Implementation Plan for Chemical Industry R&D Roadmap for Nanomaterials by Design

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Prepared by

Chemical Industry Vision2020 Technology Partnership

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Acronyms and Abbreviations

ACS, American Chemical Society

ACC, American Chemistry Council

AML Advanced Measurement Laboratory

ANL, Argonne National Laboratory

BAA, Broad Agency Announcement

BCP, Block co-polymers

BNL, Brookhaven National Laboratory

CAN, Computer Aided Nanodesign

CBAN, Consultative Board for Advancing Nanotechnology

CCR, Council for Chemical Research

ChI, Chemical Industry

CINT, Center for Integrated Nanotechnologies

CNT, Carbon Nanotube

DARPA, Defense Advanced Research Projects Agency

DHS, U.S. Department of Homeland Security

DOC, U.S. Department of Commerce

DOD, U.S. Department of Defense

DOE, U.S. Department of Energy

DOJ, U.S. Department of Justice

EERE, Office of Energy Efficiency and Renewable Energy

EHS, Environmental Health and Safety

EM, Electromagnetic

EPA. Environmental Protection Agency

FY, Fiscal Year

ITP, Industrial Technologies Program

HHS, Department of Health and Human Services

LANL, Los Alamos National Laboratory

LDA, Local Density Approximation

MANTECH, Manufacturing Technology

MEMS, Micro-electro-mechanical systems

MOU, Memorandum of Understanding

MRSEC, Materials Research Science and Engineering Center

NASA, National Aeronautics and Space Administration

NCN, Network for Computational Nanotechnology

NER, Nanoscale Exploratory Research

NSEC, Nanoscale Science and Engineering Center

NIH, National Institute of health

NIOSH, National Institute for Occupational Safety and Health

NIRT, Nanoscale Interdisciplinary Research Teams

NIST, National Institute of Standards and Technology

NNI, National Nanotechnology Initiative

NNIN, National Nanotechnology Infrastructure Network

NRL, Naval Research Laboratory

NSF, National Science Foundation

NSRC, Nanoscale Science Research Centers

OM. Optical Metrology

ORNL, Oak Ridge National Laboratory

PCA, Program Component Area

QC, Quality Control

SEM, Scanning Electron Microscope

SBIR, Small Business Innovation Research

SNL, Sandia National Laboratory

SRC, Semiconductor Research Corporation

STTR, Small Business Technology Transfer

TEM, Transmission Electron Microscopy

USDA, U.S. Department of Agriculture

Executive Summary

The purpose of this effort is to develop an implementation plan to realize the vision and goals identified in the *Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function.* This Nanotechnology Implementation Plan aims to achieve the following:

- Define industry's specific research needs for priority roadmap technical areas
- Develop R&D recommendations and identify potential funding sources
- Identify options for transitioning research in commercialized products
- Provide opportunity to access potential benefits, such as energy savings

A workshop was held on February 15, 2005 to identify the priority needs from the roadmap and to develop research recommendations targeted to the goals of National Nanotechnology Initiative (NNI). The workshop was attended by representatives from industry and government, and nanotechnology experts from academia, DOE, and NSF Nanoscale Science Research Centers. These attendees together identified seven prioritized needs areas in four topical areas of nanomaterials science and engineering for manufacturing:

Manufacturing and Processing

- Develop unit operations and robust scale-up and scale-down methodologies for manufacturing. Five classes of unit operations for nano-chemical engineering were identified: Synthesis, Separation, Purification, Stabilization, and Assembly. Specific needs include:
  - developing robust dispersion and surface modification processes that retain functionality, and
  - developing manufacturing processes for nanostructured catalysts, coatings, ceramics, sorbents, and membranes.

Characterization Tools

- Develop analytical tools for measuring and characterizing nanomaterials
- Develop real-time analytical tools for measuring and characterizing nanomaterials, particularly online and in-process tools for process control and robust measurement tools for quality control

Fundamental Understanding and Synthesis

- Develop new paradigms for creating nanoscale building blocks based on understanding of physics and chemistry at the nanoscale
- Develop new paradigms for controlled assembly of nanocomposites and spatially resolved nanostructures with long-range order

Modeling and Simulation

- Develop computational tools to predict bulk properties of materials that contain nanomaterials
- Develop methods for bridging models between scales, from atoms to self-assembly to devices

These interconnected needs areas span a range of Program Component Areas (PCAs), the research focus areas introduced in the NNI Strategic Plan of December 2004. PCAs are used by NNI to track federal investment in research areas critical to accomplishing NNI goals.

There is currently a significant level of effort in nanotechnology R&D, with federal funding exceeding $1B in FY 2005. The challenge and opportunity for industry in NNI's fundamental research appears to be in ensuring that the research is relevant to industrial needs. In contrast to fundamental research, topics more directly related to enabling nanomanufacturing are funded at much lower levels. Funding for nanomanufacturing and instrumentation research or nanoscale technology currently lags that for the more fundamental PCAs or nanoscale science.

Apparent gaps in knowledge or activity between the existing programs and the chemical industry's priority needs as identified in this effort include the following:

- Manufacturing and Processing – Few programs are dedicated to issues of nanomanufacturing, and scale-up issues are not fully addressed. A research center, or virtual center, dedicated to process development may provide sufficient focus for progress in this area.
- Characterization Tools – Most current NNI efforts in Instrumentation Research appear to be aimed at developing new tools for research. Additional focus is needed on developing instruments for rapid characterization and in-process monitoring for nanomanufacturing.
- Fundamentals and Synthesis – There is currently a large amount of activity in this area; however, there is a perception among some in industry that much of the work is not relevant or sufficiently connected with issues of importance (such as scalability of synthesis) for industrial implementation. Industrial input to fundamental research programs may help to provide greater relevance.
- Modeling and Simulation – Multiscale modeling is seen as an important, long-term effort. A stronger connection of computational user centers to industry or industrially relevant problems is desirable.

Joint efforts developed by NNI and Semiconductor Research Corporation (SRC) are being used by the chemical industry to model new initiatives. Specific research needs in each gap area were identified by industrial teams. Three of the areas (Modeling and Simulation, Characterization Tools, and Fundamental Understanding and Synthesis) were being addressed by joint semiconductor/chemical industry teams formed in recognition of their common interests in priority R&D. Chemical industry-specific research needs in manufacturing and processing were identified by a chemical industry team. These priority needs were presented and discussed at the Chemical and Semiconductor Joint Research Needs Meeting hosted by NIST in November 2005 and the resulting needs statements are integrated into this document.

The primary target agencies for interactions with the chemical industry may be identified by budget (NSF, DOD, and DOE have the largest nanotechnology-related budgets), and by relevant agency activities, as summarized in the NNI Supplement to the President's 2006 Budget. Primary target agencies for each priority need area are given in Table 1, along with suggested actions for promoting R&D. Several other efforts are currently underway by NNI-ChI CBAN toward the recommended actions and include the following:

- A letter to NSF centers has been drafted to identify ongoing center activities relevant to priority need areas and possibilities for industrial guidance of research.
- The chemical industry nanotechnology liason group, together with the semiconductor industry have initiated interactions with NIST to identify collaboration along the lines of a "nano-center of excellence" for industry.
- One project in the DOE MPLUS program on real-time nanoparticles characterization was identified by the Manufacturing and Processing team and has been initiated.
- The chemical industry proposes a new initiative to expand activities in nanotechnology, including greater interactions with research centers, government agencies, and other industrial groups.

1. Introduction

The purpose of this effort is to develop a plan to forward the vision and goals identified in the Vision2020 nanotechnology roadmap, *Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function*. The project was commissioned by the Chemical Industry Vision2020 Technology Partnership and funded by Chemicals Plus initiative of the Industrial Technologies Program, Office of Energy Efficiency and Renewable Energy, U.S. Department of Energy. This Nanotechnology Implementation Plan aims to achieve the following:

- Define industry's specific research needs for priority roadmap technical areas
- Develop R&D recommendations and identify potential funding sources
- Identify options for transitioning research in commercialized products
- Provide opportunity to access potential benefits, such as energy savings

To attain these goals, a workshop was held on February 15, 2005 with attendees from industry and government, and nanotechnology experts from academia, DOE and NSF Nanoscale Science Research Centers (NSRCs). The workshop goal was to identify the priority needs from the roadmap and to develop research recommendations targeted to missions, interests, and needs of National Nanotechnology Initiative (NNI) agencies. Subsequent to the workshop, input was obtained from nanoscale science and technology experts and from industrial and government members of the NNI-Chemical Industry Consultative Board for Advancing Nanotechnology (NNI-ChI CBAN). Information was also gathered from internet surveys and NNI reports.

1.1 Priority R&D Needs Areas Identified in the February 2005 Workshop

The priority needs areas identified by the workshop participants are grouped into four major areas and are summarized below. These needs areas span from discoveries in nanoscience to applications for commercialization of nanotechnology (Figure 1).

(i) Manufacturing and Processing

- Develop unit operations and robust scale-up and scale-down methodologies for manufacturing. Five classes of unit operations for nano-chemical engineering were identified: Synthesis, Separation, Purification, Stabilization, and Assembly. Specific needs include:
  - Develop robust dispersion and surface modification processes that retain functionality.
  - Develop manufacturing processes for nanostructured catalysts, coatings, ceramics, sorbents, and membranes.

(ii) Characterization Tools

- Develop analytical tools for measuring and characterizing nanomaterials.

- Develop real-time analytical tools for measuring and characterizing nanomaterials, particularly online and in-process tools for process control and robust measurement tools for quality control.

(iii) Fundamental Understanding and Synthesis
- Develop new paradigms for creating nanoscale building blocks based on understanding of physics and chemistry at the nanoscale.
- Develop new paradigms for controlled assembly of nanocomposites and spatially resolved nanostructures with long-range order.

(iv) Modeling and Simulation
- Develop computational tools to predict bulk properties of materials that contain nanomaterials.
- Develop methods for bridging models between scales, from atoms to self-assembly to devices.

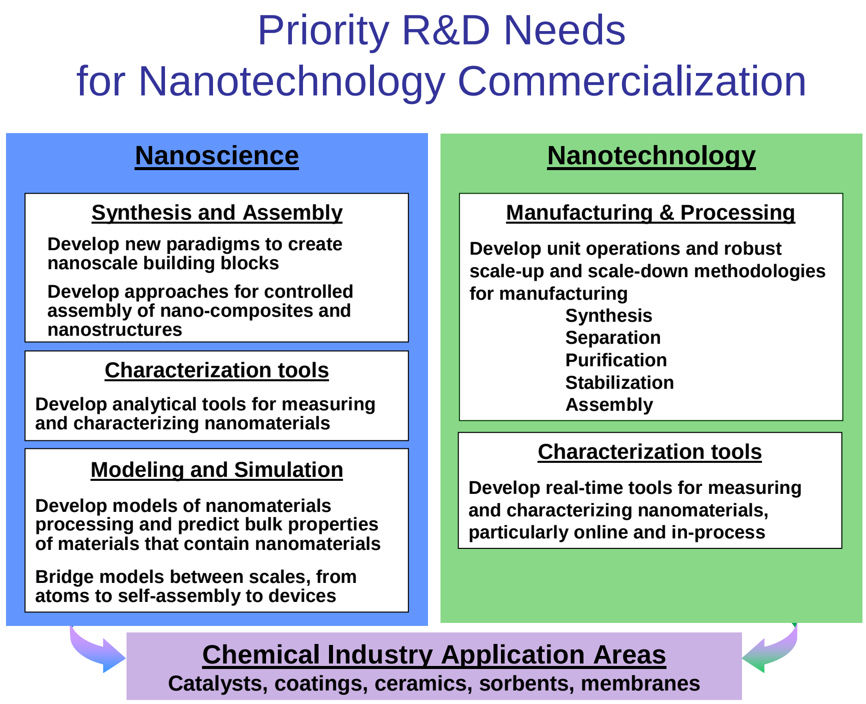


Figure 1: Priority research needs in nanoscience and nanotechnology

Due to areas of common interest between the chemical and semiconductor industries, working groups comprising members from both the industries were established to identify specific key areas for research efforts. The following three areas of common interests were addressed by joint semiconductor/chemical industry teams: modeling and simulation; characterization tools; and fundamental understanding and synthesis. Chemical industry research needs in manufacturing and processing were identified by a chemical industry team. The Chemical and Semiconductor Industry Joint Nanotechnology Research Needs Teams met November 29-30 at NIST-Gaithersburg to finalize description of common priority research need areas and to communicate the needs to representatives of NIST and other NNI-sponsored groups. The specific research needs areas identified by these working groups are incorporated into this report.

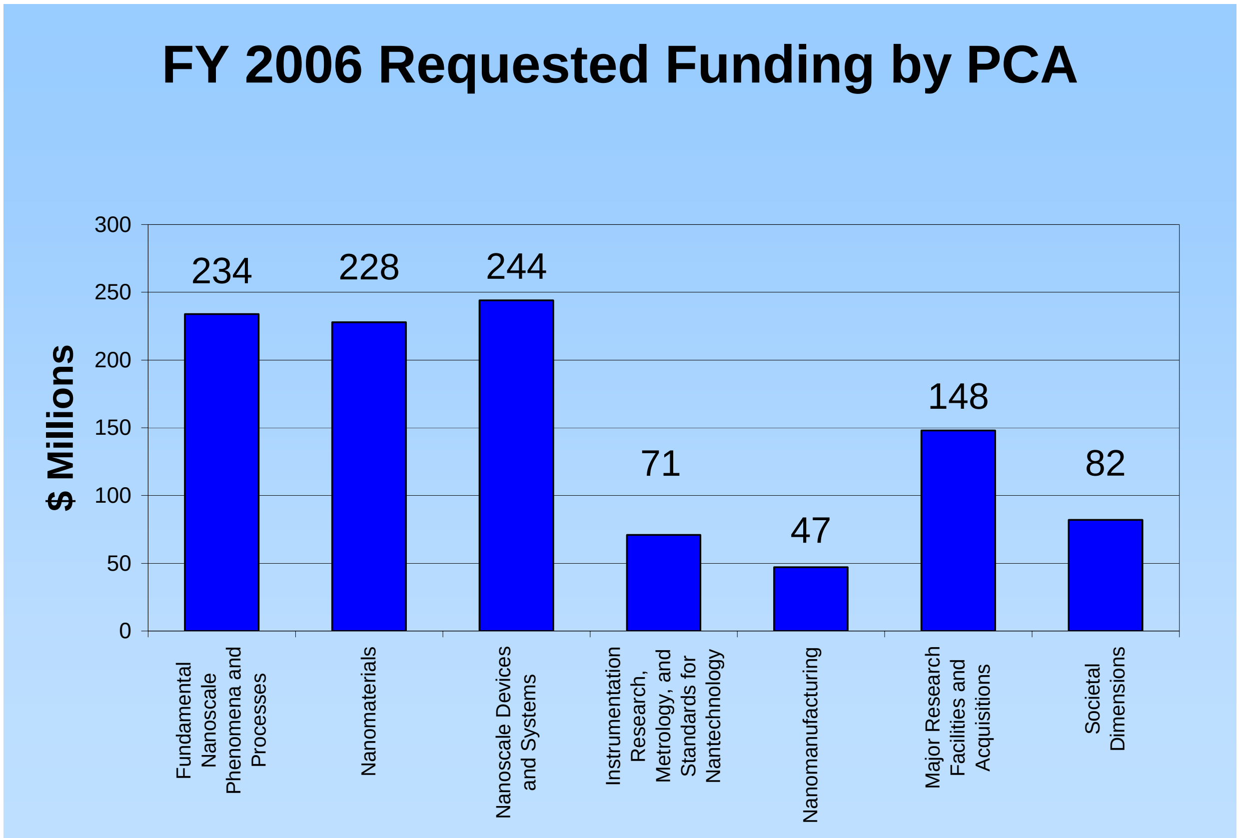
The Council for Chemical Research (CCR) and Vision2020 have agreed to continue collaboration with the semiconductor industry on research in areas of common interest, including these specific priority needs:

- Synthesis & Self Assembly*
  - Synthesis of nanostructured materials
  - Directed & self assembly
- Nanomaterial Structure Properties*
  - Magneto-electronic & transport properties
  - Nano-surface properties & mechanisms
  - Nano-mechanical & interface properties
  - Thermal properties of nanostructured materials
- New Metrology Capabilities
  - Large-volume electronic property characterization
  - In situ nano-particle (sub-50 nm) monitoring
- Chemical Industry Manufacturing
  - Fundamental engineering knowledge of the unit operations for manufacturing organic and inorganic nanomaterials
  - Real-time characterization techniques for process monitoring and process control
  - Scale-up path for self-assembly processes for commercial-scale unit operations

* Modeling of synthesis and nanostructure properties over multiple length and time scales is a common theme.

1.2 Current Status of Funding and Agency Efforts in Nanotechnology Research

There is currently a significant level of effort in nanotechnology R&D, with federal funding exceeding $1B in FY 2005. An impressive array of scientific infrastructure and research programs has been initiated over the past five years. Research on nanoscale science topics is well funded, where the challenge and opportunity lies in ensuring that the fundamental research is relevant to the industrial needs. In contrast to fundamental research, topics more directly related to enabling nanomanufacturing are funded at much lower levels. Figure 2 presents data from the NNI Supplement to the President's FY 2006 Budget. Funding for nanomanufacturing and instrumentation research currently lags that for the more fundamental R&D needs areas.



(Source: National Nanotechnology Initiative Supplement to the President's FY 2006 Budget)

Figure 2: NNI FY 2006 Funding by Program Component Area

As indicated in the NNI Strategic Plan of December 2004, liaison with industry groups is important for success of the initiative. The chemical industry interaction with NNI has high visibility; industry can use this opportunity to positively influence the course of NNI efforts as they transition nanoscale science to technology. However, the interaction of the chemical industry with NNI is not as mature as that of the semiconductor industry with NNI. Joint efforts developed by NNI and Semiconductor Research Corporation (SRC) are being used by the chemical industry to model new initiatives, such as those resulting from the November 2005 NIST meetings. In addition, joint advocacy of research by semiconductor and chemical industry groups may be expected to have greater effectiveness.

Apparent gaps in knowledge or activity between the existing programs and the chemical industry's priority needs were identified and are presented as potential actions in Table 1.

Table 1: Target Agencies and potential actions to promote R&D in priority roadmap areas

Priority R&D Needs Areas	Target Agencies	Potential Actions
Manufacturing and Processing	DOE	• Interact with EERE ITP (MPLUS as initial step) to develop programs • Advocate a center on transition to commercialization • Provide input to SBIR program
	NIST	• Continue Vision2020-semiconductor-NIST interaction • Develop roadmap for actions related to priority industry needs
	NSF	• MOU with Nanomanufacturing Program • Provide input to SBIR program
Characterization Tools	NIST	• Continue Vision2020-semiconductor-NIST interaction • Develop roadmap for actions related to priority industry needs • Communicate needs defined by SRC/ChI/NIST team to NSET
	NSF, DOE	• Engage appropriate centers and encourage collaboration among agencies in virtual center on characterization for nanomanufacturing
Fundamental Understanding and Synthesis	NSF	• Engage NSECs and appropriate MRSECs – guide research and identify opportunities through letter to centers • Employ unique tools available at user centers to conduct pre-competitive and proprietary R&D • Participate in SBIR/STTR research as appropriate and provide guidance to SBIR/STTR managers
	DOE	• Engage NSRCs – initiate workshop to encourage communication of industry needs and NSRC goals and operations
	DOD, NASA	• Interact with specific program managers
Modeling and Simulation	NSF	• Utilize user centers • MOU with nanomanufacturing – guide research to relevant systems
	DOE	• Interact with user centers • Review funded research
	NIST	• Continue Vision2020-semiconductor-NIST interaction • Develop roadmap for actions related to priority industry needs

2. Priority Needs Areas

2.1 Manufacturing and Processing

A. Unit Operations *(Ref: Roadmap p.33)*

Description
The unique physics and chemistry at the nanoscale requires new approaches in many cases beyond that of the classical chemical engineering unit operations in order to commercialize nanotechnology. Five classes of unit operations for nanochemical engineering were identified:

1. Synthesis – form desired nanomaterial building blocks from precursors in commercial quantities, with consistent quality
2. Separation – separate nanomaterials from precursors, reaction media, etc.
3. Purification – tailored isolation of nanomaterials by function (separate by desired property, such as size, composition, charge, magnetic, electrical, optical, functionalization, etc.)
4. Stabilization – processes such as surface modification, dispersion, etc. that allow a consistent nanomaterial product to be utilized while retaining desired functionality
5. Assembly – integration into devices/products through a variety of top-down and bottom-up processes, including self-assembly, directed assembly, etc.

It is recognized that not all processes will require all unit operations and that some processes will combine unit operations. Multidisciplinary teams will be needed, working at the laboratory and pilot scale, to translate the discoveries of nanoscience into new processes for effective nanomaterial production. Government support, in the form of test beds at research centers, may be useful to overcome the barriers presented by the risk of capital investment in unproven technology.

Current Work
According to the 2005 NSF solicitation announcement for *Manufacturing Processes at the Nanoscale,* "Research in this area will focus on creating nanostructures and assembling them into nanosystems and then into larger scale structures. This research should address understanding nanoscale processes, developing novel tools for measurement and manufacturing at the nanoscale, developing novel concepts for high-rate synthesis and processing of nanostructures and nanosystems, and scale up of nanoscale synthesis and processing methods. Examples are synthesis of nanostructures for various functions, fabrication methods for devices and nanosystems, design concepts for manufacturing, simulation of the manufacturing methods at the nanoscale, and evaluation of the economic and environmental implications of manufacturing at the nanoscale. Possible benefits include improving understanding of manufacturing processes in the pre-competitive environment, generating a new group of nanoscale manufacturing methods, increasing the performance and scale up of promising techniques, and establishing the physical and human infrastructure for measurements and manufacturing capabilities."

Recent awards from the NSF-NER/NIRT (National Science Foundation-Nanoscale Exploratory Research/Nanoscale Interdisciplinary Research Teams) program include:

- University of New Orleans for directed assembly
- North Carolina State University for surfactant directed self assembly
- State University of New York, Stony Brook for synthesis of boron-containing structures

The round of NER proposals that were funded in fall of 2004 were mostly in directed self-assembly. Predominant funding from this mechanism was to investigate self-assembly of nanoparticles. Several programs in this round also had modeling components, while only 2 of approximately 30 had large-scale synthesis as a focus.

NSF 04-043 Call for Proposals for the Center on Hierarchical Manufacturing (CHM) addresses the following additional components:

- A systems-level focus that drives the research from discovery through proof-of-concept, including the design and/or development of nanosystems, structures, enabling tools technology, processes or devices, and proof-of-concept test beds that pull together disparate research efforts to test a system or complex concept and thus identify where further research efforts are required;
- Collaboration with other centers on nanomanufacturing, including two Nanoscale Science and Engineering Centers (NSECs) established in 2003 and grantees from other agencies. The new NSEC is expected to:
  - collaborate with grantees from other agencies with similar programs;
  - share resources with those programs for mutual advantage;
  - work toward a nanomanufacturing network that encourages extensive industrial collaboration;
  - participate in joint nanomanufacturing program evaluations.
- Plans for a nanostructured materials and nanomanufacturing database, and
- Plans for clearinghouse activities that the Center will undertake including plans for involvement of a wide range of shareholder groups, and coordination and/or compilation of appropriate data for material properties, manufacturing processes, best practices, educational materials, etc.

This particular NSF program at this time focuses on combining top-down microfabrication with bottom up self-assembly. The program will have great impact on microelectronic and biomedical industry, but will require outreach to meet chemical industry needs.

While the chemical industry has identified specifically Dispersion and Unit Operations, these are not significantly covered under the NSF program. The majority of grants funded are still laboratory-scale programs with only a few addressing scale-up.

Existing Infrastructure

The research scope of several NSECs includes some aspects of nanomanufacturing. However, there is no center dedicated to scale-up of manufacturing and processing of nanoscale materials.

Application Areas
The Office of Naval Research has a Manufacturing Technology Division focused on coatings and sol-gel processes. The target in these programs was for low-friction or anti-wear coatings for drive shafts and similar uses. Several other specific applications that are targeted by solicitations from mission agencies are described in Appendix C.

B. Dispersion *(Ref: Roadmap p.34)*

Description
The development of scalable dispersion and surface-modification techniques are needed to enable reproducible nanomaterial stabilization and dispersion of nanomaterials into other materials. Fundamental R&D is required to develop a general understanding of the basic principles that allow processing that retains the nano-derived functionality. In addition, work will be needed with specific systems to develop unit operations that work across a range of materials of commercial interest, such as inorganic oxides, clays, carbon materials, etc., and matrices, such as polymers, pure liquids, solution gels/sols and metals.

Current Work
These areas are mainly covered under the Particulate and Multiphase Processes effort of NSF's Chemical and Transport Systems division. The work is described as follows: "The Particulate and Multiphase Processes Program supports fundamental and applied research on mechanisms and phenomena governing single and multiphase fluid flow, particle formation and transport, various multiphase processes, nanostructures, and fluid-solid system interaction. Research is sought that contributes to improving basic understanding, the design, predictability, efficiency, and control of existing systems that involve the dynamics of fluids and particulates, as well as the innovative uses of fluids and particulates in materials development, manufacturing, biotechnology, and the environment."

C. Manufacturing Processes for Nanostructured Catalysts, Coatings, Ceramics, Sorbents, Membranes

Description
Catalysts, coatings, ceramics, sorbents, and membranes are priority materials for application of nanotechnology in the chemical industry. Development of manufacturing processes is needed to accelerate the controlled, high-rate synthesis of functional materials for these applications and integration of the engineered materials into devices.

Current Work
Several mission agencies identify chemical industry applications (see solicitations in Appendix C). However, it is not clear if there is significant work on controlled, high-rate synthesis of functional materials for these applications, or on the integration of the engineered materials into devices.

D. Specific Priority Research Needs in Manufacturing and Processing

The development of engineering techniques for nanomaterial processing is currently at an early stage. Key capabilities to be developed include large-scale production of nanoparticles of controlled size and shape, manufacture of ordered and oriented nanostructures, and chemical processing of complex nanocomposite structures by design.

The primary research needs for manufacturing and processing were presented at the Chemical and Semiconductor Joint Research Needs Meeting hosted by NIST in November, 2005. These research needs include:

- engineering knowledge of the unit operations for manufacturing organic and inorganic nanomaterials;
- real-time characterization techniques for both process monitoring and process control;
- the identification of a scale-up path for self-assembly processes for use in commercial-scale unit operations such as synthesis, separation, purification, stabilization and assembly; and
- concurrent development of processes to mitigate emissions of nanomaterials to the workplace and external environment.

The development of a fundamental engineering knowledge of unit operations that can be used in the integrated manufacture of organic nanomaterials will help to achieve several basic goals of the chemical industry. This information could lead to high purity and low cost materials synthesis, superior catalysts that improve product yield and improved separations that will ensure product purity. In addition, improving unit operations will also yield better control of nanotube chirality, diameter and length.

The same type of developments in engineering will be important for producing inorganic nanoparticles by improving the understanding of nucleation and growth mechanisms, interparticle and interfacial phenomena, transport process, kinetics and thermodynamics. These advances will lead to improved control of particle morphology and development of particle control techniques that reduce agglomeration, allow continuous reactive processing of nanoparticles and allow assembly of nanoparticles into macrostructures.

The real-time characterization techniques for process monitoring and process control are similar to those needed for metrology, and include optical and spectroscopic analyses, mass spectroscopy and small angle X-ray scattering. Pathways for extension of these techniques to the unit operations of synthesis, separation, purification, stabilization/functionalization and assembly are needed.

Taking nanotechnology from the promise of the laboratory to the practice of the manufacturing plant will require a scale-up path for self-assembly processes that will have practical uses in commercial-scale unit operations. This pathway will require the application and adaptation of current lab- and pilot-scale techniques of molecular or biological self-assembly to larger-scale processes. It will also require the development of appropriate in situ diagnostics and process control schemes that will ensure consistent, low-cost manufacture of nanostructures.

2.2 Characterization Tools

A. Analytical Tools for Measuring and Characterizing Nanomaterials:

Description
Characterizing nanomaterials and the dispersion level of nanoparticles requires establishing publicly available nano-centers that provide the necessary infrastructure, tools, and trained personnel. These nano-centers for characterization of nanomaterials must ensure equitable and affordable access to all parties. Cutting edge analytic tools must also be made available to outside third parties through access to NNI-funded universities or government labs (via pay-as-you-go or collaborative arrangements).

Additionally, these centers need to focus on developing tools and methods to measure materials and physical properties of commercial interest. These properties include mechanical, electrical, magnetic, optical, transport (heat, mass, momentum), diffusion, thermodynamic, surface-surface, and absorption/adsorption properties.

Current Work and Infrastructure
There are currently efforts in several agencies to develop new analytical tools for nanoscale science and technology, and to provide access of cutting-edge tools to researchers in academia and industry.

1. **NSF** provides tools and access primarily through the National Nanotechnology Infrastructure Network (NNIN). NNIN facilities provide support in nanoscale fabrication, synthesis, characterization, modeling, design, computation, and hands-on training, in an environment available to all qualified users from industry and government. Users do not have to be associated with any university or know someone at the site. Historically, about 25% of users are from companies. NNIN facilities house over 700 major tools, which are detailed in a searchable database at http://www.nnin.org/nnin_tool.taf; the tools are available in the following general categories: lithography; deposition and growth; etching; wet-chemical processing; other traditional thin-film and device processing; electrical characterization; structure and materials characterization; biological and chemical processing; synthesis and molecular assembly; particles and nanomaterials; and process integration.

2. **DOE** contributes through its creation of five Nanoscale Science Research Centers (NSRCs) (http://www.sc.doe.gov/bes/BESfacilities.htm#NSRC). The NSRCs are co-located with other major national user facilities supported by DOE at national laboratories. NSRCs are involved in development of new tools and provide users a wide array of cutting-edge tools for nanoscience research. In contrast to NNIN, free access to the tools is mediated by peer review and is subject to open publication. Proprietary access is available at full cost recovery, and a standard intellectual property agreement will be available. Examples of tools can be found at http://www.cnms.ornl.gov/workshops/spm/SPM_NSRC_Workshop_Report.pdf.

3. **NIST** provides Advanced Measurement Laboratory (AML) which is the most environmentally stable laboratory in the world for next-generation nanometrology requirements. NIST's Nanomanufacturing Program (http://www.mel.nist.gov/proj/nm.htm) has annual program funds of $5.029M and aims to achieve the following: "Develop and deliver timely measurements, standards, and infrastructural technologies that address identified critical U.S. industry and other government agency needs for innovation and traceable metrology, process-control and quality in manufacturing at the nanoscale."
   FY 2005 projects include:
   - Scanning Electron Microscope (SEM) for Nanoscale Measurements
   - Optical Metrology (OM) for Nanoscale Measurements
   - Atom-Based Metrology for Nanoscale Measurements and Standards
   - Scanning Probe Microscopy for Nanoscale Measurements
   - Force Metrology for Nanoscale Measurements and Standards
   - Advanced Control Systems and Positioning for Nanoscale Measurements and Standards
   - Optical Tweezers for Nanoscale Manipulation and Metrology
   - Advanced Lithography for Nanoscale Measurements and Standards
   - Development of Nanomachining Technologies for Nanomanufacturing

Application Areas
These nanocenters support a broad range of nanoscale science and technology needs.

B. Real-Time Characterization Tools *(Ref: Roadmap p. 35, 40)*

Description
In addition to ongoing efforts in development of advanced characterization tools for R&D, there is a need to develop deployable process-monitoring tools that can be used to ensure nanomaterial and nanoproduct consistency on a manufacturing scale. Such instruments would include real-time, on-line characterization tools and rapid quality control (QC) tests for samples. Nanomaterial characterization capabilities needs include monitoring the following:

- in situ particle size and shape
- in situ composition or function (including charge; surface energy; functionalization; magnetic, electrical, or optical properties, etc.)
- surface chemistry at nanoscale, including fractional coverage and thickness of coatings on nanoparticles
- quality of particle dispersion in a solid phase

Current Work
No specific NSF programs related to real-time characterization have been found as yet; this area might be covered under other existing programs. If any program is in the offing, a focus on rapid assay should be high priority, which might be a strong component of any NSF-oriented program. Best match in interests was found in the NIST Nanomanufacturing Program goals of "process-control and quality in manufacturing at the nanoscale."

Infrastructure
The President's FY 2006 Budget (http://www.nist.gov/public_affairs/releases/budget_2006.htm) includes three research initiatives that "target pressing national priorities," with an increase of $19.6 million for Advances in Manufacturing. A key part of this initiative is $10 million for a national nanomanufacturing and nanometrology facility at NIST.

C. Specific Priority Needs in Characterization

The specific primary research needs for metrology were identified by the Chemical and Semiconductor Industry Joint Research Needs Team and were presented at the Chemical and Semiconductor Joint Research Needs Meeting hosted by NIST in November 2005. The goals identified by this group are to develop techniques for in situ monitoring of the particle size and critical electronic properties of nanomaterials. Efforts should be focused on finding techniques for characterizing bandgap distribution, and determining particle size and particle surface roughness. Large-volume electronic property characterization of one-dimensional nanomaterials and in situ nano-particle (sub-50 nm) monitoring are the primary research need areas identified by the working group. Size distribution capability is needed for manufacturing controls and as environmental health and safety monitors.

Large-Volume Electronic Property: Work in large-volume electronic property characterization is needed because there is currently no single tool that can characterize bandgap distributions of large numbers of carbon nanotubes. Fluorescence appears to be the most useful potential characterization tool as it may yield information on cross-sections of carbon nanotubes (CNT) vs. diameter, chirality and bandgap in different chemical environments. However, more research is needed to identify applicable conditions. Quenching of fluorescence from conditions such as the presence of bundles, SiO_2 or other chemicals and high dielectric constant (K) could limit the applicability of this technique and will require new concepts to cancel the quenching.

In Situ Monitoring: Current analytical techniques for nano-particles cannot yet be used for in situ monitoring. Small angle X-ray scattering can measure particle size distribution and surface areas, and has demonstrated compatibility with flow cells. Micro-electro-mechanical systems (MEMS) based particle detectors may prove useful. A proposed particle mass spectrometer to characterize particle weight, composition and surface could be valuable in development and excursions, but not for in situ applications. Brownian motion techniques are sensitive to flow, and so will not be useful for in situ applications. TEM holography has been used to study particle size and surface morphology in development or excursion, but is also not compatible with in situ monitoring.

Further research is needed in the use of small angle X-ray scattering, mass spectroscopy (particularly in the correlation of models to particle size and surface area distribution for different particles and in the development of smaller more compact sources for commercial applications), and novel approaches such as MEMS-based techniques.

A summary of the utility of the application of various research tools to the characterization of particular nanomaterial properties is given in Table 2.

Table 2: Utility of various research tools in nanomaterial property characterization

Nanomaterial Properties	Research Tool Application		
	Small Angle X-ray scattering	Mass Spectroscopy	Microscopy (SEM/TEM)
Particle size	Yes	Yes (1000 particles/sec)	Yes (5000/hour SEM, TEM ?)
Particle size distribution	Yes	Yes	Yes
Bulk composition	No	Yes (photo ionization of sample)	No
Surface composition	No	?	Yes
Surface composition-ligands	No	?	?
Particle structure (Architecture)	?	?	Aberration Corrected TEM carbon sensitivity?
Level of dispersion/aggregation	Yes	?	Yes (if in matrix)
Particle shape	?	Yes, with ion mobility measurement	Yes
Particle aspect ratio	?	No	Yes
Surface charge	No?	?	?
Surface functionality	No?	?	Yes?
Homogeneity/Heterogeneity (surface, size, composition)	?	No	Yes (dependent on statistics)
Heterogeneity of population	?	?	Depends on statistics
Heterogeneity of single particle	?	?	Yes

? indicates utility still to be determined based on input from other experts

The research needs identified for measuring nanomaterial properties can be grouped into four areas: 1) Magneto-electronic and transport properties, 2) Nano-surface properties and mechanisms, 3) Nano-mechanical and interface properties and 4) Thermal properties of nanostructured materials.

1) Magneto-electronic and transport properties: The experimental capabilities essential for further understanding these properties of nanostructures include:

- Statistical measurement of the electronic transport properties of nanostructures
- Correlation of electronic transport properties with atomistic structure in the nanostructure
- Measurement of the properties of contacts to nanostructures, and correlation with atomic structure of nanostructure/metal interface
- Measurement of the optical properties of nanostructures and of opto-electronic processes
- Measurement of the temperature dependence of nanotube bandgaps, addressing the role of phonons
- Effect of adsorbates on nanowire conductivity
- Large-volume electronic properties

2) Nano-surface properties and mechanisms: The capabilities for characterization determined to be essential for further understanding of these traits include measurement of structure and composition, and an understanding of their control.

3) Nano-mechanical and interface properties: The essential experimental results required to feed models for the understanding of these properties in nanostructures include:

- Measurement of the three-dimensional mechanical response of nanostructures to controlled applied strain
- Measurement of the mechanical response of nanostructures to electronic, magnetic, optical, and thermal stimulation
- Atomic imaging of defects, failure modes, dislocations, grain boundaries, interfaces, and similar properties
- Effect of substrate interactions on nanostructure deformations

4) Thermal properties: The experimental results required to feed models as determined essential for the understanding of thermal properties of nanostructured materials include:

- Characterization of phonon dispersion in nanomaterials and interfaces
- Measurement of thermal transport in nanostructures, including role of interfaces
- Temperature dependence of thermal properties

2.3 Fundamental Understanding and Synthesis

A. New Paradigms for Creating Nanoscale Building Blocks *(Ref: Roadmap p.27)*

Description
Continued research is directed at developing new, more efficient ways of synthesizing high-quality nanomaterials. In addition to current wet-chemistry, gas-phase, and self-assembly technologies, new concepts involving new solvents and processes are sought. Points of emphasis include the need to develop methodologies for synthesis based on scientific understanding rather than from discovery. Research should focus on materials of relevance to specific applications, such as catalysts, sorbents, coatings, adhesives, resins, nanofibers, etc., and on materials that exhibit properties of commercial interest, such as mechanical, electrical, magnetic, optical, thermodynamic, transport, surface, and absorption/adsorption properties. R&D goals should include the need for scalability, reproducibility, and controllability.

Current Work
Several approaches are currently being investigated for nanoscale materials synthesis:

1. Gas-phase synthesis based on evaporation and condensation: This method is mainly used to produce nanoparticles of metal oxides. The advantage includes high purity of materials and some control of particle size. The disadvantage includes the limit of scale of production, aggregation and the difficulty to control particle morphology.
2. Direct gas phase synthesis, with or without the use of catalysts: This approach has been extensively used to produce a wide range of nanoparticles, nanowires, carbon nanotubes,

semiconductor nanobelts, etc. Gas-phase synthesis is flexible and is particularly suitable for producing semiconductor compounds that are not accessible to solution-phase synthesis. *However, the production cost may be high, and the processes are very sensitive to temperature, atmosphere, and multiple other experimental conditions. Producing high-quality, uniform products remain a challenge*. Commercially, high temperature gas phase reaction is used for some important nanoparticles, including high surface area silica and titania that are widely used in paints, fillers, and catalysts.

3. Solution-phase synthesis: This approach includes production of quantum dots, hydrothermal or solvothermal particle production and co-precipitation. Solution-phase synthesis is the least expensive approach for production of nanoscale particles and is widely investigated for a wide range of materials. These methods are already widely used for commercial production of a range of products, although they may not be labeled as "nanomaterials." Examples of current commercial materials include products of sol-gel processes, zeolites, powders for chemical mechanical polishing, many ceramic precursors, and numerous catalyst materials. *Solution-based approach has great potential for commercialization, but scientific understanding of the principles governing chemical reaction, diffusion, mixing, nucleation and growth, etc., is very poor. Many processes are not predictable, repeatable, and scalable at this time. Impurities and contamination could be another problem for high-performance products.*
4. A special solution synthesis method based on encapsulation: In this approach, the chemical reaction and nanomaterials growth are limited within a reaction vessel such as a micelle or a vesicle. *This method is useful in controlling particle size and agglomeration, but the quantity is limited and the cost is high. The organic coatings on the particle surface are difficult to remove, and may significantly alter the physical and chemical properties of the particles.*
5. Mechanical grinding: This approach is widely used to produce ceramic particles, but it is difficult to reduce the particle size to nanometer scale. Also, contamination on particle surfaces and grain boundaries is a serious problem.
6. Supercritical fluid processing: This is an emergent technology for producing novel nanomaterials, but the application of this technology has not been widely explored.

A large amount of work on synthesis of nanoscale materials is currently underway, funded by several NNI agencies, including discovery research and applied fundamental study for mission agencies. *Focus on scalability of synthesis is not universally present*.

Existing Infrastructure

Facilities and infrastructure exist in some industries for producing high surface area nanoparticles and catalysts. However, these facilities and infrastructures are not particularly designed for most of the advanced nanomaterials. The environmental, safety and heath hazards associated with the manufacturing processes have not been systematically evaluated. Most facilities and programs in national laboratories and universities are related to research on small quantities of materials and are not suitable for industrial processes.

Application Areas
Synthesizing nanomaterials has numerous applications: structural materials and nanocomposite materials for improved mechanical properties, reduced weight, or improved thermal properties (such as flame retardants); packaging materials for improved mechanical and chemical properties; ceramic slurries for chemical mechanical polishing; coating materials and films; highly efficient catalysts; catalyst supports and selective sorbents; cosmetics; fuels and explosive additives; ceramic materials for fuel cells; ceramics and metals for batteries; carriers for drugs and pharmaceutical products; and other biomedical applications.

B. New Paradigms for Controlled Assembly *(Ref: Roadmap p.28)*

Description
Improvement in methods for assembly of nanoscale building blocks is needed to develop commercial-scale approaches for fabrication of products/devices incorporating newly discovered nanomaterials and nano-derived functionalities. High-rate nanomanufacturing processes related to applications of interest to chemical industry are sought, in addition to current efforts related to electronics and medical applications.

Current Work

1. <u>Bioinspired materials manufacturing</u>: Many groups have studied how to genetically engineer proteins and other biomolecules, and organisms to produce tailored nanomaterials. Initial work focused on minerals that are not of engineering significance, such as calcium carbonate. Recently, great progress has been made in making metal oxides, semiconductors, metals and non-oxide materials. Extensive study is also under way on how to use this approach to assemble useful microdevices and bulk materials. While this is a very inspiring and promising approach, near-term products are difficult to anticipate.
2. <u>Molecular assembly</u>: This approach takes advantage of the self-assembly properties of many functional molecules, such as surfactants, proteins, polymers, dendrimers, DNA molecules, etc., to form functional nanomaterials. The functional molecules either function as a structural directing agent (determining the final products) or as a template. Zeolite is a primitive example. In zeolite synthesis, small template molecules function as the structural directing agent to control the cage structure. Recently, micelles formed from surfactants and polymers have produced a new class of self-assembled nanomaterials with tightly controlled nanoscale features such as pore size and pore geometry. Such materials have great potential as in catalysis and absorption. Although promising results have been reported, these materials have not yet achieved their potentials in terms of efficiency, selectivity and cost saving for practical applications.
3. <u>Assembly and consolidation from nanoparticles and other nano-building blocks</u>: Traditionally, colloidal processing and consolidation has been widely used to fabricate ceramic and metal products from particles. However, this approach becomes extremely difficult for ultrafine nanoparticles because of the small sizes and the tendency of these particles to agglomerate. First, most of the processing techniques used, such as pressure filtration, sedimentation, centrifuge, slip-casting, etc., are not applicable because of the small sizes. Second, in order to stabilize the suspension of nanoparticles, a repulsive interaction is introduced between the particles either electrostatically or through

surfactant/polymer absorption. The range of the repulsive forces is at least comparable with the size of the nanoparticles. As a result, the consolidated state contains a small fraction of the particles by volume. This will lead shrinkage, cracking, defects and difficulty in fabrication.

4. Continuous nanomaterials production: Recently, several groups have initiated research activities in continuous production, realizing the limitations of commonly used batch reaction and the problem of quality control. One way to study continuous production is through a microfluidic reactor. In a microfluidic reactor, the materials flow, diffusion, the temperature and many other parameters are tightly controlled. In addition, the reaction process can be followed using in-situ microscopic and spectroscopic techniques. The microfluidic platform has the potential to provide the fundamental understanding of nanomaterials manufacturing. *Although continuous production is in the early stage, it represents an important future direction for nanomaterials manufacturing in terms of reliability, scalability and cost.*
5. 3D assembly: Self-assembly has been explored to assemble 3D functional nanostructures from nanoparticles, nanowires and nanobelts. Here the challenge is to control the defect density, the long range alignment, and range of structures that are useful for practical applications. Many groups are also interested in direct assembly of functional nanomaterials and structures by combining self-assembly and top-down approaches. So far some individual components and functions have been demonstrated, but true functional devices and materials are yet to emerge.

Existing Work and Infrastructure
Most groups working in this area are conducting small-scale, benchmark research. Many universities and most nanocenters funded by DOE and NSF are involved in some aspects of the novel approaches. A few groups (one or two with the DOE-funded nanocenters) are conducting research in continuous reaction and microfluidic platforms.

NSF has established three nanomanufacturing centers focused on elements of controlled assembly. Another center focusing on hierarchical nanomanufacturaing was to be awarded funding in 2005. DOE Nanoscale Science Research Centers (NSRCs) primarily focus on overarching science issues related to assembly, and provide infrastructure and collaborative support to users. *Infrastructures and facilities suitable for investigation of issues related to scale-up to industrial processes are not widespread.*

Application Areas
Relevant areas include microelectronic devices, microdevices, sensors, medical applications, catalysis, smart coatings, absorbents, etc.

C. Specific Priority Needs for Fundamentals and Synthesis

Specific primary research needs for Fundamental Understanding and Synthesis were identified by both the Synthesis and Self Assembly, and the Nanomaterial Properties teams of the chemical and semiconductor industries. These needs were presented at the Chemical and Semiconductor Joint Research Needs Meeting hosted by NIST in November 2005. The goals identified by these teams are focused on the synthesis of nanostructured materials and on directed and self assembly.

Synthesis of Nanostructured Materials

The goal for understanding the gas phase synthesis of carbon nanomaterials (e.g., nanotubes and nanowires) is to encourage experiments and modeling to understand the fundamental relationship between catalyst nanostructure, growth conditions and resulting nanotube and nanowire structures. To achieve this goal, an experimentally validated model of nucleation, growth and the interaction of growth with fields, which includes temperature, catalyst structure, composition, gas, in addition to surface and field interaction, is needed. Also, it is necessary to understand what determines the nanostructure of the catalyst through fundamental understanding of catalyst nucleation and growth, mechanisms to predefine or self-assemble catalyst structure and operation and combinatorial design of experiments. Finally, experiments and analysis are needed to comprehend the statistical nature of factors that are convoluted by the experiment.

The primary goal for understanding the solution phase synthesis of nanoparticles, nanowires and other nanostructures is to establish the relationships between synthesis, material structure and property relationships. Experiments are needed to understand dynamics of growth for improved control of nanostructure in terms of size, shape and poly-dispersity. Topics to be addressed should include the spatial and temporal control of solutions, process conditions, and nucleation and growth (e.g., micro-fluidic studies to understand nano-particle nucleation, growth & structure). Better control of solvents, composition, fields, temperature is also needed. Experimental work to better understand the influence of external fields such as topology, electromagnetic (EM), gradients, and stresses is needed. End results of this work should be the ability to predict the final products and structures and the ability to control shape of nanostructure and composition.

Directed and Self Assembly

The primary goal for understanding self assembly is to design experiments that determine what limits the size, shape, separation, location, cure time, phase behavior, and composition of self-assembled structures. These basic experiments should include:

- Block co-polymers (BCP), homo-polymer, monomer, surfactants/solvent mixtures, and additives (e.g., inorganic or organic monomers)
- Block-copolymer or surfactant shape, bonding, rigidity and side groups
- Variations in block co-polymer or surfactant combinations, χ mismatch, and characterization of χ (interaction energetics)
- Characterization, including temperature dependence, of BCP and surfactant surface and interfacial energy on different material surfaces
- Characterization of diffusion, kinetics, nucleation, size, shape, and defect density

Experiments to understand interaction of self assembly with external fields should investigate:

- Interaction with topology, edges, openings, non-uniformities (e.g., integration of top-down patterning and bottom-up self assembly) and fields (topology, EM, flow fields, gradients, stresses, etc.)

- Dynamics of nucleation and growth
- Characterization of composition, size, shape, and orientation
- Characterization of defect density with and without directed assembly (confining structures) and of nucleation and kinetic models of defects

2.4 Modeling and Simulation

A. Computational Tools to Predict Bulk Properties of Materials That Contain Nanomaterials
(Ref: Roadmap p.25 & 44)

Description
Modeling and simulation efforts that may provide the most quickly realizable benefit to industry include the development of computational tools to predict the properties of materials that contain nanomaterials. Modeling and simulation of materials properties can provide a means to screen options for nanomaterials design. University and/or national laboratory efforts utilizing supercomputers will be necessary; industry involvement would likely involve guidance, with limited validation. To accelerate application, computations should target commercially interesting materials and be focused on a problem of intermediate complexity – one that could be solved in a near-to-mid-term time frame, but not too small as to be a trivial advancement.

A common challenge in addressing industry needs is providing nanomaterials input parameters within existing manufacturing and engineering software. Since finite element codes break down at nanoscale, new software tools are required at the nanoscale to analyze materials properties. There are two challenges: understanding nanoscale properties, and then finding a way to interface those results with the existing software. Until this happens, widespread implementation/integration of nanomaterials within existing manufacturing infrastructure will be slow to come.

In addition, there may be some near-term benefit from the development of models of nanomaterials processing operations. Such modeling, even initially including semi-empirical efforts, can provide value by accelerating the transition from small-scale synthesis to commercial production.

B. Develop Methods for Bridging Models between Scales, from Atoms to Self-Assembly to Devices
(Ref: Roadmap p.45)

Description
The ability to seamlessly transfer data among quantum, molecular and mesoscale and to simulate processes on multiple time scales is needed. Basic code development is required with an engineering focus. Interfacial properties, thermal effects and reaction mechanisms are still poorly understood. The development of models that bridge multiple scales is seen as a valuable long-term effort. Some challenges and recommendations for research are described in the report, "Opportunities for Discovery: Theory and Computation in Basic Energy Sciences." (http://www.sc.doe.gov/bes/reports/files/OD_rpt.pdf).

Current Efforts

Accelrys is building commercial software (Computer Aided Nanodesign or CAN tools) to solve these issues. There is ongoing work with consortium partners (led by industry and members from academia). The Accelrys consortium (http://www.accelrys.com/materials/nano/nano_consortium/index.html) efforts may be complementary to other nanotech activities within academic/government labs. For commercialization to happen, industry participation at an early stage is critical, and the research must be tailored to existing needs and to problems that can be solved within a 2-3 yr time frame to justify industry return on investment. Mid- to long-term requirements are best met via academic research/government labs, with practical input from industry. Government agencies should start active funding at the interface between physical sciences and engineering (esp. chemical engineering).

Current government-funded efforts include work at the following centers:

- The Network for Computational Nanotechnology (NCN) (http://www.ncn.purdue.edu/)
- National Nanotechnology Infrastructure Network's computational drive (NNIN/C) (http://www.nnin.org/nnin_compsim.html)
- National Center for Supercomputing Applications at University of Illinois at Urbana-Champaign (http://www.ncsa.uiuc.edu/)
- Nanomaterials Theory Institute at ORNL (http://www.cnms.ornl.gov/nti/nti.shtm)

The DOE Office of Science recently announced awards from the solicitation on multiscale modeling (http://www.science.doe.gov/grants/FAPN05-16.html). Following projects related to nanomaterials were awarded:

- *"Multiscale Design of Advanced Materials based on Hybrid Ab-Initio and Quasicontinuum* Methods" (Luskin, University of Minnesota) – Focuses on interfacial catalysts, metal-organic framework (MOF) materials for hydrogen storage and fusion materials.
- *"Northwest Consortium for Multiscale Mathematics and Applications Educational Strategies and Critical Problems in Thermo-mechanics of Materials"* (Panchenko, Washington State) – Addresses inadequacy of continuum models (solid mechanics, fluid mechanics and heat transfer) as industrial focus shifted from traditional engineering problems – first to micro-scale problems and, recently to nano-technology.
- *"Localized Scale Coupling and New Educational Paradigms in Multiscale Mathematics and Science"* (Graham, LANL) – Aims at developing a numerical simulation capability for suspension flows that incorporates effects spanning diverse time and length scales.
- *"Micro-Mesoscopic Modeling of Heterogeneous Chemically Reacting Flows Over Catalytic/Solid Surfaces"* (Pannala, ORNL) – Modeling of heterogeneous reacting flows over catalytic surfaces, characteristic of applications in combustion, catalysis, materials production, etc.

In addition, multiple DOD solicitations identify modeling and simulation as research goals.

C. Specific Priority Needs in Modeling and Simulation

Specific primary research needs for Modeling and Simulation were identified by both the Synthesis and Self Assembly, and the Nanomaterial Properties teams of the chemical and semiconductor industries. These needs were presented at the Chemical and Semiconductor Joint Research Needs Meeting hosted by NIST in November 2005. The goals identified by the Synthesis and Self Assembly group are focused on the synthesis of nanostructured materials and on directed and self assembly.

Modeling and simulation can serve several purposes in the research on nanomaterials:

1. Gas-phase Synthesis: The goal for the modeling and simulations aspect of understanding the gas phase synthesis of carbon nanotubes and nanowires is to predict the size, structure, composition, orientation to surface, and the influence of catalyst and applied fields to these structures. To achieve this goal, simulation and models should include multi-scale modeling across scales from atomic to nanoscopic and models of the kinetics of growth. Kinetic models will need to incorporate a wide range of factors including the following:
    - Temperature dependence
    - Gas composition and structure
    - Catalyst nanostructure, shape, and energetics
    - Catalyst nucleation and growth
    - Gas decomposition, diffusion, and segregation
    - Gas interaction with catalyst and catalyst nanostructure
    - Nanostructure nucleation and growth
    - Fields (topology, electromagnetic (em), gradients, stresses, etc.)

2. Liquid synthesis: The modeling and simulations aspect of understanding the liquid synthesis of nanostructured materials has the same goal to predict the size, structure, composition, orientation to surface, and the influence of catalyst and applied fields to these structures. For multi-scale modeling, important questions are long-range fluid-solvent interactions, stereo-chemical effects and confining boundary conditions (e.g., the role of passivating ligands and mixtures). Topics critical to modeling the kinetics of growth are similar to those for gas phase synthesis and include the following:
    - Temperature dependence
    - Solution composition and solution phase segregation
    - Ligand interactions with the solution and crystal faces
    - Nucleation and growth
    - Reactant diffusion, and segregation
    - Reactant solid state growth
    - Oxidation-reduction reactions (for example, nano-electrochemistry)
    - Fields (topology, EM, gradients, stresses, etc.)

3. Directed and self assembly: Modeling and simulation efforts targeted toward directed and self assembly span a wide range of topics including the following:

- Multi-scale modeling (atomic, macromolecular and mesoscopic scale) of equilibrium and kinetic models including long-range fluid-solvent interactions and confining boundary conditions
- Component interaction energetics
- Polymer block or surfactant size, density, shape, diffusion, chain length, persistence length
- Material functional properties as related to the structure
- Shear/elongation, temperature, solvents
- Fields (topology, EM, gradients, stresses, etc.)
- Surface and interface interactions
- Prediction of nanostructure space group, shape, orientation, size, and size variation
- Material functional properties as related to the structure

4. Characterization: The modeling and simulation research needs identified for the purpose of characterization can be grouped into four areas: 1) Magneto-electronic and transport properties; 2) Nano-surface properties and mechanisms; 3) Nano-mechanical and interface properties; and 4) Thermal properties of nanostructured materials.

(a) Electronic structure and electronic transport properties: The modeling and simulation steps determined to be essential for further understanding of the electronic structure and electronic transport properties of nanostructures include the following:

- Develop ab-initio and semi-empirical approaches to model the interactions of nanostructures with environmental factors such as photons, adsorbates or magnetic fields
- Study the role of phonons in electronic transport and bandgap renormalization
- Develop approaches beyond local density approximation (LDA) to calculate electronic structure and electronic transport
- Model interfaces in nanostructures (contact to metals, organic/inorganic interfaces, etc.) and their effect on electronic and transport properties

The Columbia University Center for Electronic Transport in Molecular Nanostructures Nanoscale Science and Engineering Center (NSEC) is recommended as the primary point of contact for this topic.

(b) Nano-surface structure and mechanisms:

- Measurement of surface structure and composition and understanding of their control
- Understanding mechanisms of functionality and surface reactivity

(c) Nano-mechanical and interface properties: The modeling and simulation capabilities determined to be essential for characterization for further understanding of nanomechanics and interfaces in nanostructures include:

- Understanding of the issues of failure modes, interactions with substrates and other materials at the nanoscale

- Predictive models to study the mechanical response of nanostructures to electrical, optical and magnetic stimuli
- Approaches to calculate the effects of mechanical deformations on electronic properties

Contacts with NSECs or Materials Research Science and Engineering Centers (MRSEC) doing work in this area should be established. The Materials Research Laboratory at the University of California, Santa Barbara (MRSEC) currently has a task addressing characterization for polymers and possibly nanocomposites.

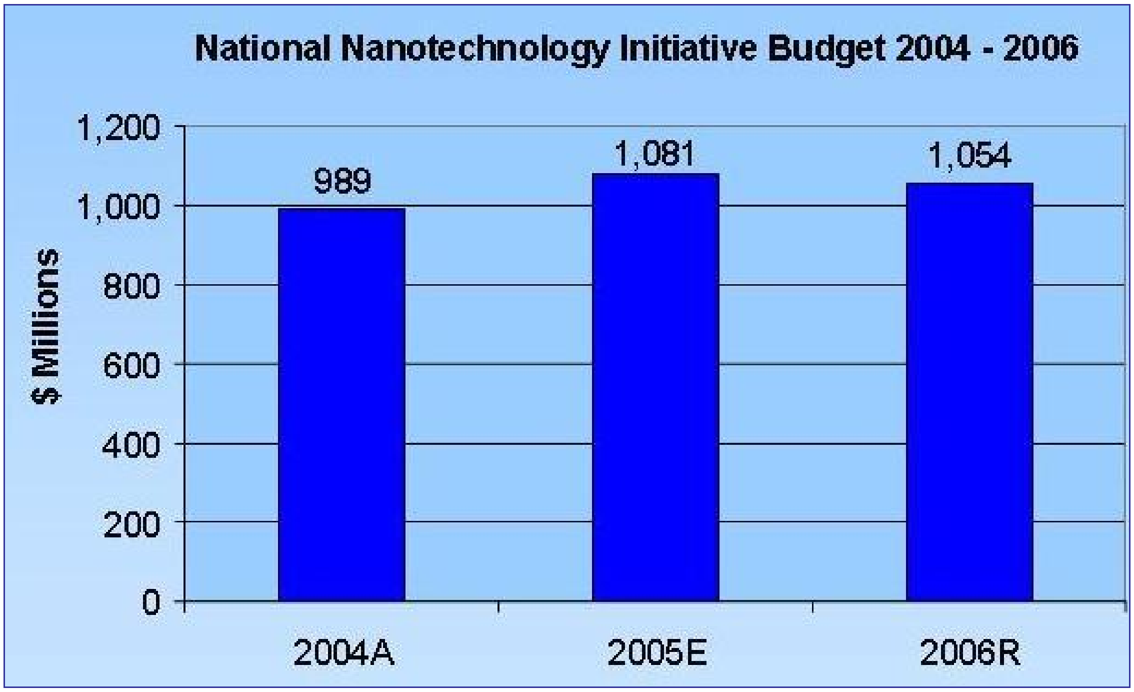
(d) Thermal properties: The modeling and simulation capabilities to be developed for characterization that are essential for further understanding of thermal properties of nanostructured materials include:

- Establishing tools to enable engineered materials with desired properties
- Modeling of transport through nano-composites
- Modeling and simulation tools for phonon scattering in nanomaterials, including the role of phonon scattering in presence of surfaces and interface

3. Current Activities of Federal Agencies

3.1 NNI Funding by Agencies and Program Component Areas (PCAs)

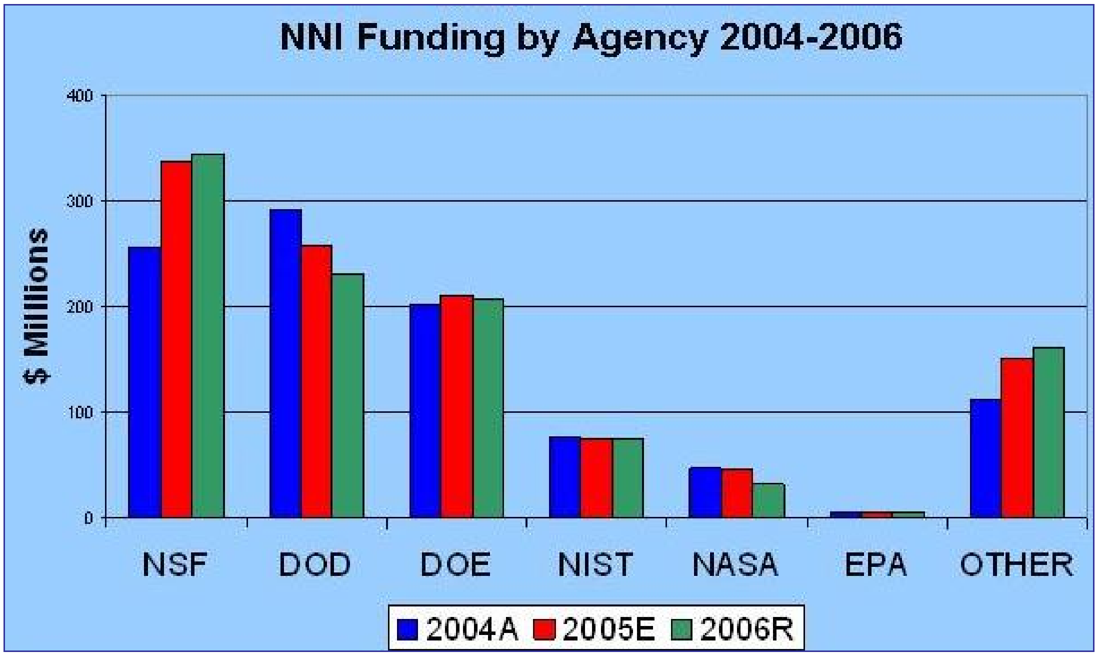
The NNI continues to be well funded, with approximately $1B allocated to activities in multiple government agencies, as shown in Figure 3.



Source: National Nanotechnology Initiative Supplement to the President's FY 2006 Budget

Figure 3: NNI Funding (2004 actual, 2005 estimated, and 2006 requested)

The bulk of NNI funding goes to NSF, DOD and DOE. Funding by agency for the period 2004-2006 is shown in Figure 4. Increases in funding for NSF have been largely offset by corresponding decreases in funds received by DOD. Agency funding included in "Other" category is primarily to the National Institute of Health (NIH).



Source: National Nanotechnology Initiative Supplement to the President's FY 2006 Budget

Figure 4: NNI Funding by Agency (2004 actual, 2005 estimated, and 2006 requested)

Government investment in nanotechnology research and development activities is coordinated through an organizational structure of seven Program Component Areas or PCAs. PCAs provide areas of investment that are critical to accomplishing the NNI goals. The seven PCAs are defined in the NNI Strategic Plan (December 2004); five of the seven PCAs relate to areas of particular interest for R&D investment that addresses chemical industry needs. These PCAs are defined in the Strategic Plan as follows:

Fundamental nanoscale phenomena and processes: Discovery and development of fundamental knowledge pertaining to new phenomena in the physical, biological, and engineering sciences that occur at the nanoscale. Elucidation of scientific and engineering principles related to nanoscale structures, processes, and mechanisms.

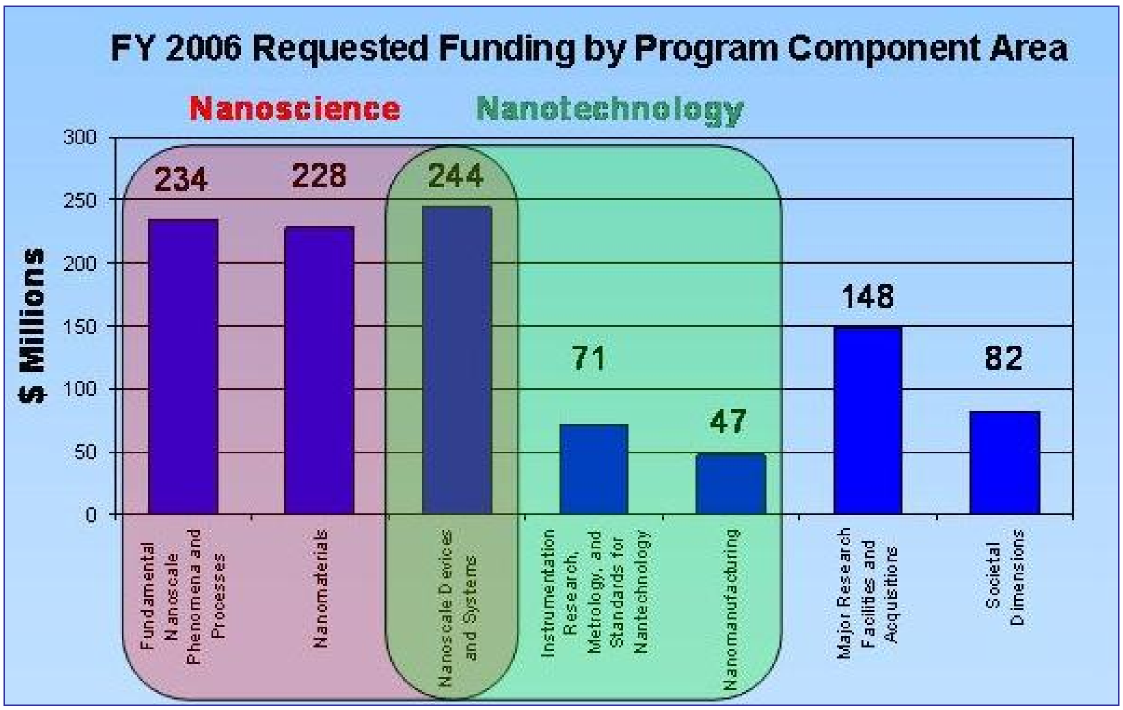
Nanomaterials: Research aimed at discovery of novel nanoscale and nanostructured materials and at a comprehensive understanding of the properties of nanomaterials (ranging across length scales, and including interface interactions). R&D leading to the ability to design and synthesize, in a controlled manner, nanostructured materials with targeted properties.

Nanoscale Devices and Systems: R&D that applies the principles of nanoscale science and engineering to create novel, or to improve existing, devices and systems. Includes the incorporation of nanoscale or nanostructured materials to achieve improved performance or new functionality. To meet this definition, the enabling science and technology must be at the nanoscale, but the systems and devices themselves are not restricted to that size.

Instrumentation Research, Metrology, and Standards for Nanotechnology: R&D pertaining to the tools needed to advance nanotechnology research and commercialization, including next-generation instrumentation for characterization, measurement, synthesis, and design of materials, structures, devices, and systems. Also includes R&D and other activities related to development of standards, including standards for nomenclature, materials, characterization and testing, and manufacture.

Nanomanufacturing: R&D aimed at enabling scaled-up, reliable, cost-effective manufacturing of nanoscale materials, structures, devices, and systems. Includes R&D and integration of ultra-miniaturized top-down processes and increasingly complex bottom-up or self-assembly processes.

The breakdown of NNI funding in the President's 2006 budget request by PCA indicates that agency activities are heavily weighted toward scientific discovery over technology development (Figure 5). The PCAs of fundamental nanoscale phenomena and processes, nanomaterials, and nanoscale devices and systems together comprise 67% of the total funding. Major research facilities and instrumentation acquisition contributes another 14%. In contrast, instrumentation research and nanomanufacturing combined represent 11% of the total investment.



Source: National Nanotechnology Initiative Supplement to the President's FY 2006 Budget

Figure 5: **NNI Funding by Program Component Area**

3.2 Agencies Involved with NNI and their Activities

The NNI Strategic Plan identifies the primary agencies involved with each PCA. Table 3 presents information from the plan, listing the agencies with nanotechnology funding in FY 05 with the relationship of their missions to the five PCAs of interest.

Fundamental Nanoscale Phenomena and Processes	Nanomaterials	Nanoscale Devices and Systems	Instrumentation Research, Metrology, and Standards for Nanotechnology	Nanomanufacturing
Primary Agencies				
DHS*	DOD	DHS	DOC (NIST)	DOC (NIST)
DOE	DOE	DOD	DHS*	DOD
HHS (NIH)	EPA*	DOJ*		EPA*
NSF	NASA	EPA		NSF
	NSF	HHS (NIH)		
	USDA	NASA		
		USDA		
Secondary Agencies				
DOC (NIST)	DOC (NIST)	DOC (NIST)	DOD	DOE*
DOD	HHS (NIH)	DOE	DOE	HHS (NIH)
EPA	HHS (NIOSH)	NSF	EPA*	HHS (NIOSH)
NASA			HHS (NIH)	NASA
USDA			NSF	USDA

Source: NNI Strategic Plan, December 2004 (http://www.nano.gov/NNI_Strategic_Plan_2004.pdf)

* indicates agencies that have not requested FY 2006 funding specifically for that area according to the NNI Supplement to the President's FY 2006 Budget

Table 3: **Primary & secondary relationships between PCAs and missions of Federal Agencies**

Overview of Federal Agencies Relevant to Chemical Industry Needs

A summary of the current and planned activities in federal agencies that are relevant to chemical industry needs is given below. Further information on agency activities is given in "The National Nanotechnology Initiative: Research and Development Leading to a Revolution in Technology and Industry, a Supplement to the President's FY 2006 Budget." A list of contact information listed by Federal Agency is provided in Appendix C of that document.

NSF –The NSF supports nanotechnology research through individual research grants and through 18 Nanoscale Science and Engineering Centers (NSECs), the National Nanotechnology Infrastructure Network (NNIN has 13 sites), and the Network for Computational Nanotechnology (NCN has seven sites). Awards for three new NSECs, including the Center for Hierarchical Nanomanufacturing, were to be announced in 2005.

The stated goals of Nanomanufacturing Program and nanomanufacturing centers appear to be appropriate and aligned with chemical industry needs. Efforts of researchers appear to be more focused on research discovery than on technology development of immediate utility to industry. The nanomanufacturing centers have more focus on issues of relevance to industry. Industrial input is encouraged at the Center for Hierarchical Manufacturing, a new NSEC site which will be awarded in FY 2005 and is expected to operational in 2006. This center is mandated to develop a "nanomanufacturing network that encourages extensive industrial collaboration." Semiconductor Research Corporation involvement in solicitations indicates agency willingness to further address industry goals; there may be similar opportunities for the chemical industry. The NSF will maintain dedicated funding for nanotechnology with its Small Business Innovation Research/Small Business Technology Transfer (SBIR/STTR) program at approximately $13 million annually for 2005 and 2006.

DOD – DOD efforts to develop innovative materials, synthesis techniques, devices, and manufacturing may present a range of cooperation opportunities for chemical industry involvement. Projects related to materials may be of special interest. Several solicitations from DOD address processing, scale-up, and characterization needs, particularly focusing toward NNI mission goals (see Appendix C). In FY 2006, DOD hopes to begin integration of nanomanufacturing into the DOD Manufacturing Technology (MANTECH) program. New nanotechnology programs are expected from Defense Advanced Research Projects Agency (DARPA) in FY 2006.

DOC – DOC's NIST is the lead agency for the Instrumentation Research, Metrology and Standards PCA. NIST research activities and solicitations address manufacturing issues, especially characterization/metrology related to processing. The newly opened Nanomanufacturing and Nanometrology Center at the Advanced Measurements Lab in Gaithersburg, MD is expected to further address relevant characterization issues.

NIST has recently prepared a draft report on the NNI Interagency Grand Challenge workshop, "Instrumentation and Metrology for Nanotechnology." This comprehensive report presents an overview of the state of the art, goals and challenges, vision for the future, recommendations for future research, and implementation strategies. Sections on nanocharacterization, nanofabrication, nanomanufacturing, and cross-cutting computational science are of particular importance to the chemical industry.

NIST is actively engaged with industry in developing a nanomanufacturing program. Participants at the November 2005 meeting at NIST agreed that there was significant overlap between the chemical and semiconductor industries and NIST in the following areas:

- Nano-particle size distribution
- Modeling over multiple dimensions and time scales
- Nano-surface properties and reactivity
    - Catalyst, nano-catalyst etc.
    - Absorbents on nanostructures
    - Electro-magnetic property characterization

A roadmapping workshop focused on these topics is planned for April 2006 to involve NIST, semiconductor and chemical industry groups, leading researchers, and representatives from other NNI agencies.

DOE – DOE's mission is well aligned with applications that exploit properties of nanoscale materials. Several examples are given in the report *Nanoscience Research for Energy Needs* (http://www.er.doe.gov/Sub/Newsroom/News_Releases/DOE-SC/2004/NREN_rpt.pdf).

DOE has established five Nanoscale Science Research Centers (NSRCs) –

- Molecular Foundry at LBNL,
- Center for Functional Nanomaterials at BNL,
- Center for Integrated Nanotechnologies at SNL and LANL,
- Center for Nanophase Materials Science at ORNL, and
- Center for Nanoscale Materials at ANL

All five centers have an emphasis on scientific understanding and applications. These user facilities are accessible to industry for scientific research and represent a significant new set of opportunities for industry-governmental cooperation. In addition, many projects funded at universities and national laboratories by the Divisions of Materials Science and Chemical Science of the Office of Basic Energy Science, Office of Science, are related to research of nanoparticles, nanomaterials, self-assembly, and catalytic science. The DOE Office of Science has recently increased funding for basic research in nanomaterials and nanoscale phenomena to support developing a hydrogen economy and in multiscale modeling. Initiatives exploring nanoscale science to address other energy-related topics may be expected in the future.

The Small Business Innovative Research (SBIR) program of DOE directly solicits industry partners for cooperative research over a wide range of topics. The most recent SBIR solicitation included a section "Nanotechnology Applications in Industrial Chemistry." That section referred to material from the chemical industry nanomaterials roadmap workshop, and focused on applications in catalysis, polymers and polymer manufacture, and composite materials. The solicitation requires plans to introduce nanotechnology into the marketplace in conjunction with major chemical companies that have capabilities for widespread technology implementation and manufacturing.

The current DOE centers do not directly address scale-up, manufacturing, real-time characterization, and nanotechnology applications which are of concern to the chemical industry. At this time, it does not appear that DOE mission offices have developed programs explicitly designed for translation of nanoscience discoveries to energy applications.

EPA – Much of EPA's limited funding in this area is directed toward tracking and removing atmospheric particulate matter, particularly mercury emissions from coal-fired power plants. A relatively small, but growing part of the EPA portfolio is aimed at determining the environmental fate of nanomaterials and the use of nanomaterials in environmental treatment processes.

NASA – The focus of NASA projects is toward materials, electronics and sensors that will be useful in space missions.

Relationship of Agency Activities to PCAs and Chemical Industry Need Areas

The relationship between agency activities, PCAs and the chemical industry's priority R& D needs areas is shown in Table 4. Agency work areas are identified by each agency's statements in "The National Nanotechnology Initiative: Research and Development Leading to a Revolution in Technology and Industry, a Supplement to the President's FY 2006 Budget." Agencies were subjectively ranked by interest in particular fields. In general, there is a good overlap between agency activities and the industry needs.

Table 4: **Agency Activity by PCAs and Industry Interest Areas**

National Nanotechnology Initiative Program Component Areas

Priority R&D Needs Relevant to the Chemical Industry

Primary Secondary	Fundamental nanoscale phenomena, processes and behavior	Nano-materials	Nanoscale devices and systems	Instrumentation research, metrology, and standards for nanotechnology	Nano-manufacturing
Manufacturing and Processing	**A**	**B**	**C**	**D**	**E**
1-Combined Manufacturing and Processing			NSF		1-NSF 2-DOE 3-DOD 4-NIST 5-EPA
Characterization Tools					
2-Develop analytical tools for measuring and characterizing nanomaterials	NIST		NIST	1-NIST 2-NSF 3-DOE 4-DOD	
3-Develop real-time, on-line and in-process tools for measuring and characterizing nanomaterials			1-NSF 2-NIST	NIST	
Fundamental Understanding and Synthesis					
4-Develop new paradigms for creating nanoscale building blocks based on understanding of physics and chemistry at the nanoscale	DOE	1-NASA, 2-NSF 3-DOD	1-NSF 2-NASA		
5-Develop new paradigms for controlled assembly of nanocomposites and spatially resolved nanostructures with long-range order			NASA		
Modeling and Simulation					
6-Develop computational tools to predict bulk properties of materials that contain nanomaterials	1-NSF 2-DOE 3-NIST	1-DOE 2-NASA			
7-Develop methods for bridging models between scales, from atoms to self-assembly to devices.	NIST	1-DOE 2-NASA	NSF		

Note: The field for each program/solicitation is identified by its column and row label, with columns A through E representing NNI PCAs and rows 1-7 the chemical industry areas of interest (see Appendix C)

This background information on the funding areas and current activities of the various federal agencies provides a means of closing the gaps in existing R&D programs that have been identified by the chemical industry. For each priority needs area, the industry can take action steps to influence one or more agencies to close these gaps. These proposed pathways for closing the gaps in the various priority needs areas are shown schematically in Tables 5A-5D.

Table 5A: Potential actions to promote R&D in Manufacturing & Processing area

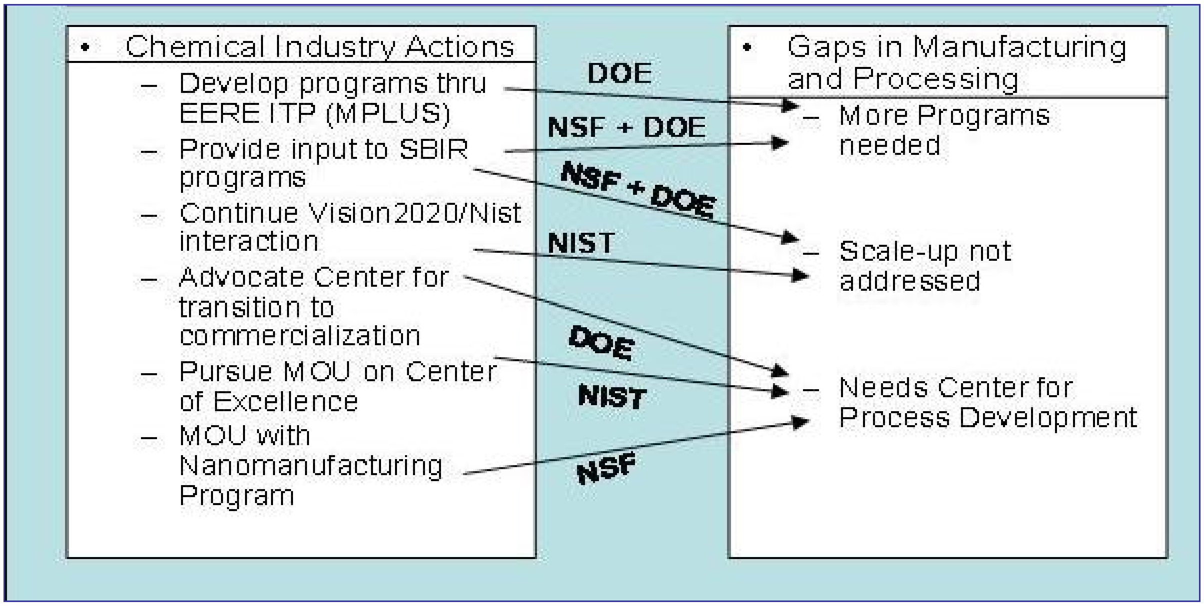


Table 5B: Potential actions to promote R&D in Characterization Tools area

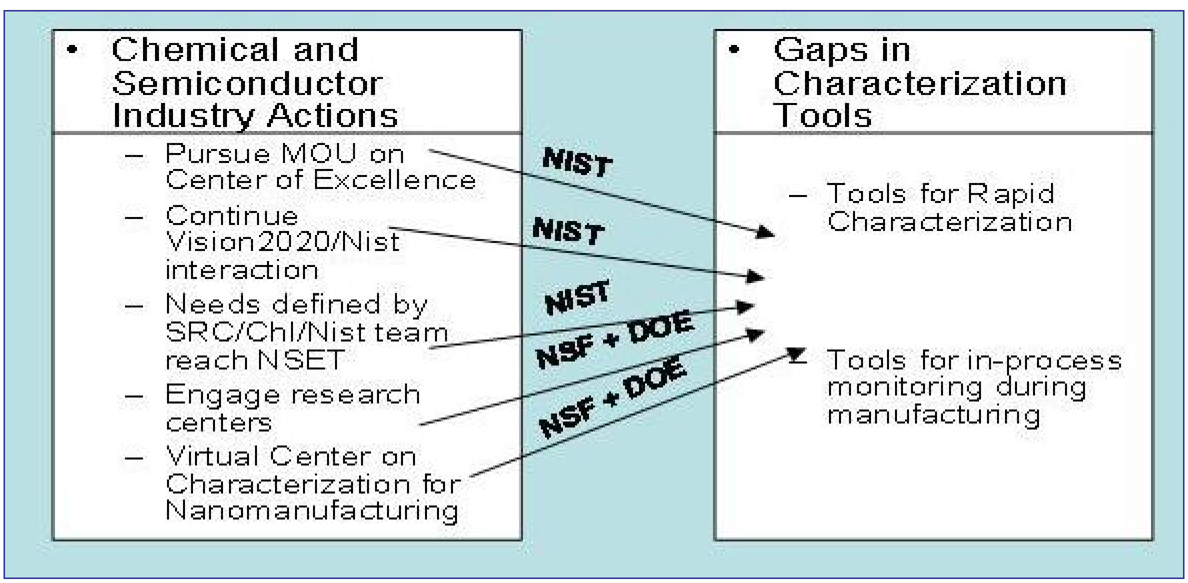


Table 5C: **Potential actions to promote R&D in Fundamental Understanding & Synthesis area**

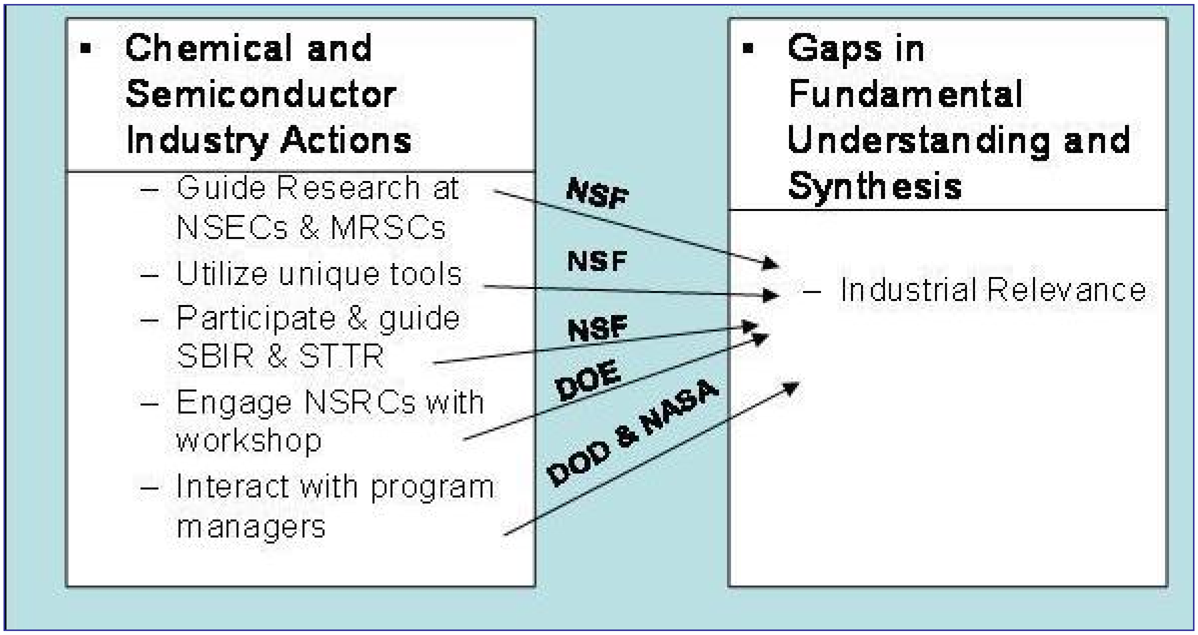
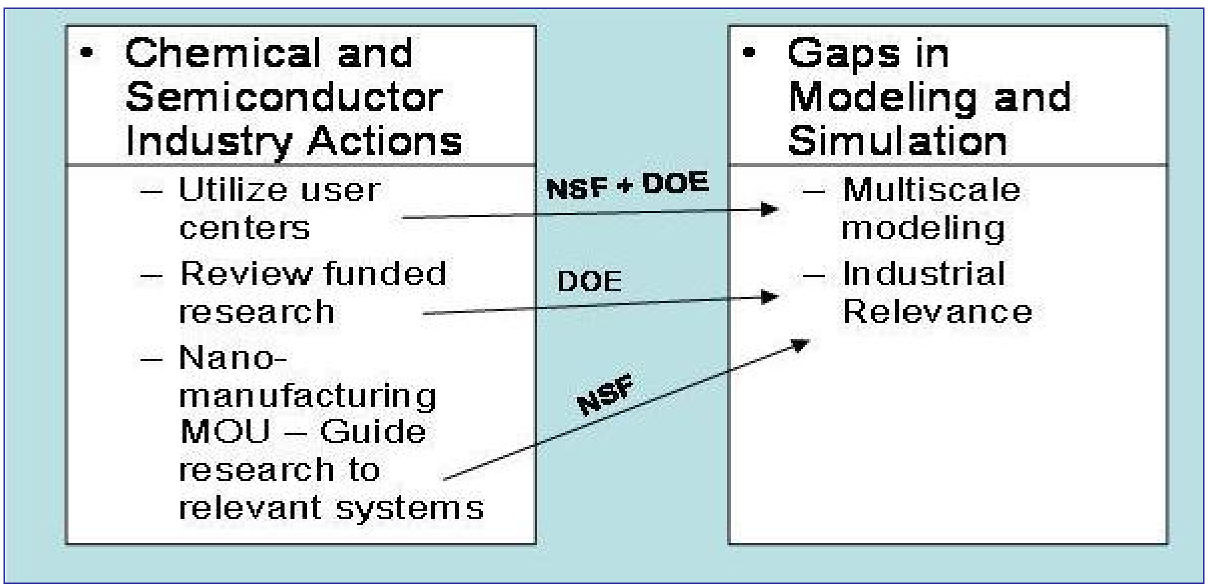


Table 5D: **Potential actions to promote R&D in Modeling and Simulation area**



4. Resources

A number of resources have been established through National Nanotechnology Initiative. A variety of research centers, user centers, funding programs and solicitations are currently actively involved in nanotechnology research. These resources together provide several pathways for the chemical industry to advance the roadmap goals.

4.1 Research Centers

A review of Web sites of nanotechnology research centers was conducted to summarize current research efforts in nanotechnology. The primary reference for this effort was the National Nanotechnology Initiative's Research Centers Web page at http://www.nano.gov/html/centers/home_centers.html. Contact information and brief descriptions of relevant research activities are included in Appendix A.

Though much of current nanotechnology research pertains to semiconductors or biotechnology, significant research relating to chemicals and manufacturing already exists. An effort was made to identify the research centers where work is currently best aligned with the needs of the chemical industry. High priority centers were identified as those working on production, process or scalability, and in areas of coatings, catalysts, high-strength materials, sorbents, or membranes. Centers were prioritized into three tiers according to their relevance to chemical industry roadmap goals: a short list of target centers (7), other potential target centers (9), and the remaining centers (37).

The target centers which appear to have the most relevant focus on priority needs of the chemical industry are:

- Center for Hierarchical Nanomanufacturing; award to be announced by NSF
- University of California-Los Angeles, Center for Scalable and Integrated Nano-Manufacturing (NSEC)
- University of Illinois at Urbana-Champaign, Center for Chemical-Electrical-Mechanical Manufacturing Systems (NSEC)
- Northeastern University, Center for High-Rate Nanomanufacturing (NSEC)
- Northwestern University, Institute for Nanotechnology, Center for Nanofabrication and Molecular Self-Assembly (NSEC)
- Rensselaer Polytechnic Institute, Directed Assembly of Nanostructures (NSEC)
- University of Wisconsin-Madison, Center for Nanotechnology (MRSEC)

In addition to targeting centers based on current published research interests, the industry plans an in-depth survey of centers to better understand their research goals and capabilities. A letter has been drafted for communication from Chemical Industry Vision2020, Council for Chemical Research, and NSF to directors of NSECs and MRSECs, asking for identification of current research activities related to the chemical industry priority needs. When complete, this information will give a more complete picture of the scope of current research activities and will allow more detailed targeting of research efforts to advance industry goals.

4.3 User Centers

User Centers provide the opportunity for outside researchers, including those from industry, industry to exploit unique instrumentation and other capabilities to conduct pre-competitive and, in some cases, proprietary nanoscale research.

A review of Web sites of nanotechnology User Centers was conducted in order to summarize where research activities are being conducted and what experimental facilities are available to outside researchers. Information about User Centers was derived primarily from links on the NNI Web site at http://www.nano.gov/html/centers/randdcenters.html and is summarized in Table 6. These User Centers are funded through the Department of Energy, National Science Foundation, National Institute of Standards and Testing, and the Department of Defense. Contact information and brief synopsis of research areas and facilities for each User Center is listed in Appendix B.

Table 6: Nanotechnology User Centers' areas of interest

Nanotechnology User Centers Summary		**Areas of Research Interest**									
		1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Agency	**Facility**	Theory/Modeling/ Simulation	Nanoscale Magnetism, Nano-photonics, Nano-electronics, & Quantum Transport	Nanomaterials Synthesis	Nanoscale Catalyst Materials	Macromolecular Complex Systems	Bio-Nanosystems	Nanoscale Imaging, Charact-erization & Manipulation	Nano-Fabrication	Nano-scale Processing	Sensors & micro/ nano-mechanical systems
DOE	Brookhaven National Laboratory		X	X	X						
DOE	Sandia & Los Alamos National Labs		X	X			X				
DOE	Oak Ridge National Laboratory	X	X	X	X	X		X	X		
DOE	Argonne National Laboratory	X	X	X			X	X	X		
DOE	Lawrence Berkeley National Laboratory	X		X		X	X	X	X	X	
NSF	Cornell University							X	X	X	
NSF	Stanford University		X								X
NSF	University of Michigan		X							X	X
NSF	Georgia Institute of Technology		X	X				X		X	X
NSF	University of Washington			X	X		X			X	
NSF	Pennsylvania State University								X		
NSF	UC Santa Barbara		X								
NSF	University of Minnesota			X				X			
NSF	University of New Mexico				X		X		X		
NSF	University of Texas at Austin		X							X	
NSF	Harvard University	X	X						X		
NSF	Howard University		X					X	X	X	
NSF	North Carolina State University								X		
NIST	National Institute of Standards and Technology	X	X	X			X			X	
DOD	Department of Defense		X	X			X				

4.3 Relevant Programs and Solicitations

The currently funded NNI programs provide the best opportunity for chemical industry interaction and guidance to address priority needs areas. A Web search of relevant programs and solicitations was conducted in order to summarize current federal funding sources for nanotechnology research. The primary source for funding information is the CINT Nanotechnology Database found at http://lmisgreen.lanl.gov/programs.

Contact information and relevant information on the programs and solicitations as listed on the Web sites were compiled. Some solicitations with expired deadlines were included in order to cover all recent funding opportunities. Solicitations that did not specify nanotechnology research but where nanotechnology research would be required were also included.

A wide variety of programs and funding sources for nanotechnology research in areas of interest to the chemical industry are already in place and compiled in Appendix C. Two major programs of interest are the NSF Nanomanufacturing (App. C, #1) and the Department of Defense Multidisciplinary Research Program of the University Research Initiative (App. C, #14). The results of this survey are summarized in Table 7, where programs and solicitations are mapped to the NNI's PCAs and the chemical industry priority research needs areas. Funding sources 7, 8, 10, and 34 were not included in Table 7 and are only listed in Appendix C.

Table 7: Programs and Solicitations by PCAs and Industry Interest Areas

National Nanotechnology Initiative Program Component Areas

Priority R&D Needs Relevant to the Chemicals Industry

Primary (orange) / Secondary (yellow)	Fundamental nanoscale phenomena, processes and behavior	Nano-materials	Nanoscale devices and systems	Instrumentation research, metrology, and standards for nanotechnology	Nano-manufacturing
Manufacturing and Processing	**A**	**B**	**C**	**D**	**E**
1-Combined Manufacturing and Processing	2, 4	2, 11, 13, 14, 16, 19, 22, 23, 24, 29 (secondary)	13, 14, 39		1, 2, 3, 4, 15, 17, 23, 27, 28, 36 (primary)
Characterization Tools					
2-Develop analytical tools for measuring and characterizing nanomaterials	2, 4, 35, 37	1, 12, 37		1, 2, 6, 26, 35 (primary)	1, 3
3-Develop real-time, on-line and in-process tools for measuring and characterizing nanomaterials			36	1, 2, 14, 24, 26, 35 (primary)	1, 3, 14, 24, 36 (secondary)
Fundamental Understanding and Synthesis					
4-Develop new paradigms for creating nanoscale building blocks based on understanding of physics and chemistry at the nanoscale	4, 19, 26, 32	1, 11, 12, 16, 18, 19, 20, 24, 25, 26, 31, 36, 38 (primary)	22, 23, 28		
5-Develop new paradigms for controlled assembly of nanocomposites and spatially resolved nanostructures with long-range order	2, 4, 19, 21, 26	1, 15, 16, 17, 21, 25, 26, 30 (primary)	1, 2, 4, 13, 14, 15, 17, 27, 28, 30, 38 (primary)		
Modeling and Simulation					
6-Develop computational tools to predict bulk properties of materials that contain nanomaterials	1, 2, 5, 14, 26, 33 (primary)	12, 26			1, 3
7-Develop methods for bridging models between scales, from atoms to self-assembly to devices.	2, 9, 33 (primary)				

__Note__: The numbers in the cells in Table 7 refer to programs/solicitations summarized in Appendix C. The field for each program/solicitation is identified by its column and row label, with columns A through E representing NNI PCAs and rows 1-7 the chemical industry areas of interest (see Appendix C)

5. Recommendations for Future Activities

Gaps in Chemical Industry's Priority Needs and Existing Efforts

Apparent gaps of knowledge or activity with the chemical industry's priority needs include the following:

- Manufacturing and Processing – Few programs are dedicated to issues of nanomanufacturing, and scale-up issues are not fully addressed. A research center or virtual center dedicated to process development may provide sufficient focus for progress in this area.
- Characterization Tools – Most current NNI efforts in Instrumentation Research appear to be aimed at developing new tools for research. Additional focus is needed on developing instruments for rapid characterization and in-process monitoring for nanomanufacturing.
- Fundamentals and Synthesis – There is currently a large amount of activity in this area; however, there is a perception among some in the industry that much of the work is not relevant or sufficiently connected with issues of importance (such as scalability of synthesis) for industrial implementation. Industrial input to fundamental research programs may help to provide greater relevance.
- Modeling and Simulation – Multiscale modeling is seen as an important, long-term effort. A stronger connection of computational user centers to industry or industrially relevant problems is desirable.

Joint efforts developed by NNI and Semiconductor Research Corporation (SRC) are being used by the chemical industry to model new initiatives. Specific research needs in each gap area were identified by industrial teams. Three of the areas – Modeling and Simulation, Characterization Tools, and Fundamental Understanding and Synthesis – were being addressed by joint semiconductor/chemical industry teams formed in recognition of their common interests in priority R&D. Chemical industry-specific research needs in manufacturing and processing were identified by a chemical industry team. These priority needs were presented and discussed at the Chemical and Semiconductor Joint Research Needs Meeting hosted by NIST in November 2005 and the resulting needs statements are integrated into this document.

The primary target agencies for interactions with the chemical industry may be identified by the budget (NSF, DOD, and DOE have the largest nanotechnology-related budgets) and by relevant agency activities, as summarized in the NNI Supplement to the President's 2006 Budget. Primary target agencies for each priority need area are given in Table 1, along with suggested actions for promoting R&D. Several other efforts are currently underway by NNI-ChI CBAN toward the recommended actions and include the following:

- A letter to NSF centers has been drafted to identify ongoing center activities relevant to priority need areas and possibilities for industrial guidance of research.
- Chemical Industry Vision2020 and Semiconductor Research Corporation have initiated interactions with NIST to identify collaboration along the lines of a "nano-center of excellence" for the chemical industry. Efforts are ongoing between the industry groups

and NIST to define and establish R&D programs focused on modeling for synthesis and properties of nanostructured materials and their interfaces.

- One project for the DOE MPLUS program was identified by the Manufacturing and Processing team and has been initiated. This project is focused on real-time characterization of nanoparticles in gas-phase production processes.

Proposed Chemical Industry Initiative

This Implementation Plan seeks the route for the most efficient development of commercial nanotechnologies. The chemical industry seeks to work with the existing federal research programs and advocate the initiation of new programs that fill the important gaps between the existing programs and the research needs most critical to translating the discoveries of nanoscale science to commercialization. To achieve these goals, it is proposed that the chemical industry expand outreach and cooperative activities with DOE, NSF, and the semiconductor industry. Initially, a single NSF nanocenter should be identified as a focal point for contacts, and two research programs in metrology and manufacturing should be funded at existing nanocenters. Subsequently, these activities should be reviewed semi-annually.

Specific action items for the Implementation Plan are:

- Explore opportunities to partner with existing NSF-funded Centers on priority topics
    - Metrology – Develop real-time analytical tools for measuring and characterizing nanomaterials, particularly online and in-process tools for environmental health and safety (EHS), process control and quality control.
    - Manufacturing – Scale-up of self-assembly processes for use in commercial-scale unit operations. Apply current lab-/pilot-scale techniques of molecular or biological self-assembly to larger-scale processes.

  Establish a relationship with the Northeastern University Center for High-Rate Nanomanufacturing as a focal point for industry interaction. Broaden industry relationships with other appropriate NSF funded centers.
- Continue to work with the semiconductor industry on directing research in areas of mutual interest. Participate in their reviews of programs in these areas.
- Interact with NSF program managers for input on program directions. Participate in program reviews as requested, especially those related to manufacturing and metrology.
- Work with the DOE's Industrial Technologies Program on nanotechnology applications, and encourage their support of roadmap activities.
- Continue interactions with DOE's Office of Basic Energy Sciences to explore opportunities to efficiently and appropriately apply capabilities at NSRCs.
- Hold semi-annual follow-up meetings.
    - Meetings could be held at Northeastern or other NSF Nanoscale Science and Engineering Centers.
    - Discuss and support new metrology and manufacturing programs at various existing NSF centers. Encourage efforts that are closely related to the Chemical Industry R&D Roadmap for Nanomaterials by Design.
    - Review other existing programs, and encourage work in areas of chemical industry interest.

Funding for nanotechnology commercialization plan should come from a combination of industry organizations and participating companies. The commercialization initiative will be headed by a representative from a contributing company. Emory Ford (Materials Technology Institute), Jack Solomon (Vision2020) and one representative of CCR will also be part of the leadership team. CCR can provide for organizational support, such as meeting arrangements, e-mail communications etc., with possible support from the DOE's Industrial Technologies Program.

References

Chemical Industry R&D Roadmap for Nanomaterials by Design: From Fundamentals to Function, December, 2003. http://www.chemicalvision2020.org/pdfs/nano_roadmap.pdf

Nanoscience Research for Energy Needs, Report of the National Nanotechnology Initiative Grand Challenge Workshop, March 16-18, 2004, Second Edition, June 2005. http://www.nano.gov/nni_energy_rpt.pdf

The National Nanotechnology Initiative: Research and Development Leading to a Revolution in Technology and Industry, a Supplement to the President's FY 2006 Budget, March 2005. http://www.nano.gov/NNI_06Budget.pdf

The National Nanotechnology Initiative: Strategic Plan, December, 2004. http://www.nano.gov/NNI_Strategic_Plan_2004.pdf

Appendix A: Nanotechnology Center Contacts for the Chemical Industry

A review of websites of nanotechnology research centers was conducted to identify centers whose research is currently aligned with the needs of the chemical industry. High priority centers have work on production, process or scalability and in coatings, catalysts, high strength materials, sorbants, or membranes. The bulk of applied nanotechnology research is electronics related, with biotechnology research next in abundance. Centers were split into three groups; a short list of target centers, other potential target centers, and remaining centers.

Target Centers for Industrial Teaming

University of California-Los Angeles
Center for Scalable and Integrated Nano-Manufacturing (SINAM)

http://www.cmise.ucla.edu/
Director Xiang Zhang, xzhang@me.berkeley.edu, (310) 206-7699

Focus on telecommunication, computing, biotechnology, health care and national security with special emphasis on lithography.

Also, Institute for Cell Mimetic Space Exploration is a NASA program

University of Illinois at Urbana-Champaign
Center for Chemical-Electrical-Mechanical Manufacturing Systems (NSEC)

http://www.nano-cemms.uiuc.edu/
Placid M. Ferreira, Center Director, pferreir@uiuc.edu, 217-333-0639

Aimed at developing techniques for high-throughput production of many different solids, liquids and chemically reacting molecules at the nanoscale. The center's mission is to create a nanomanufacturing system. Dr. Normand Paquin [paquin@uiuc.edu. (217) 244-7985] is the Industrial Programs Coordinator.

Northeastern University
Nanomanufacturing Research Institute

http://www.nano.neu.edu
Ahmed Busnaina, Director, busnaina@coe.neu.edu, (617) 373-2992

The NSF Nanoscale Science and Engineering Center for High-rate Nanomanufacturing (CHN) is focused on nano-manufacturing. The Center is developing tools and processes that will enable high rate/high volume bottom-up, precise parallel assembly of nanoelements (such as nanotubes, nanoparticles, etc) and polymer nanostructures. High throughput is achieved primarily through the use of nano-templates. The research program is organized around the creation, analysis and use of nanotemplates for high rate directed assembly. The center also focuses on reliability of assembled structures and devices as well as defect Control during manufacturing. Modeling is also used to guide Nanomanufacturing across multiple scales and involving multiple domains to support the understanding, analysis and design of various aspect of the nanotemplating process. The center is making two products; a CNT memory devices and a biosensing application to drive the research and development in the Center. The center also concurrently assesses the Environmental, Regulatory and Ethical Impacts of Nanomanufacturing. Industry partners include Intel, Motorola, Tyco, Nantero and Konarka in addition to 8 other companies.

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Northwestern University, Institute for Nanotechnology
Center for Nanofabrication and Molecular Self-Assembly

http://www.nanotechnology.northwestern.edu/
Chad A. Mirkin, Director, nanotechnology@northwestern.edu, 847-467-7302

Aimed at academic research on nanoporous materials for catalysis, membrane separations, and energy storage. The Nanotechnology Corporate Partners (NCP) Program allows members to benefit from opportunities to participate in long-range technical assessments, to provide advice on research directions, and to participate in Institute-wide events.

Institute also includes Nanoscale Science & Engineering Center (NSEC) for Integrated Nanopatterning and Detection Technologies, the Nanoscale Interdisciplinary Research Team, (NIRT) for Multiscale Modeling and

Catalysis for Green Chemistry and Engineering and The Center for Transportation Nanotechnology (http://www.ctn.northwestern.edu/index.html), which conducts research on catalysts to reduce engine emissions.

Rensselaer Polytechnic Institute
Directed Assembly of Nanostructures (NSEC)
http://www.rpi.edu/dept/nsec/
Dr. Richard W. Siegel, Director, rwsiegel@rpi.edu, (518) 276-8846

The new Center is focusing on the ability to assemble nanoscale structures and devices under well-controlled, intentionally directed conditions. NSEC's integrated research program combines computational design with experimentation to focus on the discovery of novel pathways to assemble functional multiscale nanostructures with junctions and interfaces between structurally, dimensionally, and compositionally different building blocks.
The Center's core program consists of two interdisciplinary research thrusts: Nanoparticle Gels and Polymer Nanocomposites and Nanostructured Biomolecule Composite Architectures.
Partners with the University of Illinois, and Los Alamos.

University of Wisconsin-Madison
Center for Nanotechnology
http://www.nanotech.wisc.edu/
Paul Nealey, Associate Director, (608) 877-2410

Materials Research Science and Engineering Center (MRSEC), http://mrsec.wisc.edu/, Juan dePablo, Director, depablo@engr.wisc.edu, (608) 262-0112. Research areas include "Nanostructured Materials as Interfaces to Biology" with applications including biosensors.

Other Centers with Related Research

Central Michigan University
National Dendrimer and Nanotechnology Center
http://www.dendrimercenter.org/
cmurc@cmich.edu, 989.774.2424

DOD funded with biotechnology focus. Research agenda includes "The use of **dendrimers as a catalyst** in the production of carbon nanotubes at the lowest temperatures recorded". Faculty is primarily **chemists**. Private sector partners include Dow Chemical.

Cornell University
Center for Nanoscale Systems
http://www.cns.cornell.edu/
Robert A. Buhrman, Director, rab8@cornell.edu, (607) 255-3732

Includes the research thrust areas: Nanoelectronics, Nanophotonics, Nanomagnetics, and Nanocharacterization and Processing.

Also, Nanobiotechnology, Science and Technology Center, http://www.nbtc.cornell.edu/, Dr. Graham Kerslick, Associate Director, gsk2@cornell.edu, 607-255-0629. Has the following research areas **Biomolecular Devices** & Analysis, Cellular Microdynamics, Cell-Surface Interactions, **Nanoscale Materials**, and Nanoscale Cell Biology. A list of 18 industry partners includes Agilent, DuPont, GE, IBM, Corning, and Phillip Morris.

Also, Cornell Center for Materials Research (MRSEC), http://www.ccmr.cornell.edu/, Frank DiSalvo, Director, director@ccmr.cornell.edu, 607.255.4273. Has four research groups conducting basic nanotechnology research.

Also, Cornell NanoScale Science & Technology Facility, http://www.cnf.cornell.edu/ is the University's research facility and has links to the National Nanofabrication Users Network http://www.nnun.org/default.html

Massachusetts Institute of Technology
Institute for Soldier Nanotechnologies
http://web.mit.edu/isn/
Prof. Edwin L. (Ned) Thomas, Director, isn@mit.edu, 617-324-4700

DOD funded. The ultimate goal is to create a 21st century battlesuit that combines high-tech capabilities with light weight and comfort. Representing the nanomaterials foundries at ISN, Team 5 **develops the processing and device fabrication technologies needed to manufacture and deliver functional nanomaterials**. These technologies must be capable of effectively processing a wide range of components: nanoscale fibers and films; multilayered materials; membranes and microdevices; microfluidic devices; functional hollow fibers; and field-responsive materials and devices. Team 5 has as its goal the fabrication and integration of hierarchically structured materials to achieve multiple and synergistic property combinations. The Industry Consortium includes Founding Partners DuPont, Partners Healthcare and Raytheon.

Also, Center for Materials Science and Engineering (MRSEC) http://web.mit.edu/cmse/www/, Anne M. Mayes (group leader)

NSF funded group Includes IRG-II: Nanostructured Polymer Assemblies which includes Nanoporous Anti-Reflection Coatings which has discovered a very simple, low cost method for making porous thin films with pore sizes controllable from the micro- to nanometer scale. Industry partners include Lucent, DuPont, HP, IBM, Raytheon, and Texas Instruments.

The Naval Research Laboratory (NRL)
Institute for Nanoscience
http://www.nrl.navy.mil/nanoscience/ext/index.html
Richard J. Colton, PhD, nanoscience@nrl.navy.mil

The mission of the Institute for Nanoscience is to conduct highly innovative, interdisciplinary research at the intersections of the fields of **materials,** electronics, and biology in the nanometer size domain. Their focus in nanochemistry is on the development of new sensor materials.

Also, Nanoscience Research Laboratory http://www.nrl.navy.mil/pressRelease.php?Y=2003&R=63-03r

Oregon State University
Oregon Nanoscience and Microtechnologies Institute
http://www.onami.us/index.html
Skip Rung, Executive Director and Industry Outreach: skip@onami.us

The Institute's purpose is growing research and commercialization of technology. It emphasizes research in the integration of nanostructures and microtechnology to **produce materials**, devices, and systems for high impact applications in the fields of energy, sensors, electronics, medicine, **chemicals,** environmental remediation and others. Hewlett Packard is a major partner.

Princeton University
Biologically Inspired Materials Institute (BIMat)
http://bimat.princeton.edu/html/overview.html
Ilhan A. Aksay, Director, iaksay@princeton.edu, (609) 258-4393

The principal goal for BIMat researchers is to develop bio-nanotechnology **materials and structures** for aerospace vehicles. NASA supported. Includes work on **high strength/high stiffness materials**.

Also, Princeton Center for Complex Materials, (http://www.princeton.edu/~pccm/) (MRSEC), Ravin Bhatt, Director, ravin@ee.princeton.edu, 609-258-2532. NSF supported Interdisciplinary Research Groups include Interplay Of Magnetism And Transport In Correlated Electronic Materials, Guided Self-Assembly, and Adhesion, Deformation And Transport At Contacts In Small Structures

Rice University
Center for Biological and Environmental Nanotechnology
http://cben.rice.edu//
Vicki Colvin, Director, colvin@ruf.rice.edu, 713-348-5741

Has an industry affiliates program. Focus is on basic research with applications to disease detection and treatment and to improving water treatment. One program is aimed at design of **continuous phase processes for forming nanocrystalline materials**. (http://cohesion.rice.edu/centersandinst/cben/research.cfm?doc_id=5090)

University of South Carolina
NanoCenter
http://www.nano.sc.edu/
Richard D. Adams, Director, adams@mail.chem.sc.edu, 803-777-7187

Lists catalysis, nanoelectronics, and polymer nanocomposites as technical thrust areas. The program's thrust area in catalysts appears to focus on **developing synergistic bimetallic catalysts for use in chemical manufacturing**.

Dr. Jonathan S. Fletcher is Industrial Relations Coordinator (fletchj@gwm.sc.edu & 803-777-6804).

SUNY-Albany
College of Nanoscale Science and Engineering (CNSE)
http://cnse.albany.edu/ContentManager/index.cfm?Step=Display&ContentID=2
Robert Geer, Assistant Vice President for Academic Affairs, rgeer@uamail.albany.edu, 518-956-7003
College has over 100 industrial partners and oversees five programs including:

Center for Advanced Technology in Nanomaterials and Nanoelectronics http://cnse.albany.edu/ContentManager/index.cfm?Step=Display&ContentID=41 James Castracane, Director. This center is primarily electronics related.

Nanoscale Metrology and Imaging Center http://cnse.albany.edu/ContentManager/index.cfm?Step=Display&ContentID=43> Eric Lifshin, Director, This center doesn't currently do exactly what the chemical industry says they need, but they appear to have **an industrial focus**, and would likely be receptive to their needs. Project areas include semiconductors and optics.

Energy & Environmental Technology Application Center http://cnse.albany.edu/ContentManager/index.cfm?Step=Display&ContentID=44Pradeep Haldar, Director. **Several applications of interest to chemical industry**; the opportunity for industry to use **test beds** is of interest. Specifically, it assists companies overcome technical, market and business development barriers by providing technology incubation, pilot prototyping and test-bed integration support leading to targeted deployment of advanced energy and environmental products. Research areas include distributed generation including fuel cells and photovoltaics.

The two other centers are Center of Excellence in Nanoelectronics and Interconnect Focus Center.

Other Centers

University of Alabama
Center for Materials for Information Technology (MRSEC)
http://www.mint.ua.edu/

Brown University
Center for Advanced Materials Research (MRSEC)
http://www.brown.edu/Departments/Advanced_Materials_Research/

University of California, Berkeley
Berkeley Nanosciences and Nanoengineering Institute (BNNI)
Center of Integrated Nanomechanical Systems
http://nano.berkeley.edu/coins/

University of California-Santa Barbara
Center for Nanoscience Innovation for Defense
http://www.engineering.ucsb.edu/Announce/cnid.html
Also, California Nanosystems Institute (CNSI) with UCLA
http://www.cnsi.ucsb.edu/
Also, Nanotech Fabrication Facility

Columbia University
Center for Electronic Transport in Molecular Nanostructures (NSEC)
http://www.cise.columbia.edu/nsec/index.html
Also, Center for Nanostructured Materials (MRSEC)
http://www.cise.columbia.edu/mrsec/index.php

Georgia Institute of Technology
Microelectronics Research Laboratory
http://www.mirc.gatech.edu/

Harvard University
Nanoscale Systems and their Device Applications (NSEC)
http://www.nsec.harvard.edu/
Also, Center for Nanoscale Systems
http://www.cns.fas.harvard.edu/

Howard University
Keck Center for the Design of Nanoscale Materials for Molecular Recognition
http://www.howard.edu/keckcenter/default.htm

Johns Hopkins University
Materials Research Science and Engineering Center (MRSEC)
http://www.pha.jhu.edu/groups/mrsec/

University of Maryland
Materials Research Science and Engineering Center (MRSEC)
http://mrsec.umd.edu/

Michigan State University
Center for Sensor Materials (MRSEC)
http://www.pa.msu.edu/csm/
Also, Center for Fundamental Materials Research
http://poohbah.cem.msu.edu/cfmr/

University of Minnesota
Materials Research Science and Engineering Center (MRSEC)
http://www.mrsec.umn.edu/index.shtml

University of Minnesota w/ the Univs. of Delaware, Oklahoma and South Dakota
Center for Nano-Energetics Research
http://www.me.umn.edu/%7Emrz/CNER.htm

University of Nebraska-Lincoln
Center for Quantum and Spin Phenomena in Nanomagnetic Structures (MRSEC)
http://www.mrsec.unl.edu/

University of North Carolina-Chapel Hill
Nanoscale Science Research Group
http://www.cs.unc.edu/Research/nano/

North Carolina State University and University of North Carolina
North Carolina Center for Nanoscale Materials
http://www.physics.unc.edu/%7Ezhou/muri/nccnm.html

Notre Dame University
Center for Nano Science and Technology
http://www.nd.edu/%7Endnano/title.htm

Ohio State University
The Center for Affordable Nanoengineering of Polymer Biomedical Devices
http://www.nsec.ohio-state.edu/home.htm

University of Oklahoma / University of Arkansas
Center for Semiconductor Physics in Nanostructures (MRSEC)
http://www.nhn.ou.edu/cspin/

University of Pennsylvania
The Laboratory for Research on the Structure of Matter (MRSEC)
http://www.lrsm.upenn.edu/

Pennsylvania State University
Center for Nanoscale Science (MRSEC)
http://www.mrsec.psu.edu/

Purdue University
Institute for Nanoelectronics and Computing
http://inac.purdue.edu/wps/portal//.cmd/cs/.ce/155/.s/1003/_s.155/1082/_s.155/1003

Stanford University
Center on Polymer Interfaces and Macromolecular Assemblies (MRSEC)
http://www.stanford.edu/group/CPIMA/
Also, Stanford NanoFabrication Facility

Texas A&M University
Institute for Intelligent Bio-Nanomaterials & Structures for Aerospace Vehicles

http://tiims.tamu.edu/

University of Virginia
Center for Nanoscopic Materials Design (MRSEC)
http://www.mrsec.virginia.edu/

Virginia Commonwealth University
Center for Bioelectronics, Biosensors, and Biochips (C3B)
http://www.c3b.vcu.edu/index.html

Other NNIN Facilities
University of Michigan
Solid State Electronics Laboratory
http://www.eecs.umich.edu/ssel/index2.php

University of New Mexico
Nanoscience at the University of New Mexico
http://nnin.unm.edu/

University of Texas at Austin
Microelectronics Research Center
http://www.mrc.utexas.edu/

University of Washington,
Center for Nanotechnology
http://www.nano.washington.edu/index.asp

Other DOD Related Contacts
Department of Defense Research Laboratories
http://nanosra.nrl.navy.mil/laboratories.php

Multidisciplinary University Research Initiatives and Defense University Research Initiatives on NanoTechnology
http://www.nanosra.nrl.navy.mil/muri.php

National Labs
Brookhaven National Laboratory
Center for Functional Nanomaterials
http://www.cfn.bnl.gov/default.asp

Sandia National Laboratories, & Los Alamos National Laboratory
Center for Integrated Nanotechnologies
http://cint.lanl.gov/

Argonne National Laboratory
Center for Nanoscale Materials
http://nano.anl.gov/

Lawrence Berkeley National Laboratory
Molecular Foundry
http://foundry.lbl.gov/

Oak Ridge National Laboratory
Center for Nanophase Materials Sciences
http://www.cnms.ornl.gov/

Appendix B: User Centers for Nanotechnology Research and Development

A review of websites of nanotechnology research centers was conducted to identify user centers available to outside researchers. Information about research areas, facilities, and contact information was derived primarily links on the website for the National Nanotechnology Initiative found at: http://www.nano.gov/html/centers/randdcenters.html. The user centers described below are operated through the Department of Energy, National Science Foundation, National Institute of Standards and Testing, and the Department of Defense. A summary table of research areas is also included.

DOE Nanoscale Science Research Centers

Department of Energy (DOE) Nanoscale Science Research Centers (NSRCs) must have:

An array of state-of-the-art equipment and laboratories for synthesis, fabrication, characterization, and simulation of nanoscale materials and structures,

A skilled staff to support this equipment, users, and the associated science,

A user scientific program that provides leadership in nanoscale science and technology

Two basic modes of user access are common among the five NSRCs – General User access and Partner access. There is no cost to users except for proprietary research.

General Users are individuals or groups who carry out their research, using existing equipment in the NSRCs. General Users apply for access by submission of a proposal that is evaluated by a proposal review panel (The PRPs consist of external scientists - without affiliation to the NSRC - with expertise in various research fields related to nanoscale research.) The scope of a General User proposal can vary from a single-experiment proposal to a program proposal (valid for multiple visits and substantial access to a range of equipment extended over multiple years) to a "special" proposal (i.e. rapid access, feasibility studies, or other means which have been developed by each Center based on their particular needs).

Partners are individuals or groups who not only carry out research at an NSRC, but also enhance the capabilities or contribute to the operation of the Center. Typically they develop the facility instrumentation by bringing outside financial and/or intellectual capital into the evolution of the NSRC, or by contributing to the operation of equipment and facilities. These contributions must be made available to the General Users. Partners may be allocated limited access to one or more facilities over a period of several years, with the possibility of renewal. Partner scientific programs are subject to the same peer review process as General Users.

Proprietary and Non-Proprietary Research – There may be access for a reasonable percentage of proprietary research which utilizes these unique facilities to benefit the national economy. Users conducting proprietary research may access the facility as either General Users or as Partners. Full cost recovery is required from the User, and DOE must approve the proprietary research proposal. Efforts will be made to secure appropriate intellectual property control for proprietary users to permit them to exploit their experimental results.

Center for Functional Nanomaterials (CFN), Brookhaven National Laboratory

http://www.cfn.bnl.gov/default.asp

CFN scientific theme areas:

Strongly Correlated Oxides: examining changes in the electronic response of metal oxides with nanoscale dimensions

Magnetic Nanoassemblies: probing magnetic interactions in nanomaterials

Nanoscale Catalyst Materials: studying new ways to form nanocatalysts and look at their electronic structure and reactivity

Charge Injection and Transport in Nanoscale Materials: understanding electronic conduction in molecular wires and dots

Nanostructured Organic Films: Structure and Self-Assembly: studying the self-assembly of thin organic films as well as their molecular and electronic structure

Applications of Functional Nanomaterials: building new devices and biological assemblies, such as nanoscale electronic devices, ultrathin-film optical devices, and advanced fuel cell catalysts

Laboratory facilities at CFN include:

Nanopatterning

Ultrafast Optical Sources

Electron Microscopy

Materials Synthesis
Proximal Probes
Theory & Computation
CFN Endstations at the National Synchrotron Light Source.

The contact for user administration is (631) 344-NANO, cfnuser@bnl.gov.

Center for Integrated Nanotechnologies (CINT), Sandia National Laboratories and Los Alamos National Laboratory
http://cint.lanl.gov/
CINT is organized around five research themes:

Nano-bio-micro Interfaces - understanding and controlling function at the intersection of biological and biomolecular science with nanoscale materials science

Nanophotonics and Nanoelectronics - controlling electronic and photonic properties of nanostructured materials

Complex Functional Nanomaterials - establishing the scientific principles needed to design, synthesize and integrate nanomaterials into robust nanocomposite architectures and systems with desired functions and performance

Nanomechanics - providing a scientific basis for designing machines that perform work at nanometer length scales by coupling mechanical, optical, (bio) chemical and electrical energy

Theory and Simulation - theory, modeling and simulation of nano- and meso-scale materials

Preference will be given to proposals that address the following challenges:

Integration of top-down fabrication with bottom-up assembly to create new classes of functional materials;

Electronic energy transfer, charge transport, mechanical force and fluidic transport across multiple length scales;

Integration of biological and synthetic materials, and control of the interface between biological and non-biological components.

The CINT Core Facility will feature low vibration for sensitive characterization, chemical/biological synthesis labs, clean room for device integration, interaction areas and conference rooms, visitor office space, and high-speed communications. The CINT Gateway to Sandia will focus on nanomaterials and microfabrication from the existing Integrated Materials Research Laboratory (IMRL), while the CINT Gateway to Los Alamos will focus on biosciences and nanomaterials.

The national user programs at Los Alamos Neutron Science Center (LANSCE) and the National High Magnetic Field Laboratory (NHMFL) provide a platform for CINT to lead the advancement of neutron scattering and high magnetic field techniques for nanoscale science research. With completion of the Asterix spectrometer, LANSCE will have the world's most intense source of polarized cold neutrons, which, along with neutron reflectometry and other neutron spectroscopies, will be essential for the study of complexity in nanomaterials. The National Science Foundation NHMFL pulsed field facility, represents a unique tunable nanoscale probe important for exploring nanostructured semiconductors, quantum systems, and complex materials.

CINT also provides a Nanotechnology Funding Database (http://lmisgreen.lanl.gov/programs) as a service to the scientific community.

Contact Neal Shinn, User Program Manager, Sandia National Laboratories, 505.844.5457, ndshinn@sandia.gov

Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory
http://www.cnms.ornl.gov/
The seven scientific themes for CNMS are:

Macromolecular Complex Systems: Polymers and bio-inspired macromolecular materials; polymer-nanomaterial composites.

Functional Nanomaterials: Nano-tubes, -wires, -dots, and functional composites; complex oxide films and heterostructures grown with atomic-layer control for enhanced and new combinations of properties.

Nanoscale Magnetism and Quantum Transport: Effects of reduced and experimentally variable dimensionality; magnetism and transport in nanostructured materials.

Catalysis and Nano-Building Blocks: Synthesis and characterization of highly selective catalysts and supports; use of catalysts to control synthesis and direct nanoscale organization.

Theory/Modeling/Simulation: Nanomaterials Theory Institute (NTI)

Integrated support for experimental research; development of theoretical and computational nanoscience methods to address Grand Challenges of multi-scale modeling, nanomaterials design, and virtual synthesis; development and dissemination of community-based methods/codes for user-initiated research (NanoFocULs program).

Nanofabrication: Nanofabrication Research Laboratory (NRL): Clean room, nanoscale patterning, nanomaterials processing; development of controlled synthesis and directed assembly methods; functional integration of soft and hard materials; nano-bio research (nanophase biomaterials systems).

Nanoscale Imaging, Characterization and Manipulation: Unique and state-of-the-art instruments and methods to manipulate and measure properties of nanostructures with simultaneous imaging. Includes neutron and x-ray scattering; UHV and ambient scanning probes; electron microscopy and spectroscopy

CNMS will provide users with access to a complete suite of nanoscience research capabilities housed in a new 80,000-ft^2 building adjacent to the Spallation Neutron Source at ORNL. Research capabilities are listed by theme at: http://www.cnms.ornl.gov/capabilities/cap.shtm

The User Coordinator for ORNL is Tony Haynes, hayneste@ornl.gov, 865.576.2858.

Center for Nanoscale Materials (CNM), Argonne National Laboratory
http://nano.anl.gov/
Argonne's research themes are:

Bio-Inorganic Interfaces
Complex Oxides
Nanocarbon
Nanomagnetism, Nanophotonics
Theory and Simulation

Nanopatterning
X-Ray Nanoprobe

The CNM will consist of the following primary elements:
Facilities for synthesis and fabrication of nanoscale materials, and instruments to characterize the fundamental properties of nanoscale materials

A dedicated beamline at the APS (hard x-ray nanoprobe). APS's hard x-rays, harnessed in a nanoprobe beamline, will provide unprecedented capabilities to characterize extremely small structures.

Advanced data-collection systems and remote-presence capabilities

Training and collaborative outreach facilities

Other facilities at Argonne National Laboratory include:
Advanced Photon Source
Electron Microscopy Center
Intense Pulsed Neutron Source

Contact Lori Moore, CNM User Administrative Liaison, lmoore@aps.anl.gov, 630/252-8152

Molecular Foundry, Lawrence Berkeley National Laboratory
http://foundry.lbl.gov/

Research areas include:
Nanotube Synthesis
Nanowire Synthesis
Colloidal Nanocrystal Growth
High-Resolution Nanolithography
Nanoscale Process Integration
Integration, Assembly and Testing of Biological Nanomaterials
Design, Synthesis and Characterization of Organic Molecules and Polymers
Physical and Electrical Characterization of Nanostructures
First Principles Nanoscale Phenomena Modeling

The Molecular Foundry includes facilities for:
Inorganic Nanostructures
Organic Nanostructures
Nanofabrication
Biological Nanostructures
Theory of Nanostructured Materials
Imaging and Manipulation of Nanostructures

James M. Bustillo, JMBustillo@lbl.gov, 510.486.4574 is Molecular Foundry Associate Director—User Program

NSF FACILITIES

National Nanotechnology Infrastructure Network (NNIN)

http://nnin.org/

NNIN is an integrated networked partnership of thirteen user facilities. The mission of NNIN is to enable rapid advancements in science, engineering and technology at the nano-scale by efficient access to nanotechnology infrastructure. The network provides support in nanoscale fabrication, synthesis, characterization, modeling, design, computation and hands-on training. Industrial and government users are welcome in NNIN facilities – historically, about 25% of use is from small and large companies. Users do not have to be associated with any university, and do not have to be associated with someone at the sites.

NNIN facilities house over 700 major tools supporting thousands of processes. The tools, which are detailed in a searchable database <http://www.nnin.org/nnin_tool.taf>, are available in laboratory facilities falling into the following general broad categories: lithography; deposition and growth; etching; wet-chemical processing; other traditional thin-film and device processing; electrical characterization; structure and materials characterization; biological and chemical processing; synthesis and molecular assembly; particles and nanomaterials; and process integration. Many of the processes and tools originated with the semiconductor industry; however NNIN has developed tools and processes for a variety of non-microelectronic materials.

In addition to access to tools, NNIN provides project and process support, through defined Technical Liaisons in life sciences, chemistry and chemical nanotechnology, soft lithography, materials characterization, scientific computation, nanoscale process integration, geosciences and particle technology.

Cornell NanoScale Science & Technology Facility (CNF), Cornell University
http://www.cnf.cornell.edu/

Expertise: Broad scope in Nanotechnology; Biology, Chemistry, MEMS, Characterization, Materials, Electronics, Life Sciences, Computation

CNF works in five primary areas.
Lithography
Thin Film Deposition, Synthesis and Processing
Characterization
Process Integration
Modeling and Simulation

A 10 minute video tour to available equipment and processes is at http://www.cnf.cornell.edu/cnf5_videotour.html. Lab equipment includes:

- Photolithography
- Furnace Processing
- Computing
- Electron-Beam Lithography
- Electrical Testing
- Metrology
- Packaging
- Sems / Microscopes
- Thin Film Etching
- Thin Film Deposition
- Thin Film Misc Processing

Contact: Michael Skvarla**,** User Program Manager, (607)-254-4674, Skvarla@cnf.cornell.edu

Stanford Nanofabrication Facility (SNL), Stanford University
http://snf.stanford.edu/About/About.html
Expertise: A broad range of micro- and nanofabrication tools and techniques.
SNL conducts research in the areas of optics, MEMS, biology, and chemistry, as well as process characterization and fabrication of more traditional electronics devices. It is especially committed to supporting use of micro- and nanofabrication technologies in non-traditional research applications.
Details of SNL capabilities are provided on their web site (http://www-lam.stanford.edu/SNL.htm). SNL provides high-quality SEM, TEM, and FIB capabilities.
Contact: John Shott**,** SNF Associate Directory, shott@snf.stanford.edu

The Michigan Nanofabrication Facility (MNF), University of Michigan http://www.eecs.umich.edu/ssel/
Expertise: MEMS, Electronics, System Integration, Biological Sensors
Research is focused on the theory, design, and fabrication of electronic, optoelectronic, and micromachined devices, circuits, and microsystems, as well as on novel characterization and metrology techniques. Research groups include:

- III-IV Integrated Devices and Circuits
- Center for Wireless Integrated Microsystems (WIMS)
- DeviceNet and ControlNet Conformance Test Labs
- High Performance Microprocessor Project
- Integrated Manufacturing Process Automation and Control Technologies Group
- Micro& Nano-Fabrication for Electrical/Optical Devices & Microsensors
- Modbus Conformance Test Lab
- MURI Center of Intelligent Microelectronics Manufacturing
- Optoelectronic Research Group
- Organic & Molecular Electronics
- Solid-State Chemical Sensors

MNF is part of the Solid-State Electronics Laboratory (SSEL). It provides facilities and processes for the integration of Si integrated circuits and MEMS with nanotechnology, The MNF builds on its experience in integration of Si-based electronics with MEMS transducers and micropackaging to push these interfaces into the nanometer regime with emphasis on the fabrication, packaging, and testing of integrated devices for chemical and biological sensing, electrical stimulation of biological systems, and integrated fluidic systems.
The Solid-State Fabrication Facility offers a complete laboratory for the fabrication of solid-state MEMS and integrated circuits. In the Si circuits area, an E/D Si-gate NMOS process and a 3 µm double-poly single-metal p-well CMOS, and a companion BiCMOS process are available for use as needed. All major MEMS fabrication technologies are available - bulk, surface, polymer/plastic, and molded electroplated micromachining. III-V compound capabilities are available for research on high-speed micro-, nano-, and opto-electronics, including microwave/millimeter wave devices and circuits, and integrated optical devices.
It consists of a Class 100/10 research laboratory available 24/7 with approximately 6,000 square feet of work area backed up by almost 25,000 square feet of support facilities. The research laboratory consists of five process bays (silicon lithography/diffusion, silicon LPCVD, gallium arsenide devices, thin-film deposition, and plasma dry etching) plus separate connected rooms for lithography (e-beam, contact and stepper), compound semiconductor growth (MBE and MOCVD) and RIE. The MNF has in-house characterization ability (SEM, spectroscopic ellipsometry, Hall, AFM and profilometry). Additionally, associated laboratories can provide XPS, Auger, TEM, X-Ray diffraction, X-ray reflectometry, Rutherford Backscatter Spectrometry, Nuclear Reaction Analysis and Elastic Recoil Detection.
Contact: Sandrine Martin, User Manager, 734-763-6719, sandrine@eecs.umich.edu

The Microelectronics Research Center (MiRC), Georgia Institute of Technology http://www.mirc.gatech.edu/
Expertise: Biology, Life Sciences, Integrated Systems, and Electronics
The scope of research includes: nanostructures nanoelectronics photonics, MEMS and BioMEMS, materials growth, process chemistry, and Biological and Chemical Sensors (CMOS ChemFETs, microacoustic bio/chem sensors).
The MiRC is housed in its own 100,000 sq. ft. building that includes an 8,500 sq. ft. cleanroom (75% class 100, 25% class 10). The major fabrication facilities in the cleanroom include thin film deposition, plasma processing, optical and electron beam lithography (100 keV / 4nm spot size JEOL JBX 9300FS), thermal processing, electroplating, wafer lapping, polishing, dicing, bonding and sawing, wire bonding, flip chip bonding, III-V MBE growth, and a 2-metal/2-poly CMOS and MEMS line (ion implantation outsourced). Characterization tools include optical and electron microscopy, AFM, SCM, STM, stylus and optical profileometry, low/high force scanning nanoindentation tribology, surface analysis tools, and high speed electronic and optical testing. Design and simulation tools are available on PC and workstation clusters under campus wide site licenses. Other GIT-NNIN resources include the

GIT Electron Microscopy Center and the Laser Dynamics Lab (LDL).
Contact Kevin Martin, Associate Director, (404)-894-4034, kevin.martin@mirc.gatech.edu

The Center for Nanotechnology (NTUF), University of Washington http://depts.washington.edu/ntuf/index.php
Expertise: Biology and Life Sciences Applications of Nanotechnology
NTUF gives critical support to research in many areas, e.g., catalysis, nano- and bio-materials, motor proteins, microfludics, and bio-nanosystems. The Center is committed to improving biomedical access to emerging micro- and nanoscale tools.
NTUF has the leading-edge instruments for characterizing biological samples at the nanoscale in both air and water. These include a Leica DMIRBE; FEI field emission SEM (Sirion) integrated with an EDAX system and Nabilty e-beam lithography system; Digital Nanoscope IIIa STM and AFM; Zeiss LSM 510 Confocal Microscope; plus soft lithography for rapid micro- and nanoscale prototyping. Well-established training programs allow users to master these tools quickly
Contact:, Dong Qin**,** Associate Director, (206)-616-2118, dqin@u.washington.edu

The Penn State Nanofabrication Facility, Pennsylvania State University http://www.nanofab.psu.edu/
Expertise: Chemical nanotechnology
The Penn State Nanofab is focused on developing, sustaining, and utilizing micro- and nanofabrication in the support of a wide range of areas including physics, chemistry, medicine, biology, and engineering.
The Nanofab houses extensive 150mm (6" wafer) processing capabilities in 2700 square feet of class 10 cleanroom space. There is equipment for:
Wet Chemical Etching
Lithography
Film Deposition / Growth
Dry Etching (Reactive Ion Etching)
Material Modification
Characterization
The Nanofab is a professionally staffed class 10 clean room facility providing a full range of processing capabilities for substrates as large as 6" in diameter. The Penn State Nanofab offers expertise in "top-down" (e.g. deposition, etching) and "bottom up" (e.g. self-assembling films) nanofabrication.
Contact: Jeff Catchmark**,** Operations Manager, (814)-865-6577, jcatchmark@engr.psu.edu

Nanotech at the University of California at Santa Barbara
http://www.nanotech.ucsb.edu/)
Expertise: Optics and Electronics Materials
UCSB strengths include leading expertise in compound semiconductors, photonics, quantum structures, and expertise with non-standard materials and fabrication processes. Areas of excellence include: compound semiconductor electronic and optoelectronic devices in GaAs, InP and the semiconductor nitrides; polymer and organic electronic and photonic devices; quantized electron structures and THz physics; spintronics, single electronics, and quantum computation; quantum optics; MEMS/NEMS, bio-instruments, and microfluidics.
The nanofabrication facility has comprehensive and advanced semiconductor and thin film processing equipment and provides access and professional consultation to industrial and internal and external academic users. The facility currently consists of 3,600 ft2 of class 100 and 10,000 clean space, 2,400 ft2 of other lab space, and will move to a new 12,000 ft2 class 100 and 1,000 facility in Q3-Q4 of 2004. A wide range of materials including silicon, compound semiconductors (III-V in particular), and novel and unusual materials (including polymers and ceramics) are processed in the facility. All lithographic systems have tooling for most substrate shapes, including small and irregular shapes and sizes. A 30 nm resolution JEOL E-beam lithography system is a key resource for outside users and a new FEI Sirion field-emission SEM is capable of writing 10 nm features. These tools are the foundation for nm-scale scientific exploration and technology development for a wide range of materials and devices. Dry etch capabilities are a particular strength, with seven reactive-ion-etch systems (including three advanced inductively-coupled plasma systems) available for etching many types of semiconductors, metals, and dielectrics. Thin films of metals and dielectrics are deposited onto a variety of host substrate materials by an extensive tool set including sputtering, reactive sputtering, electron-beam and thermal evaporation, and plasma-based CVD systems. The facility also houses many benches and systems for chemical processing, substrate preparation and cleaning, rapid thermal processing, oven curing, wafer cutting and polishing, and thin-film and device characterization. Materials characterization capabilities at UCSB include Atomic Force Microscopy, Scanning Electron and Transmission Electron Microscopy, Photoluminescence Spectroscopy, X-ray diffraction and Scanning Auger Microscopy.
Contact, Jack Whaley, Nanotech Laboratory Manager, (805) 893-8174, Whaley@ece.ucsb.edu

The Minnesota Nanotechnology Cluster (MINTEC), University of Minnesota
Expertise: Nanomaterials and Characterization
The node at the University of Minnesota combines the efforts of three organizations.
The Nanofabrication Center (NFC: www.nfc.umn.edu) hosts a full suite of processing tools for building micro and nano devices including a new Raith 150 direct write e-beam system along with optical lithography, RIE, ICP, ion milling, RTP, CVD, PECVD, and PVD. With an annual budget of approximately 1.6 M$, it runs a class 10 clean room with 14 permanent staff.
The Characterization Facility (CharFac: www.charfac.umn.edu) has a wide suite of electron beam, ion beam, x-ray, optical, and proximal probe tools along with the staff to train users, develop new techniques, and operate these systems. A new 300 keV high resolution TEM was added in 2004. Of particular interest are the Lab's capabilities in soft materials including cryogenic and environmental electron microscopy.

The Particle Technology Lab (PTL) is one of the leading centers for nanoparticle research in the country. The Lab occupies over 15,000 square feet of common-use lab space and has a wide variety of instrumentation. Retaining its strength in environmental nanoparticle work, the Lab has more recently moved into nanoparticle applications including 3D integrated circuits, nano energetics, super hard nanoparticle materials, and quantum dots.
Contact Greg Cibuzar, User Contact, (612)-624-8005, cibuzar@ece.umn.edu

Nanoscience at the University of New Mexico
http://nnin.unm.edu/
Expertise: Nanomaterials and Nanocharacterization
UNM has expertise and capabilities including: nanoscale interferometric lithography; nanoscale catalysis, and nano-geo-bio-chemistry. The current research at UNM's Department of Earth and Planetary Sciences (EPS) covers a broad range of important nanophase geological materials. Nanoscience @ UNM facilities include a high technology cleanroom, advanced lithography, and characterization equipment as well as to quantum nanostructure growth facilities. The routine growth of high quality self-assembled quantum nanostructures (quantum dots) based on the Stranski-Krastonow (S-K) growth of InAs and other semiconductors is another capability of the UNM NNIN site. Quantum dot laser diodes operating in the 1.0- to 2.0-um range possess the lowest threshold current density and largest tuning range demonstrated in any semiconductor laser system. We will provide users with the means for the synthesis and characterization of nanophase catalytic materials. UNM has unique capabilities in the synthesis and characterization of such nanostructured materials.
Contact: Rick Bradley, User Access Manager, (505)-272-7648, rbradley@chtm.unm.edu

The Microelectronics Research Center (MRC), University of Texas at Austin
http://www.mrc.utexas.edu
Expertise: Electronics, Chemical Nanotechnology, Instrumentation for Manufacturing
MRC provides opportunities to perform research in novel materials of interest to the IC industry, optoelectronics and nanophotonics, novel electronic devices and nano-structures, and interconnects and packaging. The UT-MRC laboratories reach users from many different fields: electronics, optics, physics, chemistry, astronomy, and chemical, mechanical, and petroleum engineering. UT-Austin has assembled one of the largest and most diverse university semiconductor research programs in the world. MRC has developed new approaches to scaling classical transistors to deep submicron geometries, resulting in high levels of integration, reliability, and performance in integrated circuits. New dielectric materials for MOS transistors and new processing techniques for low thermal budget manufacturing have been developed and are under further active investigation.
The facilities include 12,000 sq. ft. of Class 100 and Class 1000 clean-room space for Si, III-V and soft materials processing, which are available to the NNIN. The clean room also contains a JEOL-6000FS/E-based electron beam lithography system capable of 20nm resolution on masks, small substrates and 8" wafers. This e-beam system will be used to generate templates for the Step and Flash Imprint Lithography tool. The S-FIL is a nano-imprint scheme for patterning of features in sub-20nm regime with ability to perform layer-to-layer alignment through a transparent template to sub-tenth micron accuracy. Other micro/nano-fabrication facilities include sputter, e-beam and plasma deposition for Al, silicides and dielectrics, reactive-ion etching, rapid thermal processing and oxidation/diffusion furnaces for Si, Si-Ge and High-k dielectrics, LPCVD for poly-silicon, oxides, nitrides and numerous wet chemistry stations. The characterization laboratories contain the apparatus for comprehensive optical and electrical measurements.
The Optoelectronics Group at MRC has developed novel vertical-cavity, surface-emitting lasers, and radically new photodetectors. Detailed studies of the device physics that govern the performance of these lasers and photodiodes have led to significant improvements in performance and functionality. The Microelectronics Research Center has also established active research efforts in GaN and related materials, which is projected to become the dominant material for short-wavelength emitters, ultraviolet photodetectors and high-power electronics. The Microelectronics Research Center is also recognized as a leader in the area of interconnects, both optical and electrical.
Contact: Marylene Pallard, User Contact, Marylene@mer.utexas.edu

The Center for Nanoscale Systems (CNS) at Harvard University
http://www.cns.fas.harvard.edu/
Harvard University emphasizes the areas of 1) soft lithography and the assembly of nanoparticle and molecular electronics; 2) theoretical simulations of electron states and transport in nanoscale systems; and 3) the establishment of core computational resources to assist users in the understanding and visualization of new device structures. The mission is to foster leading-edge, multi-disciplinary research and education in the area of imaging and nanoscale systems, bridging the disciplines of chemistry, physics, engineering, materials science, geology, biology, and medicine.
CNS includes capabilities in the following areas:

Two Research Cleanrooms for Nanofabrication and Soft Lithography
Electron-Beam and Optical Lithography
Advanced Electron-Beam, Optical, and Atomic Imaging
Materials Synthesis and Characterization
Ion Beam Processing and Characterization
New Equipment Development

CNS has divided its facilities and tools into four main "Facilities.":

Imaging and Analysis (SEM, TEM, ESEM, FIB, XPS, sample prep etc.)
CAMS (Cambridge Accelerator f/Materials Science. RBS, FRIE, PIXE etc.)
Nanofabrication (cleanroom, lithography, RIE, and back-end tools etc.)

Materials Synthesis (diverse collection of tools not in any above facility)
Contact: James Reynolds, NNIN User Program, (617) 384-7411, nninapply@cns.fas.harvard.edu

Howard Nanoscale Science and Engineering Facility (HNF), Howard University
http://www.msrce.howard.edu/
Expertise: General Microfabrication, Electronics and Materials, Characterization Science, and Nanofiltration
HNF engaged in research and development in diverse areas such as electronics, materials science, optics, polymer science, membrane technology, medicine, physics and chemistry. The three technical areas are Electronics and Materials (wide band gap devices and applications to nanotechnology), Chemistry (Characterization Science), and materials (nanofiltration membranes and technology).
HNF has integrated facilities in the following categories:

- Lithography Facilities
- Nanofabrication Facilities
- Plasma Etching / Deposition Facilities
- CVD Deposition Facilities (SiC, GaN)
- Nanomembrane Facilities
- Characterization Facilities
- Computer Facilities

An equipment list is located at: http://www.msrce.howard.edu/EQUIP.htm
Contact: James Griffin, Lab Manager, (202) 806-6618, griffin@mscre.howard.edu

The Triangle National Lithography Center at NCSU (DUV lithography only)
http://www.tnlc.ncsu.edu/ (Affiliate)
Expertise: Deep UV (193 nm) lithography
The ASML 5500/950B, in the Triangle National Lithography Center (TNLC), is a state-of-the-art, 193 nm optical lithography system for rapid turnaround time and high volume patterning. This scanner is housed in Class 100 facilities within NC State's Nanofabrication Facility (NNF). The NNF provides auxiliary photoresist capabilities: resist coating, developing, descum, and trim. To complete the pattering process, RIE tools are available for film etching. In conjunction with the Strasbaugh 6EC chemical mechanical polishing tool, damascene pattering can be performed. In addition, a broad range of other processes (CVD, oxidation, PVD, chemical etching, etc.) are available to support nanofabrication.
Contact: Carlton Osburn, Director 919-515-5153, osburn@eos.ncsu.edu

Network for Computational Nanotechnology (NCN)
Providing modeling and simulation activities, the Network for Computational Nanotechnology (NCN), addresses research challenges through theory and computation. The NCN is creating a cyber infrastructure to facilitate collaboration, to provide access to simulation services and to develop nanoscience software for the public domain. NCN researchers produce new algorithms, approaches, and software tools with capabilities not yet available commercially. The nanoHUB (is a source of on-line resources, including a unique web-based computational user facility; users may sign up for a free account and run simulations using community codes via the internet. Results of these efforts can be seen at the nanoHub, where resources already are available to promote the application of computational science to nanotechnology. See nanoHub (https://www.nanohub.org/). The NCN has three research foci: nanoelectronics, nanoelectromechanics and nanobioelectronics.
(Contact - Mark Lundstrom, Director of nanoHUB initiative; 765.494.7715; ncn@ecn.purdue.edu)

Participants in NCN are:
Purdue University, http://www.ncn.purdue.edu/)
University of Illinois, http://www.beckman.uiuc.edu/inside/about.html
Stanford University, http://scpd.stanford.edu/SCPD/courses/contentView/nanotechnology/
University of Florida, http://web.math.fsu.edu/%7Exxu/applied_math/Nanotechnology.htm
University of Texas, El Paso, http://utep.edu
Northwestern University, http://www.nsec.northwestern.edu/index.html
Morgan State University, http://www.morgan.edu/

National Institute of Standards and Technology (NIST) Advanced Measurement Laboratory (AML)

http://aml.nist.gov

NIST's AML is the most technically advanced research facility of its kind in the world. The $235 million, 49,843 square meter (536,507 square foot) laboratory features five separate wings – two of them buried 12 meters (39 feet) underground – with stringent environmental controls on air quality, temperature, vibration, and humidity. The new facility allows NIST to provide the sophisticated measurements and standards needed for technologies such as nanotechnology, semiconductors, biotechnology, advanced materials, quantum computing and advanced manufacturing. AML will support some of the world's most delicate experiments in nanotechnology and measurement at the atomic level. NIST research efforts planned for the new facility range from improved calibrations and measurement of fundamental quantities such as mass, length and electrical resistance to the development of quantum computing technology, nanoscale measurement tools, integrated microchip-level technologies for measuring individual biological molecules, and experiments in nanoscale chemistry.

Industrial researchers can work side-by-side with NIST researchers under a Cooperative Research and Development Agreement. Under certain conditions, NIST also makes its facilities available for private research. See NIST's Domestic Guest Research Program. http://patapsco.nist.gov/ts/220/external/domesticgr.htm (contact - Jack Pevenstein 301-975-5519)

Center for Neutron Research (NCNR)
(http://www.ncnr.nist.gov/)
NCNR is part of the Materials Science and Engineering Laboratory . The activities of the NCNR are focused on provision of neutron measurement capabilities to researchers in the US. NCNR serves more than 1,700 scientists annually from industry, university, and government agencies. The NCNR is the only cold (i.e. low-energy) neutron facility with comprehensive capability in the United States, providing tools essential to study the complex biological, polymeric and composite materials that are at the forefront of nanomaterials research. Methods for obtaining beam time are described at http://www.ncnr.nist.gov/beamtime.html. (Contact - Patrick Gallagher, NCNR Director, 301-975-6210, patrick.gallagher@nist.gov)

Department of Defense Center
The Naval Research Laboratory (NRL)
http://www.nrl.navy.mil/pressRelease.php?Y=2003&R=63-03r
NRL offers the opportunity for scientists to conduct multidisciplinary research in the fields of materials, electronics, and biology in the nanometer size domain.
A 5000 square foot class 100 cleanroom, has been outfitted with the newest tools to permit lithographic fabrication, measurement, and testing of devices. This includes deposition systems for metals and insulators, optical mask aligners, and etching systems. This is supported by chemistry stations and fume hoods for spinning on photo resists, baking, and developing the patterns that ultimately result in small devices and circuits. Additional new equipment includes an electron beam writer for fabricating features down to 10 nanometers; a focused ion beam workstation for 10 nanometer-scale machining of materials; a scanning electron microscope for inspection of these small-scale devices, an optical pattern generator, several reactive ion etchers and metal deposition systems.
The cleanroom also contains an atomic force microscope, optical microscopes, optical index characterization, scanning stylus surface measurement, a probe station for electronic measurements on finished devices, and a wire bonder to connect the circuits in completed microchips to plug-in carriers.
Building 250 also contains 5000 square feet of controlled-environment laboratory space, which is available to NRL researchers whose experiments are sufficiently demanding to require this space. There are 12 of these laboratories within the new building. All provide shielding from electromagnetic interference and very low floor vibration and acoustic levels. In addition, eight laboratories will control the temperature to within ± 0.5 °C and four to within ± 0.1 °C.
Some of the current occupants include the Material Science and Technology Division with its ultra-high resolution transmission electron microscope (TEM) and a low-temperature magnetics laboratory; the Acoustics Division with its near-field scanning optical microscope (NSOM); and the Chemistry Division with its ultra-high vacuum, four-probe scanning tunneling microscope (STM) that is installed in one of the ultra-quiet laboratories and its atomic force microscopes (AFM) that are installed in one of the quiet laboratories.
(Contact – Richard J. Colton, Director of the Institute of Nanoscience, nanoscience@nrl.navy.mil)
There are two primary mechanisms by which the NRL transfers its technologies to the public sector: patent licensing agreements and cooperative research and development agreements (CRADAs). Under the scope of a CRADA, NRL scientists work with non-Federal parties to perform research and development on subjects of mutual interest and benefit. Often, such a cooperative research program will be associated

with a patent licensing agreement to adapt NRL's patented technologies to a particular product or service. Information on CRADAs with the NRL may be obtained at http://www.nrl.navy.mil/techtransfer/cradas.php, or contact NRL's Technology Transfer Office, crada@techtransfer.nrl.navy.mil.

Appendix C: Relevant Programs and Solicitations

Note: For description to Field numbers, refer to Table 7 on page 39

1) NSF Nanomanufacturing,
Field(s): A6, B4, B5, C5, D2, D3, E1, E2, E3,
Kevin Lyons, 703-292-5365, klyons@nsf.gov
http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=13347&org=DMII

2) NSF Nanoscale Science and Engineering (NSE)
Program Solicitation for FY 2005
Program Solicitation NSF 04-043,
Field(s):A1, A2, A5, A6, A7, B1, C5, D2, D3, E1

3) NSF Nanomanufacturing Solicitation,
Field(s): E1, E2, E3, E6
http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=13347
Kevin W Lyons, klyons@nsf.gov, (703) 292-5365

4) NSF Particulate and Multiphase Processes Program
Solicitation, Field(s): A1, A2, A4, A5, E1, C5
http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=13364;
Triantafillos J. Mountziaris, tmountzi@nsf.gov,
(703) 292-8371

5) NSF Division of Materials Research Condensed Matter
and Materials Theory Program Field(s): A6
http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=13623
G. Bruce Taggart, gtaggart@nsf.gov, (703) 292-4941
or, Daryl W. Hess, dhess@nsf.gov, (703) 292-4942;
Supports fundamental research

6) NSF SBIR Solicitation Small Business Innovation
Research and Small Business Technology Transfer
Programs Phase I Solicitation FY 2006 (SBIR/STTR)
http://www.nsf.gov/pubs/2005/nsf05605/nsf05605.pdf
Window Nov 8 to Dec. 8, Field(s): D2
Rosemarie D. Wesson, Program Manager and
Solicitation Coordinator, (703) 292-7070,
rwesson@nsf.gov

7) NSF Solicitation Opportunities for collaboration
between NSF and NIST
http://www.nsf.gov/pubs/2005/nsf05596/nsf05596.pdf
Jesus M. de la Garza, Program Director, Directorate for
Engineering, Division of Civil & Mechanical Systems,
(703) 292-7791 jgarza@nsf.gov (Not mapped in Table 7)

8) USDA National Research Initiative Competitive Grants
Program FY 2005 Request for Applications
U.S. Department of Agriculture, Cooperative State
Research, Education, and Extension Service
http://www.csrees.usda.gov/funding/rfas/pdfs/05_nri.pdf
(Not Mapped in Table 7)

9) Department of Energy Office of Science Financial
Assistance Program, Field(s): A7
Notice DE-FG01-05ER05-16: Multiscale Mathematics
Research and Education
http://www.science.doe.gov/grants/FAPN05-16.html
Dr. Gary Johnson, (301) 903-5800, garyj@er.doe.gov

10) DOE EERE Solicitation DE-PS36-05GO95011 –
Materials for Energy Efficient Industrial Processing
http://www.pr.doe.gov/iips/faopor.nsf/UNID/D6A485C1EE167A888525703700774A86/$file/DOEFundOpporGO95011_-_IMF_final.doc; (Not Mapped in Table 7)

11) DOE solicitation DE-PS26-05NT42472-16, University
Coal Research, Field(s): B1, B4
http://www.netl.doe.gov/business/solicit/main.html#42472 , Focus is University funding

12) DOE Office of Basic Energy Sciences – Basic
Research for the Hydrogen Fuel Initiative: Notice DE-FG01-04ER04-20, Field(s): B2, B4, and B6
Harriet Kung, Ph.D., (301) 903-1330,
harriet.kung@science.doe.gov.
Solicitation: http://www.science.doe.gov/grants/Fr04-20.html; closed 7-15-04

13) DOE 2005 SBIR: solicitation - Basic Energy Sciences,
Field(s): B1, C5
http://www.science.doe.gov/sbir/Solicitations/FY%202004/BES.htm

14) Department of Defense Multidisciplinary Research
Program of the University
Research Initiative, Field(s): A6, B1, B5, C5, D3, E3
Dr. Mihal E. Gross, 703-696-0388,
grossm@onr.navy.mil
http://www.onr.navy.mil/02/baa/docs/04_021.pdf

15) DARPA Broad Agency Announcement (BAA) 05-21,
Field(s): B5, C5, E1; Very High Efficiency Solar Cell
http://www.darpa.mil/ato/solicit/VHESC/index.htm

16) U.S. Army Natick Soldier Systems Center Broad
Agency Announcement (BAA)
Solicitation No."05 - 07 Natick BAA",
Field(s): B1, B5
https://www3.natick.army.mil/05baa.pdf

17) Air Force Flight Test Center solicitation
FY151957400093: Synthesization, Manufacturing,
and Characterization of New Sprayable
Nanocomposite Thermoplastic Elastomeric Solid
Rocket Motor Internal Insulation
http://lmisgreen.lanl.gov/programs?c=view&id=05-01055&r=98193; Field(s): B5, C5, E1

18) Air 4.3 Polymers and Composites BAA, Field(s):B4
Solicitation Number: N00421-05-R-0009
http://www.eps.gov/spg/DON/NAVAIR/N00421/N00421-05-R-0009/SynopsisR.html

Posted Date: Nov 02, 2004, Original Response Date: Sep 30, 2005

19) Air Force Office of Scientific Research BAA 2005-1, Field(s): A4, A5, B1, B4 http://www.afosr.af.mil/pdfs/BAA2005-1.pdf

20) Naval Research Laboratory BAA 63-05-04, Field(s):B4
Materials Science Of Energetic Thin-Film Deposition Processes,http://heron.nrl.navy.mil/contracts/0506baa/630504.htm

21) Naval Research Laboratory BAA 63-05-04, Materials Science of Energetic Thin-Film Deposition Processes, Field(s): A5, B5,
http://heron.nrl.navy.mil/contracts/0506baa/630504.htm

22) Army Research Laboratory (ARL), Army's Small Business Technology Transfer (STTR) Program Field(s): B1, C4
http://www.dodsbir.net/solicitation/sttr05/army05.pdf

23) Missile Defense Agency (MDA) Small Business Technology Transfer (STTR), Field(s): B1, C4, E1
http://www.acq.osd.mil/sadbu/sbir/solicitations/sttr05/mda05.htm

24) Navy STTR Program, Office of Naval Research (ONR), Field(s): B1, B4
http://www.dodsbir.net/solicitation/sttr05/navy05.htm

25) DARPA Defense Sciences Research and Technology, Sol: BAA05-19; Field(s): B4, B5
http://www.darpa.mil/baa/baa05-19pt1.html

26) Army Research Laboratory BAA DAAD19-03-R-0017, Field(s):A4, A5, A6, B4, B5, B6, D2, D3,
http://www.aro.army.mil/research/arl/fy06arlbaa.pdf

27) DARPA Very High Efficiency Solar Cell (VHESC), Field(s): E1, C5
http://www.darpa.mil/ato/solicit/VHESC/index.htm
Dr. Doug Kirkpatrick; VHESC@darpa.mil

28) US Army SBIR, Field(s): E1, C4, C5
http://www.dodsbir.net/solicitation/sbir052/army052.htm
Susan Nichols Army SBIR Program Manager, sbira@belvoir.army.mil (703) 806-2085

29) Army Research Office BAA W911NF-04-R-0005, Field(s): B2,
http://www.aro.army.mil/research/arobaa06.pdf
Dr. Stephen Lee, stephen.lee2@us.army.mil, (919) 549-4365

30) Office of Naval Research MURI ONR BAA Announcement 05-017 Field(s): B5, C5
http://www.fedgrants.gov/EPSData/USN/Synopses/4/BAA05017/FY%26%23032%3B2006%26%23032%3BMURI%26%23032%3BBAA.pdf, Dr. Bill Lukens, MURI Program Manager, (703) 696-4111, 363_MURI@onr.navy.mil

31) Naval Research Lab BAA 61-05-05 – Fabrication, Characterization and Structural Analysis of Amorphous, Nanoscale Materials for Power Sources, Field(s): B4, Karen.Lyons@nrl.navy.mil
http://heron.nrl.navy.mil/contracts/0506baa/610505.htm

32) NRL BAA 63-05-04 – Materials Science of Energetic Thin-Film Deposition Processes Field(s): A4
Hubler@ccf.nrl.navy.mil, (202) 767-4786
http://heron.nrl.navy.mil/contracts/0506baa/630504.htm

33) NRL BAA 61-05-06 – Computational Chemistry, Field(s): A6, A7, carter.white@nrl.navy.mil
(202) 767-3270
http://heron.nrl.navy.mil/contracts/0506baa/610506.htm

34) Defense Advanced Research Projects Agency (DARPA) BAA05-19
Brett Giroir, Deputy Director, DSO, (571) 218-4224, bgiroir@darpa.mil, closes Feb 7, 2006,
(Not Mapped in Table 7)

35) National Institute of Standards and Technology FY 2005 Small Grants Programs Funding Opportunity No.: 2005-SGP-01, Field(s): A2, B2, D3
http://www.fedgrants.gov/EPSData/DOC/Synopses/1251/2005-SGP01/2005%26%23032%3BSmall%26%23032%3BGrant%26%23032%3BPrograms%26%23032%3BFull%26%23032%3BAnnouncement.pdf

36) NIST FY05 SBIR, Field(s): B4, C3, E1, E3
http://patapsco.nist.gov/ts_sbir/fy05.pdf

37) NIST FY 2005 Small Grants Programs, Field(s): A2, B2
http://www.fedgrants.gov/EPSData/DOC/Synopses/1251/2005-SGP-01/2005%26%23032%3BSmall%26%23032%3BGrant%26%23032%3BPrograms%26%23032%3BFull%26%23032%3BAnnouncement.pdf
Dr. Richard R. Cavanagh, (301) 975-2368

38) NASA SBIR AND STTR 2005 Program Solicitations, Field(s): B4, C5
http://sbir.gsfc.nasa.gov/SBIR/sbirsttr2005/solicitation/index.html, NASA Official: Robert W. Nelson

39) EPA Small Business Innovation Research Phase I, Field(s): C1, Solicitation No. PR-NC-05-10246
http://es.epa.gov/ncer/rfa/2005/2005_sbir_phase1.html#D1