biosafety cabinets

Imaging and Manipulation of Nanostructures:

- JEOL 2100-F 200 kV Field-Emission Analytical Transmission Electron Microscope.
- Zeiss Gemini Ultra-55 Analytical Scanning Electron Microscope for imaging and analysis of conducing and insulating samples.
- Zeiss Gemini Supra 55 VP-SEM for in-situ microscopy with SEM in-lens and conventional secondary detectors, quadrant backscatter detector and variable pressure (10-100 Pa) secondary detector.
- Agilent (Molecular Imaging) PicoPlus Scanning Probe Microscope system for in situ imaging in air, controlled gas/humidity or in liquids, including under electrochemical control.
- Asylum MFP-3D Atomic Force Microscope system with 90 micron closed loop XY scanner Z displacement and integrated optical imaging.
- Foundry-built ultra-low noise AFM for measuring chemical interaction forces in air or liquids with 5 micron closed-loop XYZ scanner and Asylum control system
- PHI 5400 X-ray photoelectron spectroscopy (XPS) system with conventional (non-monochromatic) Al/Mg Dual-Anode X-ray source.
- PHI 660 Scanning Auger (SAM) system with CeB6 electron gun, 1.5 to 15 kV with ~1 micron spatial resolution in Auger mode at 0.4% energy resolution.
- Optical Spectro-Microscopy Lab
    - broadly tunable ultra-fast laser system (Coherant MiraTi:SAF + OPG) operating in ps and fs modes
    - visible and infrared CW laser sources
    - optical grating spectrometers with CCD cameras/detectors (nitrogen cooled and electron-multiplied), single photon counting modules
    - diffraction-limited confocal optical spectroscopy station for Scattering, Raman, and Fluorescence (both linear and nonlinear)
    - tip-enhanced (near field) optical imaging and spectroscopy and tip-enhanced Raman spectroscopy (TERS)
    - Variable temperature optical spectroscopy station for Scattering, Raman, Fluorescence (both linear and nonlinear) from 5 to 300 K
- Optical Microscopy
- Leica DM4000 Optical Microscope
- Leica MZ16 Stereo microscope for sample inspection, probing and manipulation

Theory of Nanostructures:

- 296-processor Dell Linux cluster w/ fast Infiniband network
- Annual NERSC allocation
- In-house HP graphics workstations for data manipulation and visualization