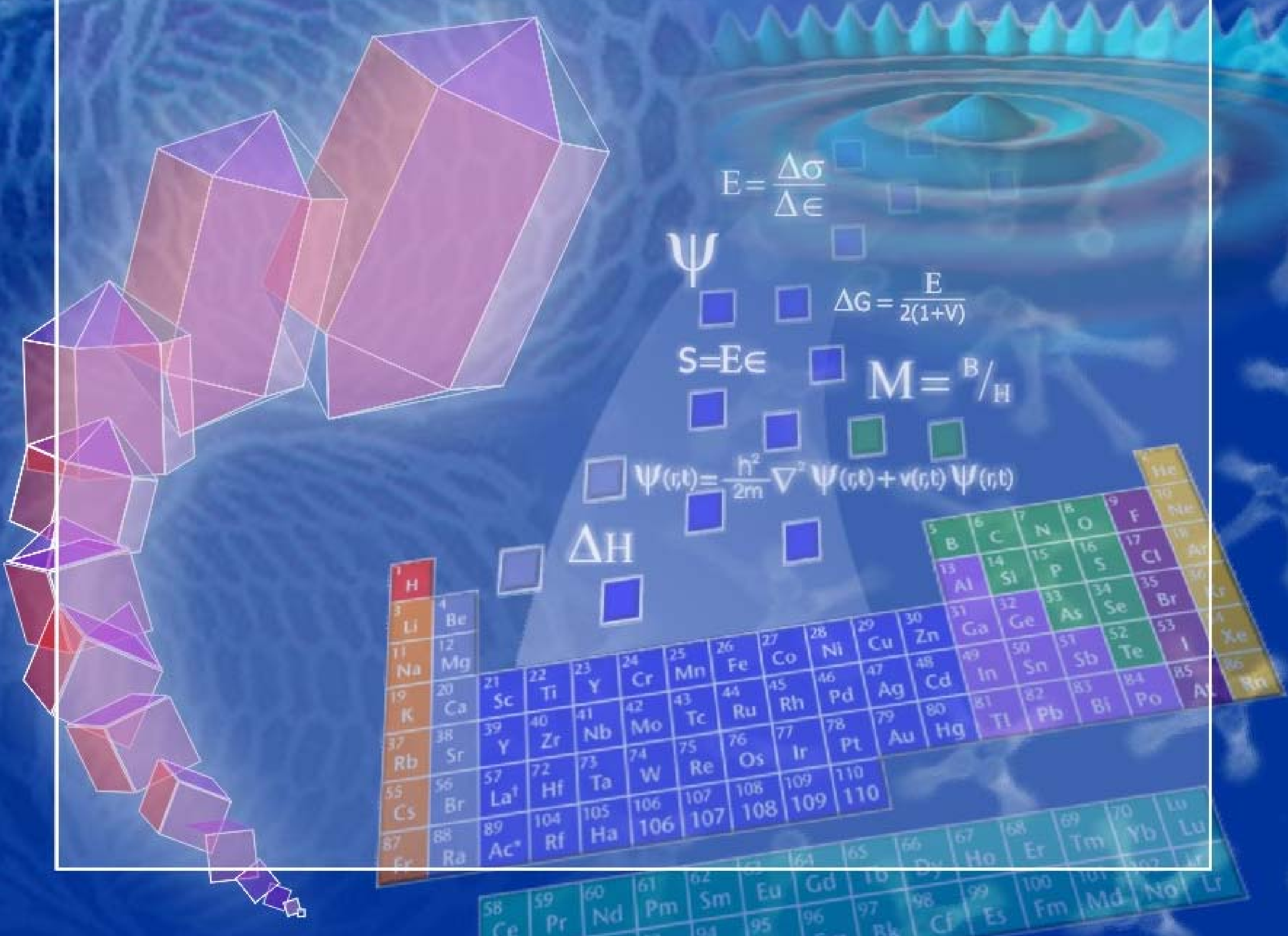
Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function

December 2003



Approved and Issued by the
Chemical Industry Vision2020 Technology Partnership

An electronic copy of this roadmap can be found at
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Chemical Industry R&D Roadmap for Nanomaterials By Design:
From Fundamentals to Function

December 2003

Prepared by

Chemical Industry Vision2020 Technology Partnership

Energetics, Incorporated

Sponsored by

Chemical Industry Vision2020 Technology Partnership

U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy

All agencies and organizations of the National Science and Technology Council's Nanoscale Science, Engineering, and Technology Subcommittee through the National Nanotechnology Coordination Office in support of the National Nanotechnology Initiative

www.ChemicalVision2020.org

To Our Readers:

The Chemical Industry Vision2020 Technology Partnership represents a broad cross-section of the U.S. chemical industry and fosters the development of technology roadmaps on topics of importance to the industry. Last year, the interagency Nanoscale Science, Engineering, and Technology (NSET) Subcommittee that guides the National Nanotechnology Initiative (NNI) approached the Vision2020 Partnership about spearheading the development of a roadmap to provide industry perspective on the NNI Grand Challenge for Nanostructured Materials by Design (see Appendices A and B for information on both organizations).

Vision2020 agreed to join NNI and the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy (DOE/EERE) in sponsoring the "Nanomaterials and the Chemical Industry Roadmap Workshop" on September 30-October 2, 2002. The event in Baltimore, Maryland, drew more than 100 scientists, engineers, entrepreneurs, and decision makers from the chemical and material processing industries, major universities, start-up companies, national laboratories, and over a dozen Federal agencies (listed in Appendix C). Through the workshop's structured forums, these participants actively exchanged ideas on research needs and approaches. Participants came to surprisingly strong consensus on the top-priority R&D needs (see www.chemicalvision2020.org/nanomaterialsroadmap.html).

This roadmap, *Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function,* is based on the scientific priorities expressed by workshop participants from the chemical industry, universities, and government laboratories. The recommendations for roadmap implementation were developed by the chemical industry and do not necessarily reflect the views of the workshop sponsors (agencies of the NSET Subcommittee and DOE). The roadmap is intended for use by the chemical industry to set corporate R&D priorities, by NSET agencies to help set funding priorities, and by legislators and the Administration to inform public policy decisions.

Members of the Vision2020 Nanomaterials Roadmap Steering Team wish to thank the many workshop participants and roadmap reviewers for generously contributing their expertise, time, and resources to this effort. The chemical industry now seeks to develop strategic partnerships with NSET agencies and the entire research community to pursue the R&D priorities outlined in this roadmap. These priorities will directly support achievement of the NNI Grand Challenges and will produce products and processes to significantly benefit all U.S. industry and society. Members of the Roadmap Steering Team, listed below, welcome the participation of all stakeholders in the next phase of this important national effort.

- Jack Solomon, Praxair, Inc., Steering Team Chair
- Susan Babinec, The Dow Chemical Company
- Frank DiStefano, Air Products and Chemicals
- Rajeev Gorowara, DuPont Company
- Catherine Hunt, Rohm and Haas Company
- Frank Lipiecki, Rohm and Haas Company
- James Murday, U.S. Naval Research Laboratory
- Frank Notaro, Praxair, Inc.
- Paul O'Connor, The Dow Chemical Company
- Bill Rafaniello, The Dow Chemical Company
- Sharon Robinson, Oak Ridge National Laboratory
- Judith Stein, General Electric Company
- Brian Valentine, U.S. Department of Energy

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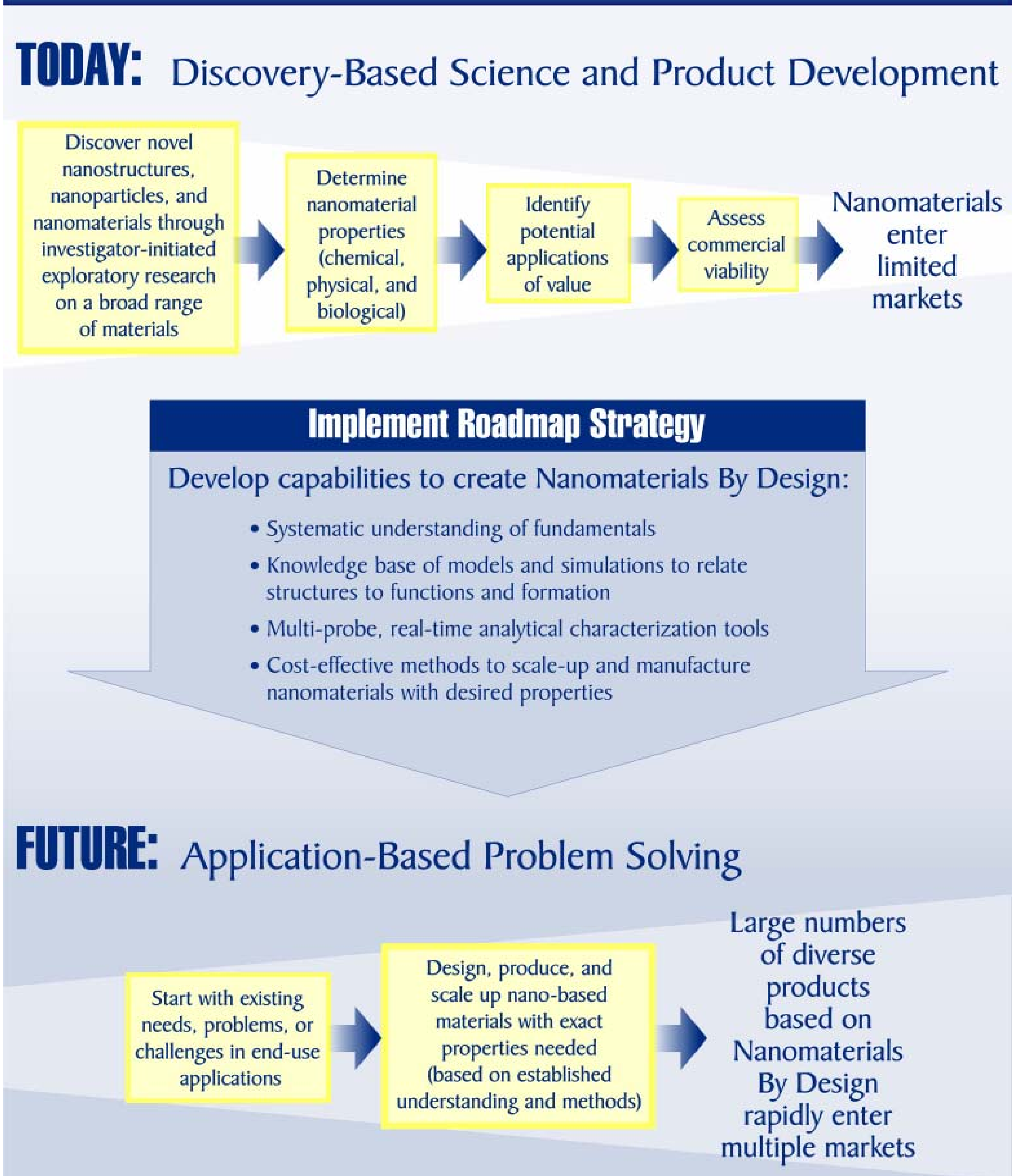
Exhibit 1: Nanomaterial Development Today and in the Future



Executive Summary

Nanomaterials present a tremendous opportunity for the U.S. chemical industry to introduce a host of new products that could energize our economy, solve major societal problems, revitalize existing industries, and create entirely new businesses. The potential economic and societal contributions of nanomaterials have prompted U.S. Federal agencies participating in the Nanoscale Science, Engineering, and Technology Subcommittee (NSET) and U.S. chemical companies of all sizes to commit significant resources to nanotechnology research and development (R&D). The race to research, develop, and commercialize nanomaterials is global. To remain competitive, U.S. stakeholders must accelerate nanotechnology development in important areas such as catalysts, separations, high-performance materials, coatings, energy conversion and storage, sensors, electronics, pharmaceuticals, and diagnostics.

> **Nanomaterials By Design**
> refers to the ability to employ scientific principles in deliberately creating structures with nanoscale features (*e.g.*, size, architecture) that deliver unique functionality and utility for target applications.

To realize fully the broad economic benefits of nanomaterials, U.S. stakeholders must invest in a new, *solution-oriented* approach to materials development—**Nanomaterials By Design.** This novel approach requires a robust understanding of the fundamental scientific principles operating at the nanoscale, including interdependent structure-property relationships. Such an understanding will enable cost-effective design, synthesis, and scale-up of materials that deliver selected properties, allowing material producers to focus on the *requirements for specific applications* as the primary drivers of the design process. The capability will accelerate nanomaterial development, moving the field from today's discovery-based science and product development to application-based problem solving in the future (as shown in Exhibit 1, see page 4).

Once the capability becomes available, large numbers of diverse products could rapidly enter global markets to solve long-standing problems and stimulate economic growth for decades to come. A library of nanomaterials and synthesis techniques could be established by 2020 for use by material producers and end users worldwide.

Vision of Nanomaterials By Design in 2020

The U.S. chemical industry will offer a "library" of diverse, high-quality nanomaterial building blocks with well-characterized compositions, stable architectures, and predicted properties. Safe, reproducible, cost-effective, and clearly defined manufacturing and assembly methods will be available to incorporate nanomaterials into systems and devices designed to perform specified functions while retaining nanoscale attributes.

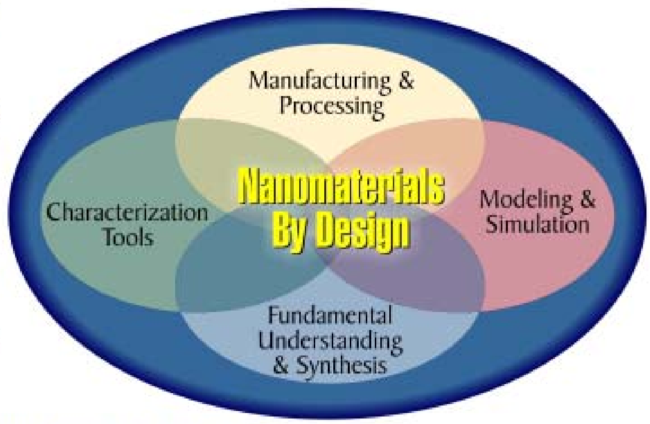
The scientific and engineering hurdles to achieving Nanomaterials By Design are enormous. Success will require significant changes in the approach to R&D (see Exhibit 2).

Exhibit 2: Required Changes in the Way Nanomaterial R&D Is Pursued

- Fundamental research must be pursued systematically to develop a complete understanding of the underlying principles of nanoscale physics and chemistry. This effort will build a solid foundation to enable deliberate material design. Systematic research to understand fundamentals and discovery-based R&D will proceed concurrently, each informing and benefiting from the other.

- The nature of working at the nanoscale dictates the need to simultaneously integrate R&D in fundamentals and synthesis, manufacturing, tools, and modeling. Breakthroughs in each area will provide capabilities to enable progress in other areas, ultimately leading to cost-effective manufacturing and integration into applications (i.e., from fundamentals to function). An exceptionally high degree of interdependent, multi-disciplinary R&D performed by diverse stakeholders is required, amounting to a cultural change in the way science and technology are pursued.

Implementation of Roadmap Strategy: Multidisciplinary, Interdependent, R&D Integrated From Fundamentals to Function



- Industry has unique expertise in application-based problem solving R&D, and should therefore help guide the direction of Federal R&D funding to implement this roadmap. Industry experts should continue to be actively engaged in identifying the scientific challenges and in planning R&D for Nanomaterials By Design.

The entire R&D effort must closely interweave developments in fundamental understanding of nanoscale properties, new synthetic methodologies, new manufacturing techniques, and new characterization and simulation tools. As shown in Exhibit 3, these concurrent, interdependent areas of R&D will also contribute to and benefit from developments in the critical research areas of safety, health, environmental impacts, standards, technology transfer, training, and infrastructure.

The priority, overarching research requirements are presented in Exhibit 4 along with expected time frames and recommended levels of investment. These requirements are discussed in depth in Section 3. Given the highly interdependent nature of the research, all of these R&D needs have a relatively high priority.

Representatives of universities, government laboratories, and industry provided input to the strategy, which is intended to

- assist the chemical industry in setting corporate R&D priorities,
- stimulate and focus university and government research,
- help guide NSET agencies to set funding priorities, and
- inform legislators and Administration officials in shaping public policy.

Recommendations for bolstering the effectiveness of the strategy are provided below. Targeted investments and a shared commitment among stakeholders are essential to attain the ultimate goal—**accelerated commercialization of innovative technology based on nanomaterials.**

Recommendations:

- Implement effective protocols to assure health and safety in nanomaterial R&D, production, transport, use, and disposal.
- Invest significantly and concurrently in the priority R&D areas—fundamentals, synthesis, manufacturing, characterization, and modeling.
- Facilitate intensive coordination and integration among these interdependent and multidisciplinary research areas.
- Encourage universities and government laboratories to conduct R&D that will systematically build an understanding of nanoscale fundamentals to enable application-based problem solving.
- Provide both large and small companies increased access to U.S. government funding for fundamentals in addition to applications R&D.
- Implement new strategies to build a shared-knowledge infrastructure.
- Provide industry access to national user facilities with equitable fees and ownership of intellectual property.
- Establish intellectual property policies at universities and government laboratories that create a more favorable climate for partnering with companies and for accelerating commercialization.
- Develop standards needed for research and commerce.
- Increase government funding in all physical sciences underlying nanotechnology.
- Work with NSET to develop an effective means of collaboration between NSET and the U.S. chemical industry to foster effective roadmap implementation.
- Encourage NSET to adopt this roadmap as a core strategy for its Grand Challenge in Nanostructured Materials by Design.

Exhibit 3: Essential Elements of the Research Pathway to Nanomaterials By Design

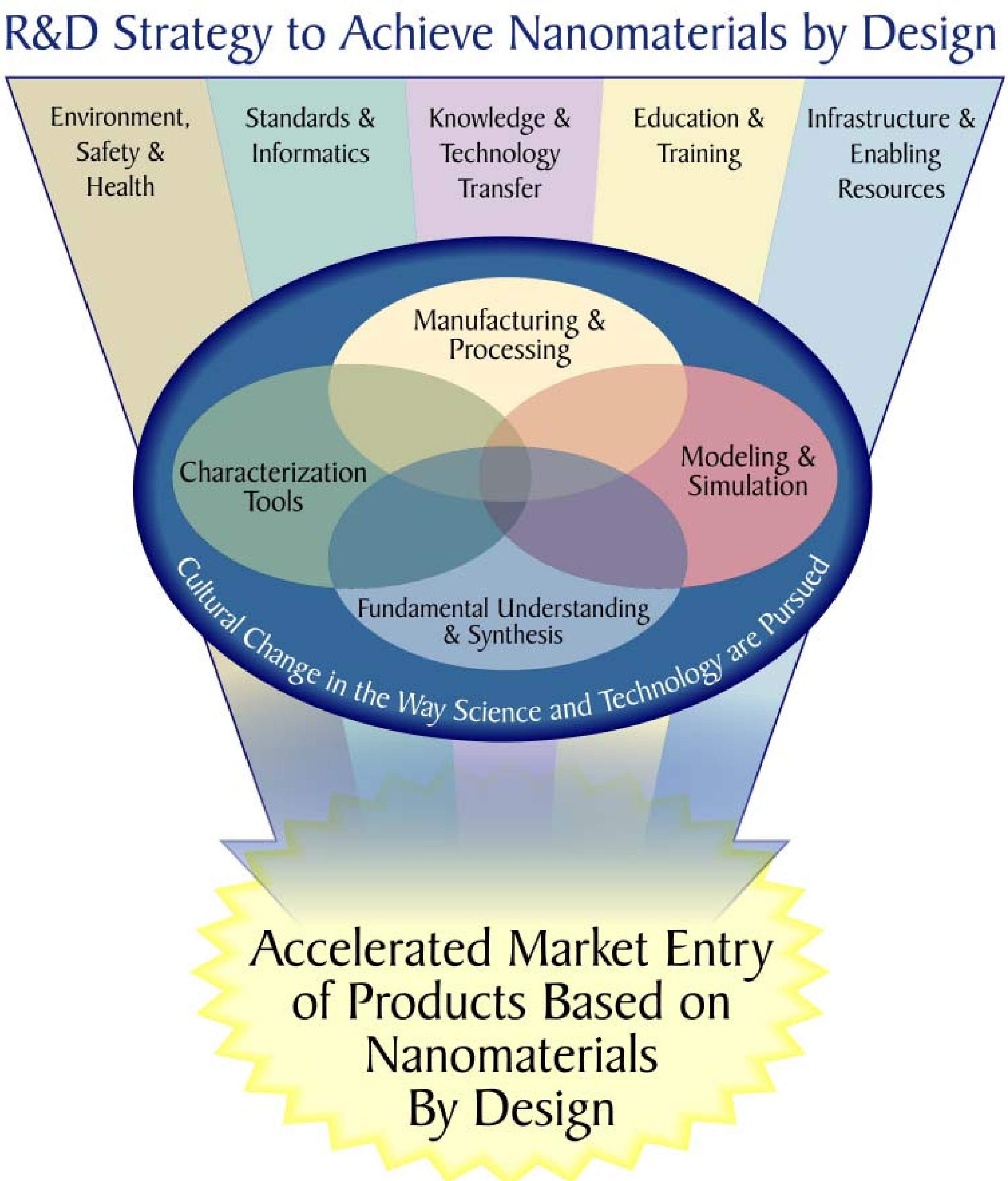


Exhibit 4: Priority Research Requirements for Nanomaterials by Design[1]

Research Requirement	Timeframe[2] (years)	Total Investment[3]
Fundamental Understanding & Synthesis		
★ Understanding of nanoscale structure-property-processing relationships		$$$$$
★ Experimentally validated models and theories of nanoscale physics and chemistry		$$$$$
★ New paradigms for creating nanoscale building blocks		$$$$
★ Design strategies for controlled assembly—nanocomposites, spatially resolved nanostructures		$$$$
★ High-throughput screening methods to determine structure-property relationships		$$$
★ Performance evaluation at the laboratory scale		$$$
● Compendium of methods to synthesize and assemble nanomaterials		$
Manufacturing & Processing		
★ Unit operations and robust scale-up and scale-down methods		$$$$
★ Manufacturing techniques for hierarchical assembly		$$$$
★ Dispersion and surface modification processes that retain functionality		$$
● Process monitoring and controls for consistency		$$$
● Integrate engineered materials into devices while retaining nanoscale properties		$$$
○ Impurity removal from raw material precursors		$
Characterization Tools		
★ Real-time characterization methods and tools		$$$$
● Infrastructure for tool development and use		$$
Modeling & Simulation		
★ Fundamental models to accurately predict nanostructure formation		$$$$
★ Bridging models between scales—from atoms to self assembly to devices		$$$$
● Infrastructure to support model advancement		$$
Environment, Safety & Health		
★ Assessment of human health and environmental impact hazards		$$$$
★ Determination of exposure potentials for nano-sized materials		$
★ Handling guidelines for operations involving nanomaterials		$
Standards & Informatics		
★ Standard procedures for nanomaterial synthesis		$
★ Reference materials for property measurement		$
★ Standard methods for physical and chemical property evaluation		$
★ Computational standards to improve information processing and transfer		$$
★ Standards for material evaluation in applications		$$
★ Standardized internationally recognized nomenclature		$
● Infrastructure to foster standardization		$$
Knowledge & Technology Transfer		
★ Technology transfer policies to foster commercialization		$$
● Infrastructure to encourage knowledge sharing		$
Education & Training		
★ Educated and trained workforce		$$
★ Greater public and industry awareness		$$
Infrastructure & Enabling Resources		
R&D areas above include these research requirements		

Priority Ranking: Importance to developing Nanomaterials by Design capability: ★ = Top ● = High ○ = Medium

1 The research requirements are discussed in depth in Section 3. The priority requirements shown here are a subset of the complete list, which can be found in the preliminary results from the "Nanomaterials and the Chemical Industry Roadmap Workshop." See www.chemicalvision2020.org/nanomaterialsroadmap.html.

Proposed starting point and duration of intense R&D efforts and investments required to make a significant impact. Ongoing activities would follow.

Cumulative investment for the duration of the R&D effort ($ to $$$$$) that considers the anticipated degree of difficulty, research duration, and infrastructure-related costs. Because of the staging and high interdependency of R&D tasks, the relative size of investment may not reflect the funding needs for a given year.

The U.S. Chemical Industry: Innovation & Value

- **The U.S. chemical industry serves a vital role in the national economy.**

  It is the world's largest chemical industry, generating more than 27% of the $1.53 trillion in world chemical sales. In the United States alone, there are 9,500 chemical companies and 13,000 operating facilities. These companies employ over one million people including 81,300 scientists and engineers engaged in R&D. Their scientific and technological innovations have led to new engineered materials and processes, which in turn propel the growth of the U.S. economy. The industry accounts for more than ten cents out of every dollar of exports and contributes $454 billion to the national GDP (12% of the total GDP).

- **The U.S. chemical industry improves our quality of life.**

  The industry transforms raw materials into intermediates and finished products that deliver tremendous benefits. These products are essential to key industries including health care, communications, food, clothing, housing, entertainment, electronics, and transportation. Every year, the U.S. chemical industry ships more than 70,000 diverse products that range from everyday items, such as toothpaste and batteries, to those used in such high-technology industries as electronics, biotechnology, and pharmaceuticals. Chemicals are an integral component of every product—even though their presence is not always obvious. For example, approximately $2,000 worth of chemical products are contained in or used in the manufacture of every automobile.

- **The strength and vitality of the U.S. chemical industry relies on innovation.**

  Every year, U.S. chemical companies invest over $26 billion dollars in R&D in order to create new products and processes to solve performance, safety, environmental, and efficiency problems in diverse industries. One clear indicator of this commitment is that the chemical industry accounts for one out of every four U.S. patents. Growing global competition has heightened the need to accelerate the development of new products for continued economic growth. New opportunities created through R&D are essential to helping the United States maintain and strengthen its position in world markets.

1. Introduction

Significant scientific and technological challenges must be overcome to realize the vast economic and societal benefits from Nanomaterials By Design.

Nanomaterials have generated tremendous interest because they present an opportunity to deliver unprecedented material performance. This opportunity is based on the unique properties (*e.g.*, magnetic, optical, mechanical, electronic) that vary continuously or abruptly with changes in the size of the material at the nanoscale (1 to 100 nanometers). These step-like changes in nanoscale properties suggest both enormous potential and challenges.

> **Nanomaterials By Design**
> refers to the ability to employ scientific principles in deliberately creating structures with nanoscale features (*e.g.*, size, architecture) that deliver unique functionality and utility for target applications.

To date, understanding of nanoscale materials and their properties has been achieved primarily through empirical or discovery-based research. While this approach will continue to make important contributions, the full understanding and development of nanomaterials will be accelerated by a systematic understanding of fundamentals (*i.e.*, chemistry and physics). In addition, the broadest and most efficient commercialization of nanomaterials will be realized by taking nanoscience to the next level: deliberate, predictive design and manufacturing capability based on the application of newly established scientific principles and focused on end-use functions. Working at the nanoscale offers the opportunity to fully exploit design and to more directly create materials with functions and properties needed to solve specific problems. This solution-oriented, "Nanomaterials By Design" approach will increase the efficiency of materials development, dramatically accelerating the commercial introduction of beneficial products.

> ***A Primer on Nanomaterials is presented in Appendix C.***
>
> **Nanometer:**
> One billionth of a meter, or about the length of ten hydrogen atoms side-by-side.

Opportunities

Nanomaterials present a tremendous opportunity for the U.S. chemical industry to generate new products that could energize our economy, solve major societal problems, revitalize existing industries, and create entirely new businesses. The ability to design materials with intrinsic properties tailored to the application opens important possibilities:

- Plentiful energy resources with significantly reduced environmental impact
- Enormously powerful computers that are easily portable
- Manufacturing equipment with vastly expanded service life
- Far more secure communications systems
- Detection and eradication of tumors that are only a few cells in size

Opportunities presented by nanomaterials have been widely documented, and examples of commercial successes appear in the media. Specific nanoscale properties are targeted for development based on their potential to address end-user needs in multiple markets, as shown in Appendix D. Virtually every market will feel the impact as nanotechnology breaks long-standing limits on materials-based performance.

The potential payoff is significant. CMP Cientifica, a nanotechnology business information company, estimates that by 2005 the nanotechnology market will reach $537 billion, driven by the material, semiconductor, pharmaceutical, and catalyst markets. These markets represent only a small portion of the markets that could be impacted by nanotechnology.[1] The National Science Foundation (NSF) projects that the worldwide nanotechnology market will surpass $1 trillion by 2015.[2] While projections of nanotechnology impacts are inherently speculative, the impacts are undeniably enormous. U.S. leadership in commercial development of nanomaterials will ensure a robust economy and growing standard of living for decades to come.

Examples of Commercialized Nanomaterials

- Catalysts in the petroleum industry
- Carbon black in tires
- Superlattices in optoelectronic devices
- Plasma spray of nanostructured coatings
- Nanocrystalline titanium dioxide in sunscreens
- Silver nucleation in photographic film
- Chemical mechanical polishing (CMP) slurries in the electronics industry

Examples of Emerging Nanomaterial-Based Technologies[3]

- **Stronger, less-expensive, high-strength steels:** Creep-resistant steel is so complex and costly to make that it is generally used only in applications like boilers and turbines in power plants. Researchers in Japan have found a way to make this steel with conventional processing methods using nanometer-scale carbonitride particles that migrate to vulnerable regions within the steel. The steel they have created takes twice as long to rupture as the most creep-resistant steel currently in use and will eventually be less expensive to manufacture.
- **Faster, smaller, safer gas sensor:** A nanotube gas ionization sensor built by researchers at the Rensselaer Polytechnic Institute could allow emergency crews to detect and identify gases swiftly in case of a terrorist attack. Traditional sensors take about five minutes to work and can be bulky (some measure 5 feet by 3 feet by 6 inches). The new device is not yet as sensitive as current sensors, but it is safer (uses lower voltage), provides instant results, and can fit in a half-inch cube.

Challenges

Nanomaterials By Design presents an immense research challenge. To realize the promise of nanomaterials, nanoscale components must be incorporated into larger-scale materials, products, and systems while retaining their novel attributes. A key challenge is to develop the capabilities (1) to precisely design and build nanoscale materials that will predictably exhibit desired properties and (2) to preserve those properties through cost-effective scale-up into safe, commercial materials that deliver needed functions.

An international race to research, develop, and commercialize nanomaterials is now underway. Governments and industry around the world are actively recruiting highly skilled researchers in the field and are investing heavily in nanotechnology—some at levels in excess of U.S. commitments. In 2002, Japan invested $900 million in nanoscience compared to $600 million by the U.S. government.[4] According to NSF, U.S. research lags behind in key areas: nanodevices, production of nanoscale instruments, ultra-precision engineering, ceramics, and other structural materials.[5] From 1992 to 2002, the number of nanotechnology patents worldwide grew by 229%. During this same time period, the U.S. share (by assignee) of these patents fell by 6%.[6] Strategic investments are needed to assure future U.S. competitiveness.

Success in the race to commercialization will require a large, highly integrated, multidisciplinary, national effort focused on predictive design and manufacturing. Nanomaterials By Design capability will require in-depth understanding of the chemistry and physics operating at the nanoscale and an extension of that understanding to the interrelationships among structures, properties, functions, and processing of nanomaterial systems.

The spectrum of invention needed for predictive design necessitates a set of parallel, highly interwoven activities oriented toward commercialization.

Bringing all of these research elements together at the required size scales will necessitate unprecedented levels of integration of multidisciplinary expertise. The R&D effort must closely interweave the concurrent development of our fundamental understanding of nanoscale properties, new synthetic methodologies, new manufacturing techniques, and new characterization and simulation tools—with the critical issues that pertain in all facets of the work: safety and health, environmental impact, standards, technology transfer, training, and infrastructure.

Strategic Approach to R&D

Given the magnitude of the research challenge and investment required to compete globally, U.S. Federal and academic research communities and chemical companies must work on all critical phases of R&D needed for early commercialization. All stakeholders must make significant, smart investments in R&D to commercialize Nanomaterials By Design within the next 10 years. Federal laboratories and university research centers must develop a knowledge base, and corporate researchers must have access to the information to expedite progress. New strategies to encourage partnering among companies (both large and small), universities, and Federal laboratories must be established to assure the greatest return from Federal investments. For their part, individual chemical companies will invest in fundamental and commercially oriented R&D as part of their own strategic plans to spur innovation and commercialize nanomaterial-based technologies in the near term and for the future.

Nanoscience must be well understood to accelerate its translation into safe, reliable, cost-effective products that will benefit society and the economy.

The chemical industry is ideally suited to help guide this national effort toward Nanomaterials By Design. The industry's unique role in the economy—adding value to raw materials and creating products to meet needs throughout society—has equipped it with vast scientific expertise, advanced manufacturing design capabilities, and detailed knowledge of product requirements in diverse applications. These qualifications are essential to understanding, coordinating, and integrating the complex array of necessary R&D efforts. With strategic investments, the market for nanomaterials will expand continuously over the next five years and will accelerate after that as predictive capabilities become more robust. This roadmap presents the recommended research pathway.

Sources:

[1] CMP Cientifica, *Nanotechnology: Atomic Engineering Presents Big Investment Opportunities*, www.angel-investor-news.com/ART_Nano.htm.

[2] National Science Foundation, *Social Implications of Nanoscience and Nanotechnology*, March 2001, p. 3.

[3] *New York Times*, July 22, 2003, p. D2-3.

[4] *The AMPTIAC Newsletter*, "The Coming Revolution—Science and Technology of Nanoscale Structures," Volume 6, Number 1, p. 7.

[5] National Science Foundation, *Social Implications of Nanoscience and Nanotechnology*, March 2001, p. 10.

[6] *Journal of Nanoparticle Research*, "Longitudinal Patent Analysis for Nanoscale Science and Engineering: Country, Institution, and Technology Field," Kluwer Acad. Publ., 2003, Vol. 5, Issue 3-4, p.8.

2. Vision for Nanomaterials by Design

By 2020, advances in nanoscience and nanotechnology will enable the routine and cost-effective use of nanomaterials to solve major problems, enhance the quality of life, and generate economic growth for the United States.

Science and technology are on the brink of a revolution. Over the next 10 to 20 years, major scientific, technical, and engineering breakthroughs in nanoscience and nanotechnology will redefine material functions and applications worldwide. Globally, these breakthroughs are expected to enable key advances in health care, such as targeted drug delivery, diagnostics, and biosensors; more efficient energy conversion devices, such as fuel cells, thermoelectric devices, batteries, and solar cells; and new materials to enable faster, cheaper, and smaller electronic devices and computers. To accelerate delivery of these potential economic and societal benefits, the U.S. chemical industry champions the development of a solution-oriented capability to produce Nanomaterials by Design.

Vision of Nanomaterials By Design in 2020

The U.S. chemical industry will offer a “library” of diverse, high-quality nanomaterial building blocks with well-characterized compositions, stable architectures, and predicted properties. Safe, reproducible, cost-effective, and clearly defined manufacturing and assembly methods will be available to incorporate nanomaterials into systems and devices designed to perform specified functions while retaining nanoscale attributes.

Nanomaterials designed from the "bottom up" will deliver the specific combination of functions needed for each application. Material developers of the future will identify the optimal material properties for each application, then select the appropriate building blocks and production technology to efficiently and economically produce the material with the desired properties and function.

Examples of Improved, Nanomaterial-Enabled Applications

- Catalysis
- Chemical Separations
- Drug or Gene Delivery
- Data Storage and Processing

Examples of Size-Dependent Nanomaterial Properties

- Electronic
- Photonic
- Magnetic
- Rheological
- Structural
- Mechanical

Vision of the Future

Revolutionary advances in science and technology will enable the solution-oriented design of nanomaterials. Enhanced understanding of physics and chemistry fundamentals at the nanoscale, combined with modern, robust, computational capability across length scales, will enable the directed design and synthesis of libraries of high-quality nanomaterial building blocks. Understanding of the fundamentals will assist in the development of models and tools, which will, in turn, help to verify the accuracy of that understanding. Knowledge of the relationships among structure, properties, functions, and processing methods will provide the basis for application-based nanomaterial design.

New paradigms for synthesizing nanomaterial building blocks will be established on the basis of thermodynamic and kinetic rules that accurately describe interactions between nanoparticles, nanoparticle-matrix interactions, and other relevant phenomena. Self-assembly and directed self-assembly methods will play routine roles in the synthesis and manufacture of nanomaterial-based products. Laboratory-scale synthetic methods will be scalable to facilitate cost-effective manufacturing. The assembly of building blocks will produce nanomaterials in technically useful forms, such as bulk nanostructured materials, dispersions, composites, and spatially resolved ordered nanostructures.

Advanced, multi-probe tools will be available to accurately measure desired properties on the nanoscale and provide real-time characterization of one-, two-, and three-dimensional nanostructures, including ensemble averages and number and type of defects. Metrology will be sufficiently advanced to validate those determinations. Robust tools will manage interfaces for property enhancement and manipulate nanostructures into predetermined two- and three-dimensional patterns.

Development of the Nanomaterials By Design approach will improve design efficiency and provide novel material solutions for use in diverse industries and applications.

Modeling and simulation efforts will link nanoscale properties to specific macroscopic properties across time and length scales. This will enable scientists to predict material function and systems from an understanding of the origin of nanoscale properties. Models will be used to foster the development of synthesis and assembly protocols that impart and preserve required functional properties at the application level. In addition, models will be used to define the functional needs and designs of nanostructures. Modeling and simulation of atomic, molecular, and nanostructure behavior will be extended to observable meso- and macro-scale properties to increase the efficiency of future research and reduce the number of design iterations and experiments as well as the number of tools required for design.

Concurrent developments will deliver multiple benefits:

Nanomaterials will deliver new functionality and material options. Libraries containing a diverse range of nanomaterial building blocks with well-defined properties and stable compositions will enable the confident design of nanomaterials that provide levels of functionality and performance not available in conventional materials. Manufacturers will combine the benefits of traditional materials and nanomaterials to create a new generation of nanomaterial-enhanced products that can be seamlessly integrated into complex systems. In some instances, nanomaterials will serve as stand-alone devices, providing unprecedented functionality.

Customized material solutions will lead to a quantum leap in performance. As customers continue to raise their expectations of product performance, predictive nanomaterial design capability will enable manufacturers and fabricators to define their application specifications and work with material suppliers to select the optimal solution. The industry will have the technical capabilities to allow customers to specify through computer models and simulations the exact composition of a system to better meet technical requirements. Designers will specify precise material locations, creating functionally gradient materials, layered materials, hybrid compositions, and virtually any other configuration that will provide value in the final product. This engineering flexibility will allow systems and products to offer performance, customization, and value that cannot be realized *via* any other process.

New synthetic strategies and design paradigms based on first principles for market-driven applications will allow the U.S. chemical industry to sustain leadership in existing markets, enter new markets, and retain global competitiveness.

Advanced manufacturing will maximize efficiency, flexibility, and value. The industry will deliver nanomaterial systems using revolutionary, cost-effective production capabilities. Manufacturing methods will allow the translation of unique nanomaterial properties through to the finished devices. Materials will be manufactured with precise control of defect quantification and location. Self-assembly processes will be employed wherever possible to reduce the cost of manufacture. Raw material volumes, byproducts, and wastes will be significantly reduced, eliminated, or produced in a manner that minimizes environmental impact. Nanomaterial manufacturing will produce new and improved materials that provide superior life-cycle benefits. Devices will be net-shaped and highly complex in a wide variety of sizes. Coupling nanomaterials and device design with advanced production capability will allow companies to offer nearly limitless options and high value to customers. Systems will be manufactured quickly, economically, and accurately to maintain cost-effectiveness. Manufacturing flexibility will allow mass customization, providing the economic and time-to-market benefits of full-scale manufacturing while offering limited production runs of specialty systems. Cost-benefit and life-cycle analysis will illustrate the value of nanomaterials in comparison to traditional materials and designs.

Innovation will create value and drive market growth. The market penetration of nanomaterials will expand continuously over the next five years and will accelerate after that as predictive capabilities for nanomaterial design become more robust. Successful demonstrations will foster use of nanomaterials in increasingly diverse applications.

New approaches will be available to develop, manage, and share intellectual assets. New knowledge gained through pre-competitive R&D at chemical companies, universities, national laboratories, and government centers will continuously expand understanding of nanoscale-to-macroscale phenomena. A national data and information repository will be available to everyone. Modified patenting and licensing practices will foster better utilization of publicly funded research results and facilitate rapid transition of knowledge into the industrial sector. Strategies for collaboration such as mutually beneficial partnerships between academia, government, and industry will accelerate commercialization of nanomaterial-based products. Government support will enable academia, national laboratories, and industry to pursue fundamentals-to-application research in nanomaterials.

Both large and small corporations, companies that supply materials and those that supply total technology solutions, will create value through nanoscience and nanotechnology advances. Chemical companies will leverage knowledge acquired from R&D at universities, national laboratories, government-funded centers, and internal R&D efforts. Collectively, companies will fill distinct markets and contribute to the development of the future economy. The U.S. government will provide incentives to large and small manufacturing organizations equitably, as appropriate, to facilitate potential value-generating activities.

Value and supply chain will be integrated seamlessly from suppliers to end users. Chemical companies will work collaboratively with suppliers and end users to design materials from fundamentals. Information technology, total process modeling, and e-business will link all parts of the value chain. A customer's system specifications will be communicated to nanomaterial producers, tooling and equipment suppliers, and device fabricators to expedite the delivery of tailored solutions.

The safety of nanomaterials will be well established and accepted widely. Nanomaterials will be produced in volume and used without detriment to animals, people, or the environment. The public will be knowledgeable about nanomaterials and how they benefit society. Public opinion of nanotechnology will be based upon factual material provided by the scientific and technical community and by the manufacturing industries. Manufacturers will understand the value of nanomaterials and preferentially employ them in new product design.

Nanotechnology will evolve into a full-fledged academic field. Nanotechnology will be a well-developed sub-discipline with clearly established fundamental principles of design, synthesis, engineering scale-up, and safety. Undergraduate and graduate-level textbooks will include nanoscale fundamentals and specialized courses will be offered on most campuses. Nanomaterial science and technology will be a recognized sub-discipline of advanced degrees in science and engineering. K-12 education will emphasize the role of nanotechnology in enhancing our quality of life.

3. R&D Strategy to Achieve Nanomaterials by Design

Developing a solution-oriented, nanomaterial design capability involves unique challenges requiring the integrated, simultaneous research of fundamentals and synthesis, manufacturing, tools, and models; this strategic R&D approach greatly intensifies the need for coordination and integration among diverse disciplines and research performers.

Major scientific and engineering breakthroughs will be required to deliberately design and manufacture materials specifically tailored to application requirements. These breakthroughs hold the potential to enable the next industrial revolution. The benefits of nanotechnology are already becoming evident, and both the public and private sectors can appreciate the value of steering nanoscience in a direction that could ultimately maximize its beneficial impacts on our economy and society.

The potential economic and societal contributions of nanomaterials have prompted the Federal agencies that are participating in the U.S. National Nanotechnology Initiative and U.S. chemical companies of all sizes to commit significant resources to nanomaterial R&D. However, a much larger and more strategic investment is required. Given the magnitude of the challenge and the global race for leadership in nanomaterial development, smart, targeted investment is imperative.

To build investor confidence and attract additional funding from the public and private sectors, representatives of universities, government laboratories, and industry have mapped out a strategic approach to focus technology investment. This technology roadmap will help to ensure that investments target the most critical needs for attaining the ultimate goal—accelerated development and commercialization of nanomaterials.

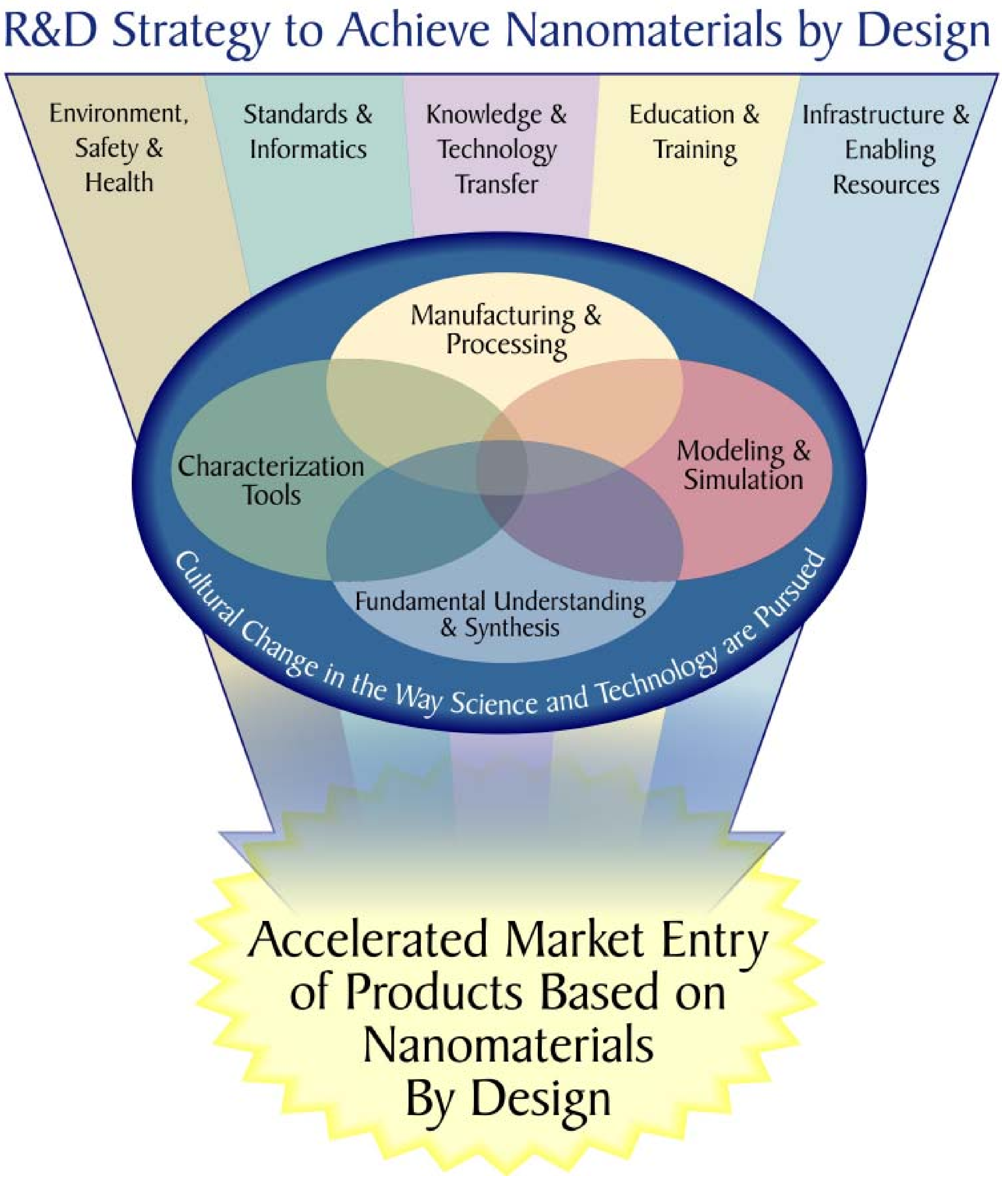
R&D Strategy

Developing the fundamentals-to-function research approach will require a cultural change in the way science and technology are pursued. Nanomaterials By Design is a uniquely solutions-based goal. It will yield a new set of tools that can provide nearly limitless flexibility for precisely building material function around the application. Such a powerful, function-based design capability holds the potential to solve critical, unmet needs throughout society. As shown in Exhibit 5, achievement of this ambitious goal demands a novel strategic approach that includes R&D and supporting activities. As shown in the exhibit, Nanomaterials By Design will require concurrent development of nanoscale fundamentals and synthesis, methods of manufacturing, multi-probe measurement tools for the nanoscale, and reliable models relating nanostructures to properties.

Nanomaterials By Design

As defined in the Introduction of this document, this phrase reinforces the preeminent role of function, *i.e.*, identifying functional needs in specific applications initiates the process by which nanomaterial-enhanced materials are conceived, designed, and produced.

Exhibit 5: Essential Elements of the Research Pathway to Nanomaterials By Design



Additional supporting activities must address environmental impacts, safety and health, standards, technology transfer, infrastructure, and education.

The ability to discern, manipulate, and assemble material at the nanoscale offers the unprecedented opportunity to design and build materials that exhibit functions tailored to specific applications. The imperative to achieve the full societal and economic benefits of nanomaterials mandates a shift from heuristic or discovery-based investigations toward disciplined development of predictive design capability. This development effort mandates a cultural change in our approach to materials production and its application to problem solving. Decisions relating to structure, composition, and other function-determining properties of materials will be made increasingly on the basis of models. Model development will require quantum leaps in fundamental scientific understanding of nanomaterials and in the ability to both observe and simulate behavior at the atomic and nanoscales. Success in attaining these objectives will require extraordinary levels of cooperation and knowledge sharing across scientific and technical disciplines.

Nanomaterials By Design will require an exceptionally high degree of solution-oriented, interdependent, multidisciplinary R&D that amounts to a cultural change in the way science and technology are pursued.

End users and developers of nanomaterials must collaborate effectively in all phases of R&D, from fundamentals through integration into end-use applications. An end-use focus will guide the direction of research and ensure that design issues are identified early. Involvement of academic and government researchers in these interactions is important to ensuring that R&D activities build the needed foundation in nanoscale science and technology. In addition, partnerships with suppliers will serve to ensure the availability of raw materials. Ultimately, chemical companies will be seamlessly integrated with end users to provide cost-effective nanomaterial solutions.

A range of researchers with diverse expertise and R&D objectives is essential to developing Nanomaterials By Design capability. Each type of researcher fills a unique niche and offers a unique orientation and perspective that should be considered in the development process. Effective R&D for Nanomaterials By Design will require close collaboration among researchers and stakeholders from all of the following types of organizations:

- Chemical companies of all sizes
- Suppliers of specialty, bulk, and reference materials
- Equipment and software manufacturers including suppliers of analytical tools
- Companies with specialized expertise, experience, and/or research facilities
- Universities, especially those with nanotechnology centers
- National laboratories, especially those with nanotechnology centers
- Government research organizations and facilities across Federal and State agencies
- Independent, non-profit research organizations
- Industrial end users and consumers of nanotechnology and related information

Essential Enabling R&D

The nature of working at the nanoscale dictates the need to simultaneously integrate R&D in fundamentals and synthesis, manufacturing, tools, and modeling. Breakthroughs in each area will provide capabilities to enable progress in other areas. The interdependency among this research is suggested by the overlapping circles in Exhibit 5 and further described below:

- **Fundamentals Underlie Functionality.** Predictive design will require a tremendous growth in understanding of chemistry and physics at the nanoscale. A full understanding of these fundamentals and how they control functionality will enable the design, control, and delivery of tailored functions to enhance material performance at the applications level.

- **Manufacturing Imparts and Preserves Function.** The process of "manufacturing" or scaling the material to the macro or applications level must preserve the specialized functions available at the nanoscale. A variety of processes (including self-assembly) will likely be needed to cost-effectively produce diverse nanomaterials. Size, composition, geometry, impurity levels, and other attributes must be pre-determined and subsequently tightly controlled at unprecedented levels. These processes are critical as nanomaterials are often unstable and may be sensitive to the surrounding environment. This sensitivity mandates that manufacturing considerations pervade the research from the exploration of fundamentals onward.

  Biological systems found in nature demonstrate complex processes that use nanoscopic control to generate macroscopic architectures (seashells are one example). Bio-inspired manufacturing processes could be developed and used to control design for function and self assembly from the nanoscale to the macro level.

- **Multi-Probe, Real-Time Analytical Tools Enhance Understanding.** Since the precise placement of atoms determines material function and performance, nanoscale tools are needed to examine nanostructures and ascertain multiple characteristics in real time. Such highly sensitive tools will expand understanding of nanomaterial fundamentals. This enhanced understanding will allow the construction of accurate models and guide manufacturing. Tools will subsequently verify that the resulting nanomaterials exhibit the desired application-defined design characteristics.

- **Modeling Enables Design and Manufacturing.** Increased understanding of fundamentals at the nanoscale will enable the construction of accurate models to test theories and guide tool development. Eventually, knowledge of nanoscale relationships will enable modeling of manufacturing processes to impart and preserve desired properties and functions.

Essential Activities to Support R&D

As indicated in Exhibit 5, the four key integrated R&D areas must also draw upon and contribute to a wide range of supporting activities to enable effective and early market entry:

- **Environmental, Health, and Safety.** The toxicological, epidemiological, and environmental impacts of nanomaterials must be fully understood and controlled. Safety concerns can constitute a major hurdle to commercial viability and market acceptance.

- **Standardization and Informatics.** Internationally recognized reference materials for calibration, standard methodologies, computational standards, and terminology regarding nanomaterial attributes will enable clear communication among researchers from various disciplines and will facilitate commerce. Informatics R&D is needed for tool and model development (*e.g.*, protocols, data acquisition, interpretation, and dissemination).

- **Knowledge and Technology Transfer.** Information sharing and effective transfer of technical knowledge among researchers will expedite progress immeasurably. Universities and national laboratories may play key roles in developing and maintaining information centers.

- **Infrastructure and Enabling Resources.** A broad array of facilities, services, networks, tools, and other resources is needed to facilitate research and commerce, and to promote collaboration, efficient information management, and technology transfer.

- **Education and Training.** Initiatives are required to attract and prepare the workforce of the future and to promote public awareness of nanoscience and technology.

While the ability to observe, characterize, and manipulate matter at the nanoscale can be accelerated by a cultural shift in R&D, the transition will necessarily be gradual. The requirements for new knowledge and new capabilities are vast. Intense resolve and cooperation across a wide spectrum of stakeholders will be crucial in achieving ultimate success, and in generating useful contributions along the way.

The strategy proposed by this roadmap—*Nanomaterials By Design*—should accelerate the early market entry of nanomaterials into the widest possible spectrum of commercial applications, facilitate the culture shift needed to maximize the national benefit from nanomaterials, increase the efficiency of future nanomaterial development, and provide the most rapid return on investment. The key priorities and critical needs of this strategy are mapped out in the following sections:

- ❒ **Fundamental Understanding and Synthesis**
- ❒ **Manufacturing and Processing**
- ❒ **Characterization Tools**
- ❒ **Modeling and Simulation**
- ❒ **Environment, Safety, and Health**
- ❒ **Standards and Informatics**
- ❒ **Knowledge and Technology Transfer**
- ❒ **Education and Training**
- ❒ **Infrastructure and Enabling Resources**

Fundamental Understanding and Synthesis

The production of nanomaterials in a controlled and predictable way will require both a fundamental understanding of nanoscale properties and new paradigms for synthesis. Fundamentals provide the rules of nanoscale chemistry and physics that will enable synthesis of nanomaterials with predictable properties and the ability to integrate material over several length scales. Understanding the fundamental relationships between structure, properties, and reactivity will provide a foundation to significantly expand nanomaterial development. Conversely, synthesis of these nanomaterials based on the predictive design rules will validate the understanding of fundamentals. These are inextricably intertwined fields and together they provide the foundation for nanomaterial manufacturing.

Adopting this methodical, predictive approach based on fundamentals will accelerate nanomaterials development and applications in which properties are designed in zero, one, two, and three dimensions (*e.g.*, dot, wire, layer, and structure) and integrated into larger structures. Predictive design is essential to address the increasing complexity of materials in the progression from nanoparticles to dispersions, to composites and finally, spatially resolved, ordered nanostructures.

Fundamentals
are the principles of chemistry and physics that govern behavior of nanomaterials such as thermodynamics and kinetics.

Synthesis
is the process that combines and isolates nanomaterial building blocks to create more complex nanomaterials.

Disciplines and skills needed:
chemistry, chemical engineering, analytical chemistry, computational chemistry, physics, biology, mechanical engineering, electrical engineering, and manufacturing engineering.

Development of fundamentals and methods of synthesis will require characterization tools and modeling breakthroughs. New characterization tools will enable researchers to observe and characterize events at the nanoscale. Modeling capabilities will provide greater flexibility for validating fundamentals based on experimentation. Ultimately, the capability to successfully predict—from first principles—structure-property relationships (*i.e.*, how various components of nanomaterials react to one another) will increase reliance on modeling and simulation, as required for cost-effective commercial production.

In addition, research must focus on extending and applying fundamental knowledge to the development of scaleable, cost-effective nanomaterial synthesis; manufacturing processes; and the integration of nanomaterials into final products. Toolkits based on fundamentals are needed for the design and synthesis of nanomaterials with unique properties and for estimating the commercial merit in a target application. Laboratory-scale validation of performance must ensure that nanomaterials and higher order materials containing nanomaterials deliver desired functions.

R&D Priorities

Develop Fundamental Understanding of Physics and Chemistry at the Nanoscale

The largest barrier to rational design and controlled synthesis of nanomaterials with predefined properties is the lack of fundamental understanding of thermodynamic and kinetic processes at the nanoscale. Today, the principles of self assembly are not well understood nor do we have the ability to bridge length scales from nano to micro to macro. This lack of basic scientific knowledge regarding the physics and chemistry of the nanoscale significantly limits the ability to predict *a priori* structure-property-processing relationships. Profitable research will result in the development of kinetic and thermodynamic rules for synthesis and assembly that can be applied to the rational design of nanomaterials at commercial scales (including hierarchical nanomaterials) from first principles.

R&D PRIORITY

Develop a fundamental understanding of structure-property-processing relationships at the nanoscale

Bulk material properties are not size-dependent. In comparison, the properties of nanomaterials are a function of size and at present cannot be accurately predicted for all sizes, structures, and compositions. The underlying principles governing the properties at all lengths, organizational complexity, and structural and property stability over time must be understood to enable the nanoscale materials by design approach. To achieve this goal, model compounds will need to be synthesized for the sole purpose of studying structure-property relationships.

Priority: Top

Timeframe: 20 years

Impacts:

- Enhanced understanding of structure-property relationships redirects R&D continuously *(ongoing)*
- Enabling capability provided for nanomaterial development *via a priori* prediction of structure-property relationships *(years 10-20)*
- Database details structure-property relationships at all length scales *(years 10-20)*

Key Challenges

Currently, material properties cannot be predicted across length scales. This will require an understanding of the laws that govern physical scaling. Nor do we understand relationships between nanostructural precision and properties. Specifically, does the building block need to be totally perfect or can it contain multiple domains? If multiple domains are acceptable, what determines the requisite length scales and what dictates their relative orientation to each other? What are the tolerance limits for defects? Researchers must determine the extent and reason for fluctuations of properties, and the fundamental limits in producing materials that have effectively "identical" structures. The impact of nanoparticle surface structure and composition on the chemical and physical properties also is not understood. New characterization, measurement, and simulation probes that can resolve all critical properties at the nanoscale are essential to this research.

Critical Needs

- Understand the origin of unexpected nanoscale behavior and develop the ability to predict behavior for properties such as:
  - Hardness and ductility
  - Electronic and optical properties
  - Mass transport
  - Reactivity
  - Catalytic properties
  - Thermoelectric and piezoelectric properties
  - Magnetic properties

R&D PRIORITY

Develop models, theories, and experimental validation of physics and chemistry at the nanoscale, including kinetic and thermodynamic principles guiding synthesis and assembly

The base set of fundamentally distinct assembly processes, their kinetic and thermodynamic limits, and the engineering scale-up implications must be understood. In many instances, synthesis and assembly may occur in one process step.

Priority: Top

Timeframe: 15 years

Impacts:

- Database of key nanomaterial properties *(years 10-15)*
- Toolkit of kinetic and thermodynamic rules for synthesis and assembly *(year 15)*

Key Challenges

Research must determine the minimum number of fundamentally distinct assembly processes, as well as their kinetic and thermodynamic constitutive elements. Phase transitions of nanoscale materials are not understood. Experimental validation of nanoscale properties and mechanisms may require development of new nanoscale characterization tools.

Critical Needs

- Development of phase diagrams for nanostructured materials to control composition and phase of nanomaterials
- Basic knowledge of self-assembly processes, particularly those governed by noncovalent forces (*e.g.*, understanding biological processes such as molecular recognition and templated synthesis and translation of these principles to man-made systems)
- Understanding of nucleation, growth, and disassembly mechanisms
- Development of mechanisms controlling interfacial interactions in the production of nanoparticles (non-agglomeration), dispersions, nanocomposites, and ordered, spatially-resolved nanostructures—especially understanding defect control and placement, uniformity and control, particle size control, and integration of dissimilar materials such as organic/inorganic/biological composites
- Understanding of mechanisms controlling heterogeneous integration across time and length scales

- A database of key nanomaterial properties (*e.g.*, physical, chemical, mechanical) that compares performance to bulk materials. This dataset will reveal unexpected similarities, differences, and unique attributes within groups of building blocks and assemblies. The database will allow determination of the minimal set of fundamental building blocks with distinct properties so that the lowest common structural denominator for a given property may be ascertained
- A toolkit of kinetic and thermodynamic rules for synthesis and assembly which researchers can use to rationally design nanomaterials from first principles

Develop Synthetic Strategies for Rational Nanomaterial Design

Today, bulk materials are based on covalent and ionic interactions. In the future, assembled nanomaterials will be formed by controlling the entire range of forces from covalent to dispersive and non-covalent. Therefore, new cost-effective, predictable, reproducible, and scalable methods for synthesis are needed to supply nanomaterials for commercial applications.

Challenges with current synthetic methods include the control of defects, particle agglomeration, inhomogeneities of composition and size distribution, and the lack of cost-effective, controllable synthetic methods amenable to scale-up. Both top-down (*e.g.,* molecular imprinting, optical lithography, E-beam lithography) and bottom-up (*e.g.,* aligned arrays, directed self-assembly, templated synthesis) assembly processes are used to synthesize nanocomposites and ordered nanostructures, but only with limited success. For example, the current technical capability for lithography at 30 nm resolution is two dimensions (2-D) with limited capability for three dimensions (3-D). Bottom-up assembly can create features from 1-100 nm in both 2-D and 3-D. However, the ability to maintain order over long distances is limited.

R&D PRIORITY

Develop new paradigms for creating nanoscale building blocks based on understanding physics and chemistry at the nanoscale

Currently, nanomaterial synthetic development occurs through an inefficient heuristic approach. Development of reproducible synthetic methods in which defects, composition, size, and order are controlled *via* an understanding of nanoscale first principles of chemistry and physics would greatly increase the commercial opportunities for nanomaterials.

Priority: Top

Timeframe: 15 years

Impacts:

- New synthetic methods available based on the understanding of nanoscale physics and chemistry *(years 5-10)*
- New materials not previously imagined are commercially feasible and cost-effective *(years 10-15)*

Key Challenges

Synthesis of nanomaterials such as quantum dots, block copolymers, and dendrimers is expensive and difficult to reproduce. Scientists do not know how to functionalize surfaces reproducibly in order to control interfacial interactions and agglomeration. New tools and processes are therefore needed to characterize the nanostructure and nanoscale properties, and to correlate macro to the nanomaterial properties as a function of the synthetic approach. Impurities, differences in defect concentrations, domain sizes, *etc.* that influence the properties of the nanomaterials are a function not only of the structure but also of the synthetic process. The effect of the synthetic approach on macro properties must be determined. The stability of the materials and assemblies over time must also be considered a function not only of structure but also of the synthetic process.

Critical Needs

- Develop new catalysts for nucleation, growth, and disassembly of nanostructures
- Develop methods to reliably and easily functionalize surfaces to control interfacial interactions and agglomeration

R&D PRIORITY

Develop new design strategies and paradigms for the controlled assembly of nanocomposites and spatially resolved nanostructures with long-range order

Priority: Top

Timeframe: 15 years

Impacts:

- Knowledge of parameters governing self-assembly *(years 10-15)*

Biological assembly demonstrates the incredible complexity and function that can be achieved by self-assembly of only a few fundamental building blocks. Unfortunately, the timescale for biological self-assembly and, in some cases the concomitant properties, are commercially unacceptable. The fundamental and practical limitations of existing processes for assembling basic nanomaterial building blocks must be understood. In addition, new design strategies and paradigms need to be developed and scrutinized.

Key Challenges

The ultimate challenge is to produce cost-effective assembled products that offer increased functionality. This will require reproducible and precise control of nanostructure size and placement, and an understanding of rate and transport limitations on assembly kinetics for each approach. Current methods to achieve long-range order are either too expensive or do not produce order over the necessary distances.

Critical Needs

- Develop new bottom-up methods based on exploitation of biological principles such as molecular recognition and templated synthesis, as well as supramolecular chemistry
- Develop methods to integrate across length and time scales with dissimilar materials (hierarchical heterogeneous integration)

R&D PRIORITY

Develop new high-throughput screening methods to determine structure-property relationships

Combinatorial chemistry has gained global acceptance for its ability to provide "out-of-the-box" materials solutions to well-studied challenges in chemistry and biology. This technique provides insights in a time frame that is significantly shorter than traditional investigation paths. High-throughput nanoscreening has tremendous potential to reveal unique structure-property relationships and to identify new synthesis strategies.

Priority: Top

Timeframe: 10 years

Impacts:

- New high-throughput screening methods *(years 5-10)*
- New synthetic strategies *(years 5-10)*
- New materials obtained via high-throughput screening *(year 10)*
- New rapid, highly efficient, parallel methods for analysis of nanoscale properties *(year 10)*

Key Challenges

New synthetic strategies for identified building blocks and assemblies that are amenable to combinatorial screening need to be developed. This will require new processes for manipulation of building blocks. New analytical methods will also be necessary, while existing analytical processes for understanding nanoscale properties will need to be applied cost-effectively to high-throughput methodology.

R&D PRIORITY

Determine nanomaterial performance at the laboratory scale

To validate the performance of nanomaterials, target applications need to be identified, and the nanomaterials must be tested to see if they satisfy application-specific design criteria. Successful laboratory validation of performance will provide information needed to accelerate the commercialization of products containing nanoscale materials. At first, nanomaterials will be employed using current design criteria. Later, a quantum leap in the benefit of nanomaterials will be realized when the unique functions of nanomaterials drive new and novel device architectures. The ultimate goal is the utilization of a total systems approach where device design and nanomaterial design are performed concurrently in an iterative real-time process.

Priority: Top

Timeframe: 20 years

Impacts:

- Total systems approach to Nanomaterials By Design is consistently employed to accelerate commercialization *(years 15-20)*

Key Challenges

A major challenge is to develop relationships between the structure of nanomaterials and material performance in applications. Knowledge is limited regarding how to "design" nanostructures, a step which must precede the next level of complexity—device fabrication based on unique nanomaterial attributes. Protocols for the evaluation of nanomaterials in applications and multidisciplinary evaluation teams are needed. Chemists, electrical engineers, mechanical engineers, and chemical engineers must find a common knowledge base and language. In some cases, additional boundaries must be crossed. For example, one institution may develop a nanomaterial, another may manufacture the nanomaterial, and another may use it in an application.

The first step in reaping the commercial benefits of Nanomaterials By Design will be to use these materials in specific applications. This will require development of protocols for application-specific targets as well as research on structure-performance relationships in real-world applications.

A new way of thinking about value creation using nanomaterials is needed, which will require unprecedented research collaboration between the end user and the material manufacturer. This communication between the researchers and end users is required to generate valid laboratory screening protocols. Materials researchers and applications researchers will have to collaborate to develop new materials and device designs.

Critical Needs

- Screen nanomaterial performance in applications at the laboratory scale
- Develop device and application design concepts and paradigms based on exploitation of the properties of the nanoscale
- Develop systems approaches to enable new, paradigm-shifting applications using nanomaterials

R&D PRIORITY

Develop a compendium of methods to synthesize and assemble nanomaterials that will perform pre-determined functions in specific applications

A number of real-time techniques must be developed and implemented to accelerate synthesis of nanomaterials with pre-determined structure, function, and purity. Nanosynthetic methods must be rigorously defined to provide a reference for both laboratory researchers and manufacturers similar to small molecule compendia that are used by the synthetic community today.

Priority: High

Timeframe: 20 years

Impacts:

- A peer-reviewed compendium of synthetic methods *(years 3-5)*
- Significant documentation of peer-reviewed synthetic methods available *(year 20)*

Key Challenges

Currently, the ability to synthesize nanomaterials with reproducible defect control, purity, and structure is limited. Because the properties of nanomaterials depend on the nanomaterial's structural integrity, it is imperative that reproducible methods for synthesis of nanomaterials be developed and disseminated *via* peer-reviewed compendia.

Manufacturing & Processing

Manufacturing and Processing

Nanomaterials and products containing nanomaterials (*e.g.*, nanotubes, inorganic powders, organic films, and coatings) are manufactured today with traditional manufacturing techniques and unit operations. These nanomaterials are prohibitively expensive for many applications due to high capital costs and low production volumes. Furthermore, byproducts, wastes, and impurities hinder commercial applications. Significant academic research is leading to discoveries of new materials. However, researchers are not focused on the requirements posed by scalable, cost-effective manufacturing. Robust and reliable production methods—consistently and correctly controlled at the atomic scale—are needed to significantly expand the commercial use of nanomaterials. In addition, production must be accomplished in a safe, environmentally friendly manner.

Successful implementation of nanotechnology will require a strong commitment to process innovation (manufacturing). The traditional focus on materials science alone will not provide the breakthroughs needed to extract the full benefits of nanotechnology. Research to understand what material structures are required for a specific application must be developed concurrently with new processing capabilities. Biological systems found in nature provide excellent examples of highly controlled and organized architectures that generate complex materials. Developing similar controlled manufacturing capabilities will require a significant research effort with close interactions among diverse disciplines.

Inherent in nanoscale manufacturing is the need to preserve the specialized functions available at the nanoscale during manufacturing and scaling the material to the macro or applications level. A variety of new processes (including self-assembly) will likely be needed to cost-effectively produce diverse nanomaterials. These processes are critical, as nanomaterials are often unstable and sensitive to the surrounding environment. This sensitivity mandates that manufacturing considerations pervade research from the exploration of fundamentals onward. Fundamental knowledge of both physical properties and chemical reactivity at the nanoscale will be necessary to manufacture nanomaterials and ensure their integrity in storage and use. For example, particles at the nanoscale may exhibit lower sintering temperatures, greater reactivity in aqueous media, or greater inter-particle attractive forces that mandate surface passivation and unique stabilization chemistry.

The application of new fundamental knowledge and synthetic inventions is essential to process development but will be limited by the constraints posed by the manufacturing environment. For example, leveraging fundamental knowledge of particle nucleation, growth kinetics, and aggregation phenomena can lead to processes with superior particle-size control and obviate the need for downstream classification steps. This is imperative because extensive classification of nanoparticles needed to achieve discrete particle size ranges is economically impractical.

Manufacturing converts raw materials and precursors safely and reliably into intermediates, finished materials, components, and devices.

Nanomaterial manufacturing involves production of products or devices with materials that have one or more dimensions less than 100 nm.

Processing is a method of operation used to produce materials and devices.

Disciplines and skills needed: chemistry, analytical chemistry, toxicology, chemical engineering, environmental engineering, and mechanical engineering.

Product consistency during scale up—from lab scale, to pilot scale, to commercial units—is essential for commercial success. Material samples for customer evaluation must be produced at the lab or pilot scale to control capital costs. However, customers must be assured that identical products can be made in a full-scale commercial unit. Mitigating the risk for both the manufacturer and the customer is critical to getting nanomaterials into application evaluations as quickly and expansively as possible. Easy access to specialized user facilities where new nanoscale manufacturing concepts can be tested and refined will enable this capability.

The smooth transition from the laboratory to commercial introduction will depend on the availability of robust modeling and simulation tools that can predict experimental outcomes. Laboratory experimentation can be cumbersome and time consuming, and often does not completely represent the final manufacturing conditions. Computer-aided modeling and simulation can supplement physical experiments, accelerate future research, and speed the time to the market by a factor of 2 to 10. For example, knowledge of cause and effect relationships based on laboratory observations can be used in models to simulate and predict the effects of environmental conditions (temperature, humidity), subtle process variances, batch-to-batch replication, and equipment scale. Computers can be used to successfully and economically mitigate the impacts of these effects.

Nanoscale manufacturing R&D and high-volume, cost-effective production will not be possible without advanced analytical tools. The development of robust manufacturing methods with nano-sized elements requires extensive process control. An effective control system requires accurate and timely measurements, rapid data assessment, and response parameters. Easy-to-use, economical tools for product assay and application-specific qualification are also needed. Integrating the process control components at the nanoscale will require a long-term commitment to R&D in diverse science and technology fields. The spectrum of invention required necessitates a series of parallel, intensely interwoven R&D activities.

R&D Priorities

R&D PRIORITY

Develop unit operations and robust scale-up and scale-down methodologies for manufacturing

New, high-yield and reproducible nanomaterial manufacturing processes are needed to reduce production costs (including labor and energy costs) and to produce materials with higher life-cycle values than today's competing materials. Unit operations that comprise these production methods need to scale up and scale down successfully and reproducibly from laboratory processes, while preserving the inherent nanoscale properties in the finished materials. In the near term, a reliable and consistent supply of nanomaterials will be required to drive application evaluations, which will ultimately lead to commercial products.

Priority: Top

Timeframe: 5 years

Impacts:

- Nanomaterial supplies available, satisfying industry needs in various applications *(year 2)*
- Identical materials supplied on gram or ton scale *(year 5)*

Key Challenges

Current methods used to isolate nanoparticles from reaction media and to separate powders and solid materials (*e.g.*, purification, separation, and consolidation techniques) result in low yields (especially at low volumes), relatively large amounts of precursor waste, compromised performance, and finished products that cannot easily be reproduced. Inefficient processes add expenses and significant manufacturing costs to nanomaterials used both directly and as raw materials to subsequent materials. Realization of the full potential of novel nanomaterials is impossible without suitable processing techniques that go beyond miniaturized traditional manufacturing. Manufacturing approaches that utilize mass production techniques, modular assembly with building blocks, and integrated assembly are needed to reduce costs and accelerate the entry of nanomaterials into commercial application. This will require basic physical and thermodynamic data that do not currently exist. For example, reliable and robust processes cannot be developed presently at low volumes.

Critical Needs

- Develop models and documented design tools to scale up or scale down processes quickly and effectively
- Design and develop processes to engineer materials at the device level that retain properties of the nanoscale (*e.g.*, retention of nanograins in sintered consolidated material)
- Develop reliable passivation techniques to allow safe handling and preservation of nanomaterial functionality
- Develop processes for nanomaterial emissions control
- Develop purification and classification processes

R&D PRIORITY

Develop novel manufacturing techniques for hierarchical assembly

Manufacturing strategies and efficient modular tools that utilize integrated synthesis and assembly methods to manufacture nanomaterial building blocks are needed. Utilizing mass production techniques and modular assembly will decrease production costs and accelerate commercialization.

Priority: Top

Timeframe: 20 years

Impacts

- Demonstrated commercial viability of self-assembly methods in select markets *(year 10)*
- Novel manufacturing techniques displace many traditional techniques *(year 20)*

Key Challenges

Although highly publicized self-assembly and biomimetic techniques have been demonstrated, these are largely limited to the laboratory scale. Nature's assembly techniques have not been effectively used at the commercial level. The commercial feasibility of using biological systems to generate nanomaterials on a full manufacturing scale should also be explored. Novel techniques of all types are needed for accelerating modular assembly, hierarchical assembly, and other self-assembly methods. These techniques could eliminate byproducts and waste typical of conventional manufacturing, reduce raw material and energy needs, and minimize labor costs.

Critical Needs

- Develop robust reproducible self-assembly techniques that integrate synthesis and assembly functions of manufacturing and minimize labor and energy input
- Develop efficient modular tools for building-block assembly

R&D PRIORITY

Develop dispersion and surface modification processes that retain functionality

Once produced, a nanomaterial (*e.g.*, nanoparticle, nanotubes) often needs to be modified for use in a specific application. Retention of the unique magnetic, electronic, mechanical, or other properties is critical. Processes and design techniques are needed to allow new nanomaterials and devices to be scaled up rapidly and with cost-performance profiles that exceed competing technologies

Priority: Top

Timeframe: 5 years

Impacts

- Incorporation of nanomaterials into polymer or liquid matrices commercially practiced in multiple industries *(year 2)*
- Standard, reproducible methods to tailor nanomaterial surfaces employed in manufacturing *(year 5)*

Key Challenges

Retaining properties and avoiding contamination, especially during scale-up from the laboratory to manufacturing, are the most important challenges faced when using a nanomaterial to meet application-specific requirements. The most common required modification is the de-aggregation and dispersion of the nanomaterial in a matrix (a *liquid*, as is the case for coatings and cosmetics, or a *solid*, as is the case for polymer composites or ceramics). Often, surface modification is required to enable dispersion. For example, functionalization of clay with organic molecules is used to improve dispersion of the clay in polymers. Additionally, surface modification is used to impart specific surface properties, such as the use of silane coupling agents with fumed silica to provide reaction with an epoxy or other matrix.

Dispersion and modification techniques suited for laboratory or pilot operations often do not translate well to full-scale manufacturing. For example, milling of aggregated nanoparticles with traditional attrition techniques may suffer from poor efficiency, excessive process time, contamination from media and equipment, and lack of particle-size control and uniformity. Ideally, the same processes employed at the product development scale will be translated to manufacturing.

Critical Needs

- Determine how much of the current microscale technology is transferable to the nanoscale
- Develop techniques for direct measurement of dispersion characteristics and surface modification in the manufacturing environment
- Develop the ability to address contamination in the process
- Develop a broad library of scalable surface functionalization and compatibilization techniques for modifying and dispersing all families of nanoparticles while retaining functionality

R&D PRIORITY

Develop process monitoring and controls to achieve nanomaterial and product consistency

Real-time, in-line measurement techniques are needed to provide reproducible control of properties such as particle size and distribution. Improved analytical tools and process control will go a long way to achieving zero defects in final materials, reducing waste, and turning nanomaterial manufacturing into a commodity.

Priority: High

Timeframe: 20 years

Impacts

- Responsive control systems developed for key physical properties, such as particle size distribution *(year 10)*
- First-pass yield reaches 100% *(year 20)*
- Process control expanded to chemical parameters, such as surface functionality *(year 20)*

Key Challenges

Inadequate monitor and control of the manufacturing process results in manufacturing that cannot be reproduced. Extra processing steps must be performed because today's techniques cannot produce purified target materials the first time. Standardized measurement techniques do not exist.

Critical Needs

- Develop robust, rapid QC tests
- Develop "smart" responsive control systems for real-time processing based on improved analytical tools that provide on-line imaging techniques

R&D PRIORITY

Develop processes to integrate engineered materials into devices while retaining nanoscale properties

Incorporating nanomaterials into devices and products will require their integration into heterogeneous materials, including organic/organic, organic/inorganic, and biological/organic materials. Integration methods will need to be cost-effective, environmentally friendly, and less labor- and energy-intensive than conventional methods.

Priority: High

Timeframe: 20 years

Impacts

- Nanoscale effects become practicable in real-world objects *(year 20)*

Key Challenges

The science of crossing material-scale boundaries and integrating nanomaterials into the macro world is in its infancy. Today, various processes have been demonstrated in isolation (*e.g.*, e-beam lithography, self assembly of block copolymers). However, little research has focused on utilizing combinations of approaches to meet criteria for a target application. High-yield, sub-100 nm integration processes and methods are needed for integrating engineered materials at the device scale that retain properties of the nanoscale. A combination of bottom-up and top-down assembly processes is expected to achieve this type of nanomaterial manufacturing and system integration.

Critical Needs

- Develop manufacturing methods that cross material-scale boundaries
- Develop and design processes that integrate engineered materials at the device level while retaining properties of the nanoscale

R&D PRIORITY

Develop the ability to remove impurities from raw material precursors to meet application specifications

Applications for nanomaterials are often very sensitive to impurities (*e.g.*, electronics, optics, medical devices) and have narrower tolerances than applications in commodity markets. Impurities in precursor materials must be removed or they can be carried forward to final products at levels that cannot be cost-effectively removed.

Priority: Medium

Timeframe: 5 years

Impacts

- Raw material quality no longer limits nanomaterial commercialization *(year 5)*

Key Challenges

The manufacture of nanomaterials poses unique challenges to raw material specification, purity, and quality control not typically encountered when manufacturing materials of larger dimensions. Purifying nanomaterials after they are produced is extremely difficult and expensive; it is far easier to control these parameters on the front end of the process. Many of the processes are gas-phase reactions in which impurities are carried through the process unaltered and, in some instances, concentrated during the process. The final product may be complex matrices of intractable materials, which do not easily lend themselves to analysis. Ultimately, industry will need to establish strong customer-supplier partnerships to clearly define application needs and work backwards through the process to raw material inputs.

Critical Needs

- Understand the raw material requirements (solids, liquids, and gases) to ensure the quality of nanomaterials produced for specific applications

Characterization Tools

Observing, correlating, and understanding structure and function at the nanoscale is essential to developing reproducible Nanomaterials By Design. To do this, analytical tool capability must move from static measurements of quenched samples to dynamic, real-time measurement. Chemical, physical, and temporal properties at the nanoscale must be monitored as reactions occur and as systems evolve (including living systems). Accurate and precise three-dimensional (3-D) characterization tools providing this capability are essential to the advancement of R&D in fundamentals and synthesis, manufacturing, and modeling as well as commercial production. Examples of needed applications of tools are listed in the sidebar.

A committed partnership of instrument vendors, national laboratories, academics, and industrial technologists is needed to develop measurement systems. These systems will need to have integrated imaging, spectroscopy, and scattering capabilities to provide the array of information necessary to characterize nanomaterial features and behavior across relevant scales. Development of these capabilities will evolve in steps, starting from an instantaneous measurement of a single property at multiple nanoscale locations, moving to multiple properties at a single nanoscale location, and finally generating a real-time, 3-D map of both chemical and physical properties. Ultimately, this tool will need to meet a demanding range of specifications (see sidebar).

These sophisticated analytical tools will provide:

- Timely, detailed, and accurate information to enable and even direct nanoscale synthesis
- Real-time process control during manufacturing to optimize production and minimize defects
- The feedback necessary to refine models that enable and verify meaningful, predictive simulations.

New analytical tools are needed to:

- Evaluate nanomaterials with a spatial resolution = 0.1 nm
- Analyze buried interfaces
- Analyze nanoscale biosystems
- Analyze high throughput in real time
- Couple theory/modeling and experiment
- Develop nanostructure/property relationships
- Understand and bridge multiple length scales

Tool Specifications for Real-time Characterization

- Three-dimensional tomographic capabilities
- Spatial resolution of 1 nm or less
- Applicable to sample volumes of 1µm^3 or larger
- Multiple probes for rapid, parallel measurement of identical properties or for simultaneous measurement of different properties
- Fast acquisition speed to monitor kinetic processes in real time
- Function in a manufacturing environment (*e.g.*, on-line process monitor)
- Easy to use
- Compact data format and storage across multiple platforms
- Function in different environments (*e.g.*, *in-vacuo, in-vivo,* and *in-vitro*)
- Function at different temperatures

With focused research, analytical tool capabilities will evolve over time, providing increasingly robust tools for research and manufacturing. As the analytical technologies improve to achieve the desired targets for nanotechnology, tool capabilities may become limited by external constraints such as building environment, information technology requirements, and the prohibitive cost for a single researcher/company to acquire advanced instrumentation. Achieving a commercially viable characterization tool with needed functionality for a given application will often require compromise and trade-offs among capabilities. For example, the routine manufacturing environment will require robust and economical tools. This may dictate the need to bundle specific features rather than implement the full range of capabilities envisioned.

Currently, traditional imaging is often two-dimensional (2-D) and surface-limited, while tomographic methods yield 3-D images. Direct optical imaging techniques are limited to objects that are equal in size to, or larger than, the wavelength of visible light. Spectroscopy today provides chemical and physical property information at an atomic level and is also capable of providing chemical and physical property information in 3-D. Typically, atomic-level resolution is sacrificed as larger and larger sample volumes are tested. Existing short wavelength scattering methods (*e.g.,* x-ray, neutron) provide structural information for objects smaller than the wavelength of visible light. Most scattering methods provide averaged structural information over large sample volumes and cannot yield information about individual objects.

Developing the analytical capability to produce Nanomaterials By Design will require a significant, dedicated research effort in imaging and detector technologies, machining and fabrication technologies, and infrastructure and information technologies. Concurrent R&D on standardization, infrastructure (people and facilities), and data management is crucial to tool development. Special funding strategies may be needed for risky, high-cost instrumentation development with uncertain marketability. Effective interactions and strong partnerships are needed to address the diversity and magnitude of the technical and organizational barriers to tool development. Industrial research laboratories which have traditionally addressed their critical technical needs internally will have to rely on collaborative partnerships to advance development of nanomaterial characterization tools.

Characterization Tools are dynamic measuring systems and devices (probes) that integrate and analyze data needed to describe physical, chemical, and behavioral properties of nanomaterials.

Disciplines and skills needed: chemistry, biology, physics, microfabrication, materials science, instrument manufacturing, electrical engineering, and information technology.

R&D Priorities

R&D PRIORITY

Develop real-time characterization methods and tools needed for research and manufacturing

Three-dimensional visual, chemical, and physical characterization at the nanoscale is essential to understanding structure-property relationships in nanomaterials. Physical properties are known to depend on size, particularly at the size scales considered for nanomaterials. Therefore, large-scale bulk measurements of physical and chemical properties may not adequately reflect properties at the nanoscale.

Priority: High

Timeframe: 20 years

Impacts:

- 1-D tools provide brighter sources, improved optics, detectors with better signal/noise, lower detection limits, improved spatial resolution *(years 1-15)*
- 2-D tools provide parallel sampling with parallel probes; advanced nanoscale machining *(years 5-15)*
- 3-D tools provide simultaneous x, y, and z sampling and processing for research and manufacturing applications *(years 10-20)*

Key Challenges

Optical methods are reaching their detection and resolution limits for probing nanoscale structures; other diffracted beam methods using electrons or x-rays hold promise for analytical tool development. Many high-resolution imaging/microscopy methods are limited to surface examination; thus, expansion of these methods to 3-D imaging methods such as optical coherence tomography and near-field scanning optical microscopy will be very important.

Similar challenges exist for spectroscopic methods. Both spectroscopy and scattering methods that utilize short wavelength radiation (*i.e.*, x-ray or neutron) are capable of providing structural information at the nanoscale. However, these methods average the information over a large sample volume. Improving the focusing ability of spectroscopic and scattering methods to examine individual features on the length-scales of 1 nm or less will be another key challenge. Accessibility to equipment is limited, however, as nuclear reactor facilities, spallation neutron sources, or synchrotron x-ray sources are used to conduct these experiments. Improved methods for rendering x-ray, neutron, and electron spectro-microscopic data into 3-D information would be an important complement to existing 2-D capability. Current technology, such as x-ray reflectivity, does provide some information on buried interfaces but has very strict sample geometry limitations.

The use of proximity probes to measure other chemical/physical properties, such as electrical or magnetic properties, with 1-nm spatial resolution or better is limited by measuring tool technology. Achieving higher raster speeds as well as manipulating and matching parallel probes remain key issues for many technologies. A key challenge is the development of nanoprobes capable of measuring certain physical or chemical properties at the desired spatial resolution. Current focus is on structural determination of chemical composition in 3-D. For the development of multiprobe or parallel-probe systems, improvements in nanofabrication are necessary to produce consistent measurements.

Critical Needs

- Develop advanced methods and instrumentation (hardware and software) to provide chemical and physical properties and structural information in *real-time*, with 1-nm or less spatial resolution—including, but not limited to:

— Spectroscopies

— Scattering techniques (Fourier Space)

— Microscopies (Real Space)

- Integrate individual techniques into 2-D, *real-time* multi-probe systems. (Develop multi-probe systems that integrate imaging, scattering, and spectroscopy functions to enable higher throughput.)

— Improved sample handling and manipulation

— Miniaturization capability

— Vibration isolation capability

— Reproducible interprobe performance

— Operation *in-vacuo, in-vitro,* and *in-vivo*

- Complete integration of single probes and multiprobe techniques into *real-time*, 3-D imaging tomography

— New data design algorithms

— Assimilation of robust tools into manufacturing environments

Infrastructure Requirements to Support R&D

PRIORITY

Develop the infrastructure essential to tool development and manufacturing

In the near term, tool development will be a capital-intensive process requiring partnerships and access to multi-user facilities. However, after intial development, external constraints may limit the performance of analytical tools or limit user access to the tools. Many of these technical external constraints will be beyond the expertise of traditional analytical technologists, in areas such as information technology and engineering.

Priority: High

Timeframe: 5 years

Impacts:

- Infrastructure available to support development of tools for research and manufacturing *(years 1-5)*
- Increased access and uniform usage policies for national laboratory facilities *(years 1-5)*
- Improved information technology hardware and software for data acquisition and analysis support progress in tool development and other research areas *(years 1-5)*

Key Challenges

The technical scope and capital requirements for developing the ultimate analytical tool will require cooperation among industrial, academic, and government laboratories. Conducting proprietary research for a direct-cost reimbursement fee at National User Facilities is prohibitively expensive for some researchers. Also, at some facilities, instrument scientists may be forbidden to handle proprietary information/data. Improved availability, reduced costs, and development of uniform usage policies are key to improving collaboration between government and industry, as well as to removing economic barriers to participation in commercializing nanotechnology.

The delicate instrumentation developed in research laboratories must be successfully transferred to demanding manufacturing environments. Successful analytical tools developed in broad-based user facilities must be transferred to instrument manufacturers for commercial distribution. Instrument manufacturers must participate in developing new measurement technologies and cost-effective means for controlling the environment surrounding the new analytical tools (*e.g.*, vibration isolation, clean room environment) to avoid interference with measurements and to ensure robust quality control. Also, significant capital resources must be directed towards constructing new facilities to meet the requirements of the new tool.

Analytical tool requirements present numerous computer science and data management challenges. Large amounts of data will have to be processed, stored, managed, interpreted, and disseminated. Identifying statistically significant trends will be difficult. Managing access to data will also be a challenge. In this rapidly changing field, maintaining an up-to-date knowledge of key advances and the options generated by the many scientists in a diverse research community is a significant challenge.

The research priorities identified for development of the ultimate analytical tool are based on existing measurement technologies. Novel approaches are needed to fully realize the potential of nanoscale material design. Examples of such novel approaches include combinatorial materials characterization approaches and "lab-on-a-chip" designs. Identifying and encouraging these novel approaches will be key for advancement in the field.

Critical Needs

- Provide affordable access to specialized government tools and facilities
  - — Improved access to facilities with high-end technologies (*e.g.*, beamlines) for proprietary projects including standardized procedures
  - — Uniform, user-friendly policies across all Federal laboratories and agencies (*e.g.*, standardized forms and policies, especially regarding intellectual property and access)
  - — Additional user facilities
- Build partnerships to ensure the development of high-end, next-generation analytical tools
  - — Develop a network between instrument makers (research and commercial) and users for feedback and expediting tool development
  - — Foster multidisciplinary collaborations for new tool development:
    - o Across disciplines: analytical, modeling, and processing
    - o Across industries
    - o Among vendors and users
- Determine the facility requirements for analytical tool development and operation
  - — Identify facility requirements
  - — Support retrofitting existing analytical facilities to satisfy the requirements for nanoscale analytical tools so that individual users (individual companies and researchers) can economically upgrade and maintain their own facilities
- Foster the commercial development of affordable, robust analytical tools suitable for both research and manufacturing environments
  - — Develop a training program at user facilities
  - — Develop robust, user-friendly tools capable of operating in a manufacturing environment
- Develop effective data acquisition and management strategies and tools
  - — Establish a central repository for data. Identify an organization to address data management issues and establish appropriate methods for exchange of pre-competitive information

Modeling and Simulation

Modeling & Simulation

Robust, high-confidence models and simulations are needed to predict the properties and behaviors of new nanomaterials and assembled systems across scales—from synthesis of particles through their integration into devices, and finally, to their performance in final products. Models and simulations will aid the development of synthesis and assembly protocols that impart and preserve required functional properties across scales. At the application level, they will define the functional needs and probable designs of nanostructures.

A new modeling paradigm is needed to combine lessons learned from experiments across the field of nanotechnology. It will be used to extrapolate properties (such as electronic, chemical, structural, toxicological, and environmental properties) from known conditions and apply them to novel cases. These models will be able to help design experiments, increase the efficiency of research, recognize and assess emergent properties, accurately predict performance, reduce the required number of design iterations and experiments, and reduce the number of tools required for design. Ultimately, a library of validated protocols will couple modeling and experimental results and will help researchers find customized material solutions for specific needs.

Informatics infrastructure and R&D is needed to develop information exchange protocols and to help researchers acquire, interpret, and disseminate data. Volumes of discrete data and algorithms will need to be transferred to material designers when simple equations are not adequate to represent nanoscale systems. Standardization of data exchange is essential to information management and simulation development and use.

The ability to develop accurate predictive models will depend on theoretical understanding of chemistry and physics fundamentals, methods that bridge time and spatial scales, data protocols and standards, and an *a priori* focus on the requirements of manufacturing during model development. A modeling center to focus model development and a national data depository will be essential.

Modeling
is the mathematical description of the fundamental relationships between material properties, behavior, composition, and the external environment. This type of expression allows the connection of individual experimental data across a continuum of conditions.

Simulation
is the combined computation of multiple modeled interactions, which allows the prediction of properties of complex systems with many different discrete parts. As parts get smaller, the number density goes up, along with their interactions.

Disciplines and skills needed:
physics, chemistry, chemical engineering, statistical science, computer science, applied mathematics, biology, computational science, data systems, software development, data analysis, data mining, data visualization, expert curating, and annotation.

R&D Priorities

R&D PRIORITY

Develop fundamental models to accurately predict nanostructure formation

Models of fundamental material properties at the nanoscale are needed, as well as models to screen formation and synthetic pathways. An understanding of nanoscale chemistry and physics, in addition to newly discovered nanomaterials, will encourage an understanding of nanostructure formation processes. This data could be used to develop models and simulations with predictive capability that accelerate research and integration.

Priority: Top

Timeframe: 20 years

Impacts:

- Models provide insight into nanostructure formation for continuously improved processes *(year 3)*
- Models connect lessons learned between discrete experiments, facilitating cross-application of knowledge *(year 10)*
- Predictive models available for multiple types of nanostructures *(year 20)*
- Novel nanostructured materials identified from theoretical understanding *(year 20)*

Key Challenges

Physics and chemistry data are currently only available for select material systems based on experimental discovery. A systematic approach to studying nanomaterial formation that is applicable across classes of materials does not exist. The lack of consistency in modeling and simulation protocols makes comparing approaches difficult. Existing models must be assessed to determine where and why nanoscale prediction is inadequate.

Critical Needs

- Develop methods to include chemistry (reaction and degradation) in force-field modeling to understand nanostructure formation
- Modeling of the chemistry of deformable interfaces
- Integrate the chemical functionality of nanomaterials into models
- Link molecular simulation to constitutive models
- Develop methods for comparing equilibrium, non-equilibrium, and kinetically trapped systems

R&D PRIORITY

Develop methods for bridging models between scales, from atoms to self-assembly to devices

Accurate predictive models and simulations linking nanoscale properties across time and length scales to specific macroscopic properties are needed. These models will help enable the design and engineering of nanomaterials.

Priority: Top

Timeframe: 20 years

Impacts:

- Nanomaterial use increases as new performance characteristics are discovered *(year 3)*
- Predictive models for macroscopic performance inspire the use of new materials *(year 10)*
- Nanostructure - macroproperty relationships predict performance *a priori (year 20)*
- Nanostructures reverse engineered from desired macroscopic properties *(year 20)*

Key Challenges

Current models and simulations predict atomistic behavior from quantum calculations as well as macroscopic continuum behavior of particles and structures. Computational tools and techniques required to bridge these two areas through the nanoscale are under development. This is a significant challenge, as scales need to be bridged across nine orders of magnitude in length and, if one assumes hours to femtoseconds, seventeen orders of magnitude in time. When nanodimension properties provide a discrete difference in material performance, continuum modeling is insufficient. Nanomaterial behavior often cannot be extrapolated from a single particle to multi-particles. Equilibrium, non-equilibrium, and kinetically trapped systems need to be compared.

Ideally, *ab initio* methods—methods derived from fundamental laws of physics and chemistry—could be used in either direction to extend atomic/molecular calculations into the nanoscale, or to extract required atomistic contributions from observed nanoscale properties. Integrating *ab initio* and combinatorial approaches at this level would be valuable.

Critical Needs

- Link modeling and simulation results to experimental data
- Simultaneously incorporate atomistic and mesoscale techniques in *ab initio* methods to predict properties or extract atomistic contributions from observed properties
- Develop advanced molecular dynamics (MD) simulation methods
- Develop models of properties that apply to industry and consider unique scaling laws from nano to meso to macroscale (*e.g.*, mechanical, electrical, magnetic, optical, convective transport [heat, momentum, mass], diffusion, thermodynamic equilibria, including adsorption, surface-surface interaction, and chemical reaction)
- Extend models to recognize and predict new and unexpected emergent properties of self-assembled systems
- Expand models to understand and predict toxicology and environmental impact
- Develop and validate extensions of continuum models from the macroscale to the nanoscale
- Combine simultaneous effects (such as flow dynamics and thermodynamic driving forces) to provide a powerful tool for evaluating potential technologies
- Integrate *ab initio* and combinatorial modeling approaches to improve simulation efficiency

Infrastructure Requirements to Support R&D

PRIORITY

Improve research infrastructure to support model advancement

The R&D needs for modeling and simulation will require innovative improvements in infrastructure to bring experts together, develop computational capabilities, and develop effective data management.

Priority: Top

Timeframe: 10 years

Impacts:

- Increased production of models and simulations for nanostructured materials *(year 5)*
- Specialized tools and techniques to facilitate nanomaterial simulation *(year 10)*
- Highly trained workforce available in theoretical and practical modeling, simulation, and informatics of nanomaterials *(year 10)*

Key Challenges

Research expertise needed to significantly improve modeling capability is currently dispersed among research centers, while current simulation methods require very large and expanding computing resources. Research is needed to improve computational feasibility through shared and innovative architectures. The efficiency of data assessment methods cannot be determined because numerous data protocols are used.

Critical Needs

- Support and integrate national centers for advancement of nanoscale modeling, simulation, and informatics:
  - — Develop and validate new models and simulation methods
  - — Provide a “moon shot-like” intellectual focus for the research community (actual centers, not ‘virtual’ centers, as personal interactions are vital to cross-fertilizing techniques)
  - — Conduct multidisciplinary research with a team focus
  - — Facilitate sabbaticals for industrial, university, and government researchers
- Develop new computational architectures for breakthrough performance in quantum mechanical simulation and calculation
- Develop information exchange protocols and infrastructure for data acquisition, interpretation, and dissemination

The informatics needs for modeling and simulation are presented in the Standards and Informatics section.

Environment, Safety, and Health

As with any new material, broadscale nanomaterial commercialization will require an understanding of the material's environmental, safety, and health (ES&H) impact, and the development of exposure and handling guidelines for production, transport, use, and disposal. Generally accepted ES&H protocols will have a significant impact on attracting employees to support accelerated scientific research; manufacturers willing to fabricate with nanomaterials; consumers willing to purchase entirely new products or products with new attributes; and a public eager to gain the benefits provided by nanomaterials.

The chemical industry applies rigorous methodologies and regulatory guidelines to determine the ES&H impact of new materials. This involves identifying human health and environmental hazards, determining human and environmental exposure, and establishing an exposure-based risk assessment to indicate the probability of adverse effects. While some data can be applied broadly to classes of materials, studies are often material-specific, particularly when related to reactivity, toxicity, and other areas. The use of approaches similar to those currently employed, and the use of existing knowledge and databases will be necessary to establish safety guidelines for nanomaterial research, production, and commercial application.

Today, knowledge is just emerging on environmental chemistry/transport and toxicokinetic processes applied to nanoscale materials. Developing this understanding is a significant challenge for this young industry because the form, quantities, and, in some cases, specific types of nanomaterials have not been defined by commercial applications. Nevertheless, the industry will benefit significantly from addressing these issues early in the technology development process. Also, the traditional approach of hazard identification-/exposure-based risk assessment is made considerably more challenging by the added complexity of variables related to nanotechnology. Size (*e.g.,* large surface area of insoluble particles, movement of nanoscale materials in the body or environment), structure (*e.g.*, carbon nanotubes, buckyballs), reactivity, and the surface functionalities of atomically designed materials add to this difficult task.

Tools and protocols are needed to characterize nanomaterials and their environmental and health effects. Tools that allow detection of nanomaterials in the environment and workplace are critical to accurately assessing potential concerns. Accordingly, tool development must progress rapidly and address the needs of detection. Protocols that employ relevant existing experimental data, models, and material-specific evaluations are needed to determine long-term and life-cycle impacts. Because of the breadth of potential nanomaterial types, initial studies should adopt a model-material approach. Model nanoscale systems can provide the opportunity to uncover general trends and issues relevant for these new materials. Model materials should also be chosen to represent classes of nanoscale products and provide data with the broadest and most immediate benefit. Handling guidelines need to be developed immediately to support commerce today and will need to be updated as new materials and new information become available.

It is essential that all stakeholders share the rapidly expanding knowledge base in this area.
A shared database that structures, qualifies, and interprets all relevant data should be developed and accessible for broad use. While industry has several examples of databases that can be used individually

or collectively as templates, enhancements will be required to accomodate categories and key properties specific to nanomaterials. Information in this database can include physical properties, environmental chemistry, ecotoxicity, and mammalian toxicity. To develop the database, assessment processes for nanomaterials will need to be generated. Once developed and validated, this protocol can be applied in an ongoing manner similar to those currently used for more traditional, high-production materials. Publication of research findings should be encouraged to support rapid and broad dissemination.

Disciplines and skills needed:
industrial hygiene, occupational health, general toxicology, inhalation/respiratory toxicology, epidemiology, pathology, analytical chemistry, environmental chemistry, environmental microbiology, and atmospheric chemistry/modeling.

Over the next decade, consumers must develop confidence in the use of products containing nanomaterials. Accurate information about benefits and any costs associated with nanomaterials must be widely available. High public acceptance is crucial to the development of an economically viable nanotechnology industry. Independent, government-sponsored research is vital to establishing consumer confidence in nanomaterial development and use, and in validating industrial efforts in this area. The anticipated growth in nanoparticle utilization warrants parallel efforts in hazard identification, exposure evaluation, and risk assessment. Chemical companies are prepared to serve a major role in this process as leaders in characterizing materials, identifying their potential risks, and providing guidelines for their safe and effective utilization. However, the task requires the support infrastructure within national and academic facilities to accelerate these investigations.

R&D Priorities

R&D PRIORITY

Assess human health and environmental impact hazards

Human health and environmental hazard identification are based on established health and environmental test guidelines of regulatory authorities such as the Organization for Economic Cooperation and Development (OECD)/Environmental Program, Occupational Safety and Health Administration (OSHA), and Environmental Protection Agency (EPA). An understanding of how specific nanosized materials may affect health and the environment needs to be established so that, if necessary, regulatory guidelines can be updated to consider novel chemistry, size, morphology, higher order structures (if any), and utilization.

Priority: Top

Timeframe: 20 years

Impacts:

- Compilation and survey of pertinent literature *(year 1)*
- Identification of model systems to perform in-depth analysis *(year 2)*
- Acute toxicology studies on model systems completed *(year 5)*
- Exposure protocols and relevant testing established *(year 5)*
- Chronic and developmental toxicology studies on model systems completed *(year 7)*
- Environmental impact of model systems determined *(year 20)*

Key Challenges

In the case of inhalation exposures, generating and maintaining stable atmospheres of nanomaterials is extremely difficult, especially during accelerated testing where high material concentrations are utilized. As the concentration increases, aggregation may occur and thus nullify experimental objectives. Anticipating other exposure routes and determining the most relevant route for administering the nanomaterial exposure is difficult without a thorough understanding of the environmental composition.

Critical Needs

- Determine the health, toxicological, and epidemiological effects and environmental impacts resulting from the creation and existence of nanostructures
- Determine the biological fate of nanomaterials
- Identify model systems to extend findings across classes of materials
- Establish and fund an accessible national ES&H database that collects peer-reviewed research from all sources. Encourage industrial researchers to participate in the process
- Encourage research investment in ES&H by all interested parties and collaboration between researchers to provide peer-reviewed analysis
- Conduct independent, government-funded research to validate health and environmental impacts and to promote confidence in research findings and acceptance of nanomaterial use

R&D PRIORITY

Determine exposure potentials for nano-sized materials

Understanding the make-up of product, emissions, and waste streams and determining the existence and persistence of nanomaterials are essential to establishing exposure potentials. They are also required, along with the hazard potential for these materials, to prioritize control strategies, environmental testing, and a rationale for testing procedures (*e.g.*, relevant route, concentration, duration).

Priority: Top

Timeframe: 5 years

Impacts:

- Nanomaterial product/waste streams characterized *(year 1)*
- Real-time monitoring incorporated into control/containment systems *(year 5)*

Key Challenges

Because an extremely high surface area-to-volume ratio exists for nanomaterials, surface energy significantly impacts stability assessments. Desired nanomaterial attributes such as enhanced solubility, increased reactivity, and a propensity for agglomeration may affect their environmental state. Determination of the existence of isolated nanoparticles is a critical first step in undertaking this exercise. *In situ* testing without biasing the results during sampling is an immense challenge. Characterization is difficult and requires state-of-the-art technologies because of the extremely fine size of nanomaterials. Significant advances in sampling and analysis, including new characterization tools and analytical technologies, are needed.

Critical Needs

- Determine the make-up of product and waste streams needed to establish nanomaterial exposure potentials
- Develop new methodologies for exposure sampling and analysis, both in the environment and in the workplace
- Determine transport mechanisms for nanomaterials in various environmental media
- Develop accurate real-time monitoring of environmental nanomaterials
- Determine the environmental persistence and bioaccumulation potential of nanomaterials
- Estimate impacts through the entire product life cycle using Responsible Care® principles
- Develop science-based exposure limits from research results

R&D PRIORITY

Establish handling guidelines for operations involving nanomaterials

Safe handling guidelines for nanoscale materials are needed to supplement standard industrial hygiene practices. Industry, academia, and government will apply these approaches to R&D, product development, commercialization, disposal, and transportation.

Priority: Top

Timeframe: 5 years

Impacts:

- Communication document providing safe work practices distributed *(year 1)*
- Effectiveness of existing personal protection equipment (PPE) determined *(year 2)*
- Best practices for exposure control of nanomaterials established *(year 5)*

Key Challenges

Because of the characterization challenges, ensuring the effectiveness of engineering controls, personal protection equipment (PPE), and handling equipment presents a formidable challenge. Development of technology to provide affordable solutions for exposure control implementation and exposure monitoring is critical.

Critical Needs

- Develop best practice exposure control methods for R&D and manufacturing environments involving nanoscale products
- Determine effectiveness of current PPE for nanoscale materials
- Manufacture affordable new PPE equipment, handling, and monitoring systems
- Develop control/containment systems for nanoscale materials (filtration, fluid/powder handling)
- Develop an education program to communicate appropriate safe work practices
- Foster National Institute for Occupational Safety and Health (NIOSH) and American Conference of Governmental Industrial Hygienists (ACGIH®) involvement and encourage completion of an independent assessment
- Recommend protocols guiding nanomaterial handling

Standards and Informatics

Reference standards, standardized methods for synthesis and analysis protocols, and effective information management and communication are vital to the development of nanoscience and nanotechnology as a new discipline. They each will make an essential contribution to accelerating the pace of discovery and commercialization.

Researchers, manufacturers, and end users must be able to reliably and confidently compare and reproduce chemical and physical properties of materials regardless of the organization performing the experiments or manufacturing the product. Comparing and testing a material to a standard provides a way to understand the material's reliability and performance under specific conditions, and its compatibility with other materials, thereby reducing the risk of designing with the new materials. Consistent material specifications that are accepted and recognized by design engineers will foster the use and inspection of materials, improving the reliability of material design. Standards will need to evolve to keep pace with discovery and nanotechnology innovation.

Standardization is critical to scientific communication and commerce because, in order to build on lessons learned, researchers need to quickly convey scientific discoveries across disciplines. On the user front, consumers must be able to compare material attributes.

Informatics requirements are significant. The sheer volume of data and its effective application will require extraordinary computational and management capabilities, as well as the development of organization systems and structures that foster communication and assist in the application of new technologies.

Developing standards and informatics will require significant participation by the scientific community. Support from Federal agencies is needed to establish internationally recognized synthesis and evaluation procedures, calibration standards, validated measurement technologies, robust protocols, and nomenclature. Ongoing communication between the lead Federal agencies and the nanotechnology community, especially the chemical industry, is essential to the effort. Because commerce is international in scope, the standards and standardization must be internationally recognized.

Disciplines and skills needed:
materials science, synthetic chemistry, analytical chemistry, physical chemistry, physics, computational chemistry, surface science, and computer and information science.

R&D Priorities

R&D PRIORITY
Develop standard procedures for nanomaterial synthesis

The current state of nanomaterials synthesis is similar to that of organic chemistry 50-100 years ago. At that time, synthetic methods were regularly being discovered and reported in the literature, yet a compilation of peer-reviewed synthetic methods was not available. The publication of the compilation "Organic Synthesis" resulted in an exponential increase in both the preparation and use of organic materials. A similar growth in inorganic chemistry resulted from the publication of standard peer-validated synthetic methods in "Inorganic Synthesis." It is believed that the development of standard methods for nanomaterials synthesis would similarly accelerate their commercialization and use.

Priority: Top

Timeframe: 20 years

Impacts:

- A peer-reviewed journal dedicated to standard nanomaterial synthetic methods *(now)*
- A documented list of standard nanomaterial synthetic methods *(years 2-10)*
- Standard procedures to control the composition, size, dispersivity, and functionalization of nanomaterials *(years 5-10)*
- Standard procedures to control dispersion of nanomaterials *(years 5-10)*
- Standard methods for self assembly *(year 20)*
- Source of well-characterized nanomaterials for property determination/validation *(years 10-20)*

Key Challenges

One of the major factors inhibiting widespread use of nanomaterials is the lack of reproducible synthetic methods, which results in materials with irregular properties. Because the properties of nanomaterials are size-dependent, reproducible methods for preparation that always yield the same size, composition (bulk and surface), dispersivity, for example, are necessary. Another factor is the lack of reproducible functionalization methods, which, again, results in the production of materials with non-reproducible properties.

Critical Needs

- Develop reproducible methods for synthesis of high-quality nanomaterials with agreed-upon analytical criteria
- Conduct round robins to validate synthetic methods
- Publish validated synthetic methods in dedicated, peer-reviewed publications

R&D PRIORITY

Develop a set of reference materials for property measurement standardization

Reliable reference materials for standardization of property measurements are needed to calibrate new measurement tools developed for nanomaterials. Without assurance that newly developed analytical tools are providing consistent results, measurement feedback into synthetic, calculational, and engineering efforts will be unreliable. Current reference materials may be unsuited for use as nanomaterial standards due to incompatibility with new instrumentation and potential size effects.

Priority: Top

Timeframe: 20 years

Impacts:

- New analytical tools generate data, enabling other research areas *(years 3-20)*
- Reliable standard reference materials available as physical standards for all desirable properties *(years 3-20)*

Key Challenges

The current form of certain calibration standards may not be compatible with the new analytical toolset. Simply downsizing current standards is inadequate because of nanoscale phenomena. For example, the melting point of gold is known to lower as size decreases. Standards for macroscale size and other physical characteristics exist today, but developing commercially available NIST Traceable Reference Materials for nanotechnology is a major challenge due to property variation with fluctuations in environmental conditions and other issues. Development of reliable nanometer or smaller length standards and fostering a supplier of such standards will be a major challenge.

Critical Needs

- Identify appropriate reference standards for the chemical industry
- Manufacture a commercially available library of high-quality standard reference materials for property measurements and disseminate it throughout the chemical industry
- Conduct round robins to calibrate reference materials and standards

R&D PRIORITY

Develop standard methods for physical and chemical property evaluation

Evaluation methods are needed for physical size and size distribution, chemical composition, material properties (*e.g.*, modulus, viscosity), electric properties (*e.g.*, resistance, conductivity, capacitance), optical properties (*e.g.*, refractive index, absorption) and electronic and magnetic properties. Property standards are needed to ensure reliable performance of the analytical tools and to exploit new properties identified at the nanoscale.

Priority: Top

Timeframe: 20 years

Impacts:

- Publication of various ASTM or other certified methods for measuring diverse nanoscale chemical and physical properties *(years 3-20)*
- Analytical tools conform to certified methods *(years 10-20)*

Key Challenges

For the measurement of physical and chemical properties on the nanoscale, tool development to measure a specific property may be accomplished by more than one method. Cross-validation of the different techniques and approaches is a key challenge for reliably determining a specific property. Comparing the various techniques to understand and correct for method-dependent systematic errors is a challenge to developing standard test methods.

Critical Needs

- Identify the best methods for obtaining any given physical or chemical property
- Rapidly disseminate round robin results to tool and method developers
- Ensure that certified methods possess the flexibility to adapt to novel approaches and incorporate key lessons learned to maintain the most up-to-date practices
- Develop statistical evaluation techniques for validation and analysis of the properties of nanomaterials
- Conduct round robins to validate standard methods
- Document standard methods in American Society for Testing and Materials (ASTM), International Union of Pure Applied Chemistry (IUPAC), and other publications

R&D PRIORITY

Develop computational standards to improve information processing and transfer for modeling and simulation

Current simulation work is fragmented by multiple approaches to defining and manipulating data at every level. In this cross-disciplinary effort, significant amounts of time and energy are spent simply ensuring common language and taxonomy between developers from different backgrounds. This difficulty extends to all types of collaborative situations in nanotechnology, and is most critical when large volumes of information are being manipulated, such as in computer simulations. A library of diverse nanomaterial building blocks must be accessible by users in an efficient way. Development of standards facilitates common usage.

Priority: Top

Timeframe: 10 years

Impacts:

- National Data and Modeling Repository established *(year 1)*
- Virtual community established in parallel with bioinformatics efforts *(year 5)*
- Improved ability to utilize knowledge developed by other practitioners *(ongoing)*
- Improved productivity of modeling and simulation efforts (faster development, cross-disciplinary application, and broader application of developed models) *(ongoing)*

Key Challenges

No well-defined standards exist for accessing models developed for nanotechnology processes. Practitioners use their own individual protocols, which hinders collaboration. Lack of common protocols in all areas slows collaboration and understanding, as time is spent in detailed meetings to establish common ideas or, worse, time is wasted due to lack of appreciation for subtle differences not explored before extensive work is performed. Another key challenge is to integrate research efforts among industrial nanotechnology practitioners, who may be able to use protocols developed by government-funded research, as well as give guidance to the development of new protocols.

Currently, materials are tested using protocols defined by the developing laboratory, rather than by a well-defined standard. This makes modeling of the phenomena more difficult and introduces more potential error from independent practitioners.

Critical Needs

- Develop an accessible and searchable National Data and Model Repository to improve information processing and transfer for modeling and simulation
- Establish standards for communication between modeling modules
- Define common taxonomy and units
- Provide remote communication to link experimentalists to modelers to facilitate virtual collaboration
- Develop library of validated modeling and simulation protocols that can be accessed by industrial users
- Establish a modeling architecture that supports modeling integration

R&D PRIORITY

Develop standards for material evaluation in applications

Standards for physical and chemical characterization of nanomaterials (*e.g.*, particle size and distribution, morphology, degree of aggregation, solubility) are required to define the material, its suitability for given applications, and product consistency.

Priority: Top

Timeframe: 10 years

Impacts:

- Standard methods for characterization and QC of nanomaterials are widely accepted and uniformly practiced, enabling accurate decisions to be made on the suitability for given applications *(year 10)*

Key Challenges

No standards for nanomaterial characterization exist. Developing protocols will be challenging given the nature of the nanoscale.

Critical Needs

- Standardized and readily implemented (*i.e.*, robust and economical) quality control (QC) protocols are required to measure key physical and chemical properties of nanomaterials
- Develop standard micro- and macro-scale integration platforms for measuring the properties of imbedded nanomaterials and devices

R&D PRIORITY

Establish internationally recognized nomenclature standards

A generally accepted standardized taxonomy and language to describe nanoscience and nanotechnology is needed to facilitate and expedite clear communication and the transfer of information. This will accelerate the pace and cost-effectiveness of scientific research, technology transfer, and commerce worldwide.

Priority: Top

Timeframe: 5 years

Impacts:

- Common nomenclature and taxonomy accepted *(year 3)*
- Common language accepted and consistently used *(year 5)*
- Significant increase in communication between researchers and consumers of nanotechnology information *(ongoing)*
- Significant improvement in the reproducibility of results and speed of technology transfer *(ongoing)*

Key Challenges

Because nanotechnology is currently a hybrid discipline, researchers were originally trained in a diverse range of disciplines, each with its own nomenclature and taxonomy. New scientific discoveries are typically described in the language of the researchers and may not be readily understood across disciplines. The inability to explain scientific information clearly is frustrating, time consuming, and thwarts the effective exchange of information. Developing a standard nomenclature for nanotechnology with specific definitions (*i.e.,* taxonomy that communicates obvious meaning, such as hexane) that will be satisfactory across disciplines is a critical challenge. A generally accepted language that goes beyond taxonomy is also needed. Keeping up with scientific progress and assuring consistent application across disciplines will be an ongoing challenge. Consumers of nanotechnology information (such as corporate purchasing managers, journal reviewers, and editors) will need to insist on the use of standard nomenclature and language to describe practices and achievements.

Critical Needs

- Define and document a common nomenclature including taxonomy and units (*e.g.*, similar to the IUPAC)
- Develop a common language for nanotechnology practitioners (definitions, glossary of terms, *etc.*)

Infrastructure Requirements to Support R&D

PRIORITY

Establish the organizational infrastructure and other requirements to foster standardization and the development of standards

The need to establish standards and standardization is an essential step in the development of a new discipline. It requires the commitment of an organization with a clear mission and dedicated resources, both organizational and scientific, as well as a committed scientific community to participate in all aspects of standards development. Standards are essential to facilitate scientific discovery and commerce.

Priority: High

Timeframe: 5 years

Impacts:

- Organization dedicated to nanotechnology standardization *(year 1)*
- Independent nanomaterial evaluation established at competent and consistent laboratories *(year 5)*
- Repository and publication of reviewed methods *(ongoing)*

Key Challenges

A key challenge is dedicating the time, personnel, and research resources required to develop standards. For example, developing test methodologies, test materials, and synthetic methods and have them reviewed by multiple users to ensure broad acceptance and reproducibility is a necessary step. The ability to reliably communicate material performance is in part, due to common definition of the experimental methods used to measure the performance, and the existence of standard reference materials.

The organizational infrastructure needs are diverse, posing a range of challenges. For example, standard materials and measurement instrumentation development must coincide with the development of synthetic-material methods. This will require cooperation and agreement on standards and the financial commitment to make it happen, even with uncertain returns. Measuring material parameters and comparing results across laboratories is time consuming and subject to variability of practices, even with standards in place. U.S. standardization activities must coincide with international activities and assure representation of U.S. interests. In addition, information processing and transfer for modeling will require a centralized depository and standards.

Critical Needs:

- Develop internationally recognized calibration standards, validated measurement technologies and robust protocols
- Establish a journal to report standard synthetic methods verified by two or more independent research groups and procedures for synthesizing reference standards for property evaluation
- Develop stable property evaluation methods; standard methods, protocols, and statistical evaluation techniques for validation; and conduct round-robins to calibrate standards, validate equipment, and determine reliability
- Encourage active U.S. chemical industry participation and leadership with international organizations and professional societies that set standards, such as IUPAC, the Versailles Project on Advanced Materials and Standards (VAMAS), and the ASTM
- Develop commercial sources for standardized materials and instrumentation
- Develop a National Data and Model Repository

Knowledge and Technology Transfer

Accelerating scientific discovery into technological innovation will require information sharing, knowledge transfer, and technology transfer in rapidly emerging areas. The speed of research and the use of research results will be dictated by the effectiveness of the infrastructure, and government, university, and corporate policies. A culture change that includes information sharing—among government, universities, and companies—will help the community to focus on developing and commercializing nanomaterials in the near term. These efforts will support R&D and help to ensure that technologies are invented, developed, and commercialized in the United States.

PRIORITY

Establish technology transfer policies that foster nanomaterial commercialization

Priority: Top

Timeframe: 10 years

Impacts:

- Reviewed effectiveness of policies to promote commercialization *(annually)*

Today, nanomaterial R&D is largely in the discovery phase. Breakthroughs will require tremendous collaboration across disciplines and research organizations. As with other areas of science, the future of nanotechnology will be shaped by intellectual property (IP) policies, patent ownership, and availability of financial resources for integrating nanomaterials into commercial products.

Current IP policies at U.S. universities put American companies at a competitive disadvantage. For example, global companies are increasingly focusing their sponsored research investments in foreign universities. To encourage industry-university collaboration and foster commercialization, U.S. universities and companies must work together to address the needs and concerns of industry sponsors regarding IP resulting from company-funded university research. In addition, new teaming approaches that facilitate technology transfer are needed before research begins in order to foster innovation and commercialization.

Key Challenges

IP policies of universities, government funding agencies, and individual companies significantly impact the level of participation in collaborative R&D. Likewise, patents shape opportunities for marketable applications—overly broad patents in the early stages of nanotechnology development can limit R&D investment. More patent examiners skilled in nanotechnology are required, while IP policies need to be modified to encourage wide commercialization of nanotechnology products.

Critical Needs

- Establish technology transfer protocols that promote commercialization, facilitate timely information exchange, and reduce the time and expense required for negotiating and establishing collaboration and licensing agreements
- Establish a nanotechnology working group within the U.S. Patent Office to foster education and communication among patent examiners
- Facilitate industry-university, industry-government, and industry-industry partnerships

Infrastructure Requirements to Support R&D

PRIORITY

Build an infrastructure that encourages knowledge sharing to facilitate nanoscience understanding and foster near-term commercialization

The cross-disciplinary, multi-scale nature of nanotechnology will require unique facilities and integrated R&D teams with synthesis, fabrication, characterization, and modeling capabilities. Mechanisms that encourage knowledge sharing and transfer are key, as well as methodologies that promote interactions across disciplines and foster collaboration.

Priority: High

Timeframe: 10 years

Impacts:

- Roadmap on shared-knowledge infrastructure completed *(year 1)*
- Roadmap implementation completed *(year 10)*

Key Challenges

Given the magnitude of the research challenges as well as the international research race, a "next-generation" infrastructure is needed so researchers can participate in virtual collaboration, build on the lessons learned by others, and improve the cost-effectiveness of research. Results from all pre-competitive, government-funded research will be the primary information source that must be easily accessible to the research and development community. This will require data sharing from basic research through full-scale manufacturing. The research centers and virtual centers will need to be networked in unprecedented ways to create a "pool of knowledge" that can be accessed by the nanomaterial research community. Mechanisms for information exchange are needed to foster reproducibility of methods and quantitative comparison of experimental methods, communication between organic and inorganic nanomaterials communities, and the development of a comprehensive database of nanomaterials.

The entire research community—including independent researchers and small companies—needs to understand how technologies become commercialized as well as the expectations and limitations of each contributor. For example, companies pursuing a proprietary niche must limit exposure to others' innovations to avoid compromising their in-house research. Nevertheless, start-ups find it difficult to simultaneously develop their core competence and find value for their products, so they depend on established companies. The expectations and limitations of customers must also be considered because they are often responsible for product development.

Knowledge and Technology Transfer

The government-funded nanomaterial research network is complex and expanding. To facilitate technology transfer, communication among researchers, program managers, and policy makers must increase dramatically. Companies, both large and small, must gain a better understanding of government programs and how to work together toward building the research foundation for Nanomaterials By Design.

Critical Needs

- Develop a roadmap for fostering a shared-knowledge infrastructure that builds on the knowledge gained from standards and informatics research
- Establish knowledge-sharing protocols in funding agreements so that results from government-funded research is readily available

Education and Training

Workforce and public education are critical to the success of the national R&D initiative. Thousands of research scientists with expertise in diverse disciplines are needed to conduct the research. The skills and expertise needed are identified in each R&D section of this roadmap. The breadth of knowledge and expertise is viewed as imperative for scientific breakthroughs in nanoscience and nanotechnology. Attracting and preparing a technically qualified workforce is a major challenge facing U.S. industry today. In addition to an educated workforce, an informed public that can draw an accurate perception of the risks and benefits of nanoscience and understand the opportunities enabled by nanomaterials is essential for their commercial success.

PRIORITY

Implement strategies to attract and prepare a workforce for nanomaterial research and manufacturing

The rapid progress in nanoscience discovery and its transition into innovative nanotechnology will require a highly trained workforce, especially innovative scientists and engineers with doctoral degrees.

Priority: Top

Timeframe: 10 years

Impacts:

- Roadmap on nanomaterial education and training completed *(year 1)*
- Nanomaterial curriculum in universities *(year 5)*
- Roadmap implementation completed *(year 10)*

Key Challenges

As the economies in Europe and Asia strengthen and education and employment opportunities expand throughout the world, fewer non-U.S. citizens may be attracted to U.S. universities and the U.S. workforce. This situation is exacerbated by recent changes to U.S. immigration policy. Shortages of physical sciences and engineering doctoral graduates in the United States and increased global investment in nanotechnology could decrease the technological dominance that the United States has enjoyed for the past 50 years. Given increasing international competition for science-educated researchers and the increasing trend to locate manufacturing sites outside of the United States, the United States must implement an education and training strategy as soon as possible. Moreover, because the nanoscale bridges various disciplines, science education will need to integrate biology, chemistry, physics, and engineering.

Critical Needs

- Develop and implement a roadmap for nanoscience and technology education and training
  - — Attract more bright U.S. students to science and engineering
  - — Provide interdisciplinary education for K-12, undergraduate, and graduate students
  - — Develop state-of-the-art nanomaterial curriculum and text books
  - — Enable rapid and cost-effective transition of knowledge into manufactured products, including new curriculum and university/national laboratory/industry partnerships
  - — Expand corporate and school (all levels) access to resources at government centers, national laboratories, and universities

— Provide opportunities for training at Federally funded centers

— Foster international collaborations in academic research, and encourage U.S. students to pursue graduate degrees abroad

— Develop professional accreditation for nanomaterial education and training

PRIORITY

Promote public awareness of nanoscience and technology

Education initiatives are needed to establish an accurate perception of risk, avert uninformed media discussions, and foster the application and use of nanomaterial-enhanced materials, devices, applications, and processes.

Priority: High

Timeframe: 10 years

Impacts:

- Awareness-raising publication available on opportunities, benefits, and risks of nanomaterials *(update annually)*
- Education implementation strategies in place, ready when research results are available *(year 2)*

Key Challenges

The public often lacks an understanding of emerging technologies and their potential benefits to society and the economy. Thus, the first step must be to ensure that the public is informed about nanotechnology and nanomaterials. Once an understanding of the environmental, safety and health impacts of nanomaterials has been established, information must be effectively communicated to the public to foster confidence in the use of nanomaterial-enhanced and nanomaterial-derived products.

Critical Needs

- Educate the public regarding the benefits, risks, and opportunities enabled by nanomaterials
- Educate the public regarding the safety of nanomaterial technology and provide the results of Federally funded studies. Include the public in discussions of nanomaterial safety

Infrastructure and Enabling Resources

Development of our nation's scientific infrastructure—the technically complex facilities and indispensable services they provide—is essential for the advancement of tools, manufacturing, and other capabilities. Cost-effective access to new capabilities at government-funded facilities is a cornerstone of the research strategy. Enabling resources such as standards, information management systems, networks for information exchange, and commercially available tools are also needed. Together, infrastructure and enabling resources provide support for successful R&D.

In this roadmap, the infrastructure and enabling resource priorities are presented under the heading "Infrastructure Requirements to Support R&D" at the end of the following sections:

- Modeling and Simulation - to support model advancement
- Characterization Tools - to support tool development and use
- Standards and Informatics - to foster development of standards
- Knowledge and Technology Transfer - to encourage knowledge sharing

4. Implementation: The Path Forward

Achieving significant societal and economic benefits from Nanomaterials By Design within 10 to 20 years will require a large, sustained, national investment in R&D. Development and commercialization can be accelerated with an effective strategy, new policies, and a commitment among the diverse U.S. stakeholders.

This roadmap presents the strategy and R&D priorities for realizing the vision for Nanomaterials By Design. It introduces a new, goal-oriented approach to materials development—one that will provide the capability to design nanomaterials as solutions in a broad range of applications. Navigating the course of research will require significant coordination and collaboration across research and funding organizations, and across scientific and technical disciplines. The required level of interdependent, multidisciplinary research constitutes a cultural shift in the way science and technology are presently pursued. To ensure success, a shared commitment is essential from key stakeholders who can provide strategic direction, technical knowledge, business acumen, and financial resources.

Nanomaterials By Design can revitalize U.S. industry and competitiveness, and help meet societal needs—from energy generation to health care—far into the future.

The roadmap is a strategic guide to investment in nanotechnology with the goal of accelerating commercialization. It is hoped that the leadership of the National Nanotechnology Initiative (NNI), diverse U.S. companies, and U.S. legislators will use the roadmap to guide investments in R&D. To implement Nanomaterials By Design within 10 to 20 years, the United States must overcome significant scientific and technological barriers. Insights and breakthroughs along the way will expand market penetration of nanomaterials continuously over the next five years and will accelerate after that as predictive capabilities for nanodesign become more robust. Effective implementation of the roadmap will ensure a focus on both near-term commercial successes and mid- to long-term R&D priorities.

Collectively, participating chemical companies—working closely with end users, suppliers, and other researchers from industry, universities, and government laboratories—will help implement the research strategy and priorities offered in this roadmap. Chemical companies will pursue government-funded R&D (pre-competitive and competitive) concurrently with corporate research focused on a broad spectrum of basic-to-applied research. By building on the science and engineering base established by Federal and private investment, the chemical industry is primed to accelerate the integration of nanoscience and nanotechnology into useful products and services that deliver superior value to customers, benefit society, and bolster competitiveness.

This section of the roadmap presents overarching implementation strategies that support the research priorities. It offers specific recommendations for changing the manner in which research is pursued to accelerate research and innovation.

Overarching Implementation Strategy

Recognizing challenges and defining a strategy are the first steps in realizing the vision of designing materials from the nanoscale. Implementing change and action will require difficult, complex steps. The best path forward will emerge from continued interactions among the key organizations and stakeholders that can lead specific efforts. Some starting points are delineated below:

- Utilize existing technical and business forums and organizations such as the American Institute of Chemical Engineers (AIChE), American Chemical Society (ACS), American Physical Society (APS), Council for Chemical Research (CCR), Materials Research Society (MRS), and the Nanobusiness Alliance to raise awareness and support for the overall roadmap strategy as well as specific research needs.
- Use the Chemical Industry Vision2020 Technology Partnership (Vision2020) and other organizations as focal points for bringing together technology partners (researchers, end users, suppliers, *etc.*) to address specific roadmap needs as well as a forum to build consensus across diverse companies within the industry who have an interest in nanodesign. Form *ad hoc* working groups to outline implementation strategies for various parts of the roadmap and seek out partner organizations to expand the network of resources available.
- Reach out to the Federal agencies participating in the National Nanotechnology Initiative and to state funding agencies that have missions and responsibilities matching the technical objectives addressed in this roadmap. Use the roadmap to leverage financial and technical support for mutual benefit. Encourage NSET to adopt the research strategy and priorities identified in this roadmap as the central strategy of the Nanostructured Materials by Design Grand Challenge. Encourage NSET to coordinate efforts across funding agencies to implement the strategy and fund the R&D priorities to the maximum extent possible, consistent with agency missions.
- Solve complex technical problems in each R&D priority area by developing and implementing more detailed technology strategies and by tracking progress toward the ultimate goal of Nanomaterials By Design. Each research area is essential and will require customized and detailed implementation plans beyond the scope of this roadmap. Plans need to be updated regularly to ensure integration and cross-communication between research areas.
- Sponsor technology forums within university and national laboratory research centers to identify capabilities and research activities corresponding to the roadmap so that they can be leveraged by industry.
- Periodically reevaluate the roadmap to ensure that the route and destinations remain appropriate.

Possible funding agencies include:

- Department of Defense (DOD)
- Department of Energy (DOE)
- Department of Justice (DOJ)
- Department of Transportation (DOT)
- Environmental Protection Agency (EPA)
- Federal Drug Administration (FDA)
- National Aeronautics and Space Administration (NASA)
- National Institutes of Health (NIH)
- National Institute of Standards and Technology (NIST)
- National Science Foundation (NSF)
- U.S. Department of Agriculture (USDA)

Specific Recommendations

To accelerate capability in Nanomaterials By Design, the chemical industry has identified priority recommendations that impact decision making, research effectiveness, and partnering relationships among diverse stakeholders. Some of these recommendations are interrelated.

Funding and Research Approach

- Implement a change in funding strategy and research approach by both NSET and the U.S. chemical industry to ensure that U.S. research efforts are focused on accelerating the development of Nanomaterials By Design.
  - — Increase government spending for research in the physical sciences underlying nanotechnology.
  - — Increase government and company in-house spending on research for fundamentals, synthesis, characterization, modeling, manufacturing and standards focused on solving important industrial challenges. Pre-competitive funding should focus on solving problems that can be leveraged in many applications.
  - — Require an *a priori* focus on the requirements of manufacturing and integration into devices, applications, and processes when implementing research plans and conducting research. Use integrated, multidisciplinary research teams with expertise ranging from fundamentals to applications. This cultural change in the way science and technology are pursued is imperative for surmounting the challenges of predictive nanodesign and accelerating commercialization.
  - — Target R&D toward developing new and improved cost-effective material functionality for market applications.
  - — Prioritize R&D initiatives based on an assessment of potential for enabling commercial value and for contributing to developing Nanomaterials By Design capability.
  - — Foster the development and participation in consortia and assist with planning and data dissemination.
- Implement changes in NSET interaction with the chemical industry.
  - — Provide more opportunities for the chemical industry to be engaged in NNI program planning, project selection, development, and management.
    - o Utilize chemical industry experts in an advisory capacity, including guiding the direction of Federal R&D funding to implement this roadmap.
    - o Include representatives from the chemical industry on the proposal review boards for center proposal and academic grants.
    - o Establish a regularly scheduled forum with representatives of the chemical industry to assess progress in incorporating manufacturing and integration requirements in NSET-funded programs.
  - — Provide funding to government laboratories, academia, and industry for fundamental and application-oriented research allocated in a manner that exploits the best capabilities of each group. Funding allocation should take steps to realize the vision of predictive design and commercialization of nanomaterials in the public interest.

— Host technical workshops and symposia for industry, university, and government researchers on important nanoscale subjects.

— Promote interdisciplinary collaborative research, the results of which should be available to industry.

— Accelerate the transfer of university and government research findings into utilization by the chemical industry by breaking down barriers between universities, government, and industry.

Essential Policies, Resources, and Considerations

- Promote studies on the environmental and health effects of nanomaterials by industry and Federally funded research centers.

  — Use current regulatory procedures to ensure worker and public safety upon exposure to nanomaterials.

  — Educate the public about nanomaterials, and provide the public with the results of the Federally funded studies of health and environmental effects of nanomaterials. Include the public in discussions of nanomaterial safety.

- Promote policies that strengthen chemical company partnerships with national laboratories and universities. For example, support equitable patenting and licensing strategies, especially granting more favorable terms to companies that actively support and collaborate with university research projects, even when significant co-funding is involved.

- Facilitate fast, easy, and no- or low-cost access to national user facilities and other resources for research.

- Provide rapid access to results of Federally funded research by establishing an effective infrastructure and policies.

  — Create a searchable national database containing experimental, modeling, and simulation results on nanomaterials. The database will use a common taxonomy and provide a link between experimentalists and theorists.

  — Create living documents to communicate information about state-of-the-art nanomaterials (*e.g.,* for characterization tools) to the R&D community *via* workshops, books, websites, and other means.

- Establish internationally accepted conventions for standards, including a common "language" for nanotechnology practitioners. The latter will provide nomenclature, definitions, and a glossary of terms to use across disciplines.

  — Authorize and adequately fund a lead government agency (NIST) to set conventions for standards for nanomaterials.

  — Promote a journal in which standard, round-robin verified, synthetic methods; characterization standards; simulation standards; property standards; and standard methods are published.

- Inform the public, manufacturers, and other industries of the benefits of nanomaterial-enhanced materials, devices, applications, and processes.

- Leverage the world-wide knowledge base in nanoscience and technology.

- Encourage government assistance in developing novel approaches to ensure that Federally funded nanotechnology research at universities, government laboratories, and small companies results in innovative products and economic benefit.
  - — Support a third year of funding to Small Business Innovative Research (SBIR) projects for product building and marketing after a compelling midpoint technical and market assessment of the product the grantee hopes to commercialize.
  - — Provide mechanisms for easy transfer of technology from universities, government labs, and small companies to industry.
- Provide funding and effective intellectual property strategies to enable early commercial opportunities such as catalysis, separations, high-performance materials, coatings, energy conversion and storage, pharmaceuticals, therapeutics and diagnostics, sensors, and displays. Concurrently, provide resources to build the foundation for longer-term opportunities such as quantum computing and nanoelectronics.
- Provide investment in workforce education.
- Provide investment in infrastructure to support R&D, including state-of-the-art user facilities, manufacturing research centers, national databases, student education, and information access.
- Create "think-tank" environments where breakaway technologies can be incubated.

Appendices

A. Chemical Industry Vision2020 Technology Partnership: An Overview

The Chemical Industry Vision2020 Technology Partnership (Vision2020) is an industry-led organization focused on accelerating innovation and technology development. The partnership leverages financial and technical resources to establish R&D collaborations in areas of promising or emerging technologies that offer broad benefits for the chemical industry. By bringing together industry, academia, and government on collaborative R&D projects, Vision2020 reduces the risk and enhances the probability of success. Participating companies work together toward common goals to protect the economic interests of shareholders and to foster a sustainable, internationally competitive chemical industry characterized by continued economic growth, new products, improved processes, and environmental responsibility.

In 2002, Vision2020 initiatives succeeded in obtaining $44 million in Federal funds for priority research projects. Chemical companies provided $48 million in matching funds and also contributed time and expenses for Vision2020 planning and activities.

Since Vision2020's inception, 240 organizations have actively participated in technology roadmap development and collaborative R&D partnerships: 143 companies, 70 universities, 12 national laboratories, 10 government agencies, and 5 professional organizations. The program is guided by the Vision2020 Steering Committee which meets quarterly to plan, coordinate, prioritize, and initiate activities. Current members include:

- Air Products & Chemicals Inc.
- BP
- Cargill
- Ciba Specialty Chemicals
- The Dow Chemical Company
- E.I. du Pont de Nemours and Company
- Eastman Chemical Company
- General Electric Company
- Honeywell
- Praxair, Inc.
- Rohm and Haas Company
- American Chemical Society
- American Institute of Chemical Engineers
- Council for Chemical Research
- Materials Technology Institute

Vision2020 is actively seeking participants. Join an activity underway or form an initiative in a new technology area and rally support from Vision2020. Visit www.ChemicalVision2020.org

Appendix B: Overview of the National Nanotechnology Initiative

NNI Program Overview: Interagency Coordination in Support of National Priorities

Organization and Management

The National Nanotechnology Initiative (NNI) is an interagency effort established in fiscal year 2001 aimed at maximizing the return on the Federal Government's investment in nanoscale R&D through coordination of funding, research, and infrastructure development activities at individual agencies. Ten of the Federal agencies participating in the Initiative have funding dedicated to nanotechnology R&D. Other Federal organizations perform related studies and research, apply technologies based on the results from those agencies performing nanoscale R&D, and participate in various NNI activities (See side box for lists of both sets of agencies).

Federal agencies with R&D budgets dedicated to nanotechnology research and development:

- Department of Agriculture
- Department of Commerce (in particular, the National Institute of Standards and Technology)
- Department of Defense
- Department of Energy
- Department of Health and Human Services (in particular, the National Institutes of Health)
- Department of Homeland Security (in particular, the Transportation Security Administration)
- Department of Justice
- Environmental Protection Agency
- National Aeronautics and Space Administration
- National Science Foundation

Other agencies participating in the NNI:

- Department of State
- Department of Transportation
- Department of Treasury
- Food and Drug administration
- Intelligence Agencies

In addition to sponsoring research, Federal support through the NNI provides crucial funds for the creation of university and government facilities with the specialized equipment and facilities required for nanoscale R&D. Federal support also helps educate the nanotechnology researchers of the future, as well as the workforce necessary for the growing use of nanotechnology in industry, primarily by providing funds for undergraduate, graduate, and postgraduate training in nanotechnology-related disciplines. The NNI plays a key role in fostering cross-disciplinary networks and partnerships, and in disseminating information to participating agencies and to the public, through workshops and meetings, as well as via the Internet (www.nano.gov). Finally, it encourages businesses, especially small businesses, to exploit the opportunities offered by nanotechnology.

The NNI is managed within the framework of the National Science and Technology Council (NSTC). The NSTC is the principal means by which the President coordinates science and technology programs across the Federal Government, providing policy leadership and budget guidance. The NSTC's Subcommittee on Nanoscale Science, Engineering, and Technology (NSET) coordinates the plans, budgets, programs, and reviews for the NNI. The Subcommittee is composed of representatives from each participating agency, the Office of Science and Technology Policy, and the Office of Management and Budget.

The National Nanotechnology Coordinating Office (NNCO) serves as the secretariat to the NSET Subcommittee, and supports the Subcommittee in the preparation of multi-agency planning, budget, and assessment activities. To adequately support the growing NNI activities, the position of NNCO Director was changed from part-time to full-time in April 2003. The NNCO also serves as the point of contact on Federal nanotechnology activities for government organizations, academia, industry, professional societies, foreign organizations, and others. Finally, the NNCO develops and makes available printed and other communications materials concerning the NNI, and maintains the Initiative's website.

The Administration is focusing significant attention on the NNI. In order to further strengthen the Initiative, the President's Council of Advisors on Science and Technology (PCAST) has begun an external review of the NNI. The PCAST review will include a comprehensive assessment of the current NNI programs, and will lead to recommendations on how to improve the management of the program. PCAST's review of the Federal nanotechnology research program is an ongoing, long-term activity.

Funding Strategy

The NNI funding strategy is based on five modes of investment, each of which builds on previous and current nanotechnology programs.

The first investment mode supports a balanced investment in fundamental research across the entire breadth of science and engineering. Such fundamental research advances knowledge and understanding of novel physical, chemical, and biological properties of nanoscale materials and systems. This broad investment is critical because the outcome of basic research cannot always be anticipated, and discoveries in one discipline can have unexpected implications in another.

The second investment mode, collectively known as the "grand challenges," focuses on nine specific R&D areas that are more directly related to applications of nanotechnology and that have been identified as having the potential to realize significant economic, governmental, and societal impact.

The nine Grand Challenge areas are:

1. Nanostructured Materials by Design
2. Manufacturing at the Nanoscale
3. Chemical-Biological-Radiological-Explosive Detection and Protection
4. Nanoscale Instrumentation and Metrology
5. Nano-Electronics, -Photonics, and -Magnetics
6. Healthcare, Therapeutics, and Diagnostics
7. Efficient Energy Conversion and Storage
8. Microcraft and Robotics
9. Nanoscale Processes for Environmental Improvement

Research directed toward the grand challenge areas aims to efficiently and effectively accelerate the transition of scientific discovery into innovative technologies that show a return on investment as quickly as possible.

The third mode of investment supports centers of excellence that conduct research within the host institution(s). These centers pursue projects with broad multidisciplinary research goals that are not supported by more traditionally structured programs. These centers also promote education of future researchers and innovators, as well as training of a skilled technical workforce for the growing nanotechnology industry.

The fourth investment mode funds the development of infrastructure, instrumentation, standards, computational capabilities, and other research tools necessary for nanoscale R&D. The centers and infrastructure developed under the third and fourth modes facilitate the basic and applied research supported under the first two modes.

The fifth and final investment mode recognizes and funds research on the societal implications of nanotechnology, and addresses educational needs associated with the successful development of nanoscience and nanotechnology.

Excerpt from *National Nanotechnology Initiative, Research and Development Supporting the Next Industrial Revolution, Supplement to the President's FY 2004 Budget,* February 4, 2003, available at www.nano.gov.

C. Workshop Participants

The results of the "Nanomaterials and the Chemical Industry R&D Roadmap Workshop" are the basis for this roadmap. Information from the workshop can be found at www.ChemicalVision2020.org. The following people participated in the workshop:

Air Force Research Laboratory
Barry Farmer, Ph.D.
Richard Vaia, Ph.D.

Air Products and Chemicals
Kevin Heier, Ph.D.
Frank DiStefano

Altair Nanomaterials
Kenneth Lyon

ATMI (CT)
Frank DiMeo, Ph.D.

BP
John Forgac, Ph.D.
Joseph Golab, Ph.D.

Cabot Corp.
Jim Menashi, Ph.D.

CNI
Dan Colbert, Ph.D.

Cornell University
Hector Abruna, Ph.D.
Emmanuel Giannelis, Ph.D.
Graham Kerslick, Ph.D.

Department of Defense
Cung Vu, Ph.D.

DOE/Center for Integrated Nanotechnologies (CINT), Sandia National Lab
Terry Michalske, Ph.D.

Dow Chemical Company
Susan Babinec
Mark Bernius, Ph.D.
Michael Elwell, Ph.D.
Gregory Meyers, Ph.D.
Gary Mitchell, Ph.D.
Paul O'Connor, Ph.D.
Bill Rafaniello, Ph.D.
Joey Storer, Ph.D.

Dow Corning Corporation
Gary Burns, Ph.D.

E.I. du Pont de Nemours and Company
Gregory Blackman, Ph.D.
Rajeev Gorowara, Ph.D.
Kostas Kontomaris, Ph.D.
William Provine, Ph.D.
Douglas Spahr, Ph.D.
Shekhar Subramoney, Ph.D.
Qian Qiu Zhao, Ph.D.

Energetics, Incorporated
Jim Carey
Melissa Eichner
Jack Eisenhauer
Nancy Margolis
Shawna McQueen
Joan Pellegrino
Richard Scheer

Food and Drug Administration
Ellen Chen, Ph.D.

General Electric Company
Pierre Bui, Ph.D.
Suryaprakash Ganti, Ph.D.
Mano Manoharan, Ph.D.
Fazila Seker, Ph.D.
Judith Stein, Ph.D.
Julie Teetsov, Ph.D.

Hyperion Catalysis International, Inc.
Robert Hoch

IBM T.J. Watson Research Center
Shouheng Sun, Ph.D.

Lucent Technologies/Bell Labs
Julia Hsu, Ph.D.

NanoScale Materials, Inc.
Kenneth Klabunde, Ph.D.
Bill Sanford

Nanotechnologies, Inc.
Randy Bell
Denny Hamill, Ph.D.

National Energy Technology Laboratory
Brad Bockrath, Ph.D.

National Institute of Standards and Technology
Robert Shull, Ph.D.
Francis Starr, Ph.D.
Stephan Stranick, Ph.D.

National Institutes of Health
Jeffery Schloss, Ph.D.

National Science and Technology Council
Mihail Roco, Ph.D.

Naval Research Laboratory
Richard Colton, Ph.D.
James Murday, Ph.D.

Oak Ridge National Laboratory
Elias Greenbaum, Ph.D.
Sharon Robinson, Ph.D.
David Wesolowski, Ph.D.

Pacific Northwest National Laboratory
Chris Aardahl, Ph.D.
Glen Fryxell, Ph.D.

Penn State University
Stephen Fonash, Ph.D.

Praxair, Inc.
Kevin Albaugh, Ph.D.
Ben Bikson, Ph.D.
Chien-Chung Chao, Ph.D.
Paul Gilman, Ph.D.
Frank Notaro, MS, PE
Jack Solomon, Ph.D.

Purdue University
Gil Lee, Ph.D.

RAND
Richard Silberglitt, Ph.D.

Rice University, Houston
Wade Adams, Ph.D.

Rohm and Haas Company
Nate Brese, Ph.D.
Susan Fitzwater, Ph.D.
Catherine Hunt, Ph.D.
Casmir Ilenda, Ph.D.
Frank Lipiecki, Ph.D.
Alan Nakatani, Ph.D.

Small Times
Doug Brown

U.S. Department of Energy
Altaf Carim, Ph.D.

U.S. Department of Energy, Office of Industrial Technologies
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U.S. EPA, ORD, NCER
Nora Savage, Ph.D.

University of California, Santa Barbara
Mathew Tirrell, Ph.D.

University of Delaware
Norm Wagner, Ph.D.

University of Pittsburgh
Anna Balazs, Ph.D.

University of Wyoming
Daniel Buttry, Ph.D.

UOP-LLC
Robert Bedard, Ph.D.

USDA/CSREES/PAS
Hongda Chen, Ph.D.

Office of Science and Technology Policy, Executive Office of the President
Thomas Mackin

WTEC, Inc.
R. Duane Shelton, Ph.D.

D. Nanomaterials Today: A Primer

As an emerging field of research, nanomaterials are unfamiliar to many individuals. This primer is intended to provide a brief background on the status of the field today.

The unique properties of nanoscale materials are size dependent; they do not naturally occur in larger bulk materials. The following explanations have been offered to account for the presence of these properties at the nanoscale:

- High surface-to-volume ratios, which can, for example, result in greater than predicted catalytic activity
- Cooperative phenomena amongst a limited number of atoms or molecules, prior to onset of bulk behaviors
- Quantum confinement effects in a nano-sized structure.

Today, nanomaterials that offer some unique properties may find application as pure materials or may be integrated into larger structures. Examples of pure materials include polymer clay nanocomposites for structural applications and quantum dots for applications in optical imaging. Examples of integrated structures include nanoparticle drug delivery systems, batteries, sensors, and fuel cells.

Nanomaterials are generally categorized into three main groups: fundamental building blocks; dispersions or composites of building blocks in randomly ordered matrices; and spatially resolved, ordered nanostructures. Exhibit D.1 provides definitions and descriptions of current capabilities for each group. Products have already been commercialized in all three categories. Nanotechnology-based products now on the market have been produced primarily as the result of empirical investigation and, to a lesser extent, the design of specific material structures. These design efforts tend to exploit niche areas in which the materials have been intensively studied for decades.

The chemistry and physics of simple atoms and molecules is fairly well understood, predictable, and no longer considered overly complex. This contrasts markedly with the current state of knowledge of nanomaterials. Our understanding is inadequate to predict the complex behavior of these materials. Although strides have been made in computational chemistry, bridging across length scales from nano to macro remains a major challenge. Biological systems have been suggested as potentially useful models for assembly, yet current understanding of biology at the nanoscale is also insufficient to allow synthesis at rates required for manufacturing based on biological principles.

Exhibit D.1 Major Categories of Nanomaterials

Nanomaterial "Building Blocks"

Base assemblies of atoms or molecules, or other elementary assemblies of atoms or molecules (*e.g.*, crystals), that have at least one of their dimensions smaller than 100 nm. Base assemblies can have normal unit structures or complex unit structures with dimensions in the nanoscale range.

Current Capability: Numerous nanomaterial building blocks are produced for commercial applications using diverse methods (*e.g.,* from vapor phase, from solution precipitation and templating, and via attrition of solids.)

Building Blocks:	Synthesis Methods:	Examples:
• Metal and ceramic nanopowders • Carbon nanotubes • Carbon nanospheres • Nanowires • Quantum dots • Dendrimers • Protein and structured polymer strands	• Colloid and emulsion chemistry • Sol-gel • Strained layer growth • Mechanical attrition • Gas phase condensation • Molding • Solution phase templating	• Building blocks for higher order structures, preferably with self assembly capability • Transducers for sensing • Fluorescent tags • UV laser cavity • Semiconductors for photovoltaic energy conversion and for flexible electronics

Dispersions

Three dimensional, solid or liquid matrices that incorporate uniformly dispersed nanomaterials.
Current Capability: Dispersion of particulates in liquid, solid, or gel phases.

Building Blocks:	Dispersion Methods:	Examples:
• Nanosize carbon (carbon black) • Nanosize clay • Nanosize metal oxides	• High energy milling • High shear mixing • Sonication • Extrusion	• Reinforcement of automotive tires with carbon black • Nanoclay dispersed in polypropylene for high strength composite • TiO_2 formulated into sunscreen • Field modified liquid properties (*e.g.,* ferrofluids)

Ordered Nanostructures

Spatially resolved nanometer scale objects via precise placement of nanomaterials and arrays of nanomaterials prepared from the building blocks and ordering methods.

Current Capability: Top-down methods–Optical lithography can provide 30 nm resolution with limited capability for 3-D resolution. Bottom–up methods–Ability to create structural features with physical dimension from 1 nm to 100 nm in both 2-D and 3-D arrayed structures, with limited capability for extension into high-fidelity long-range ordered structures.

Building Blocks:	Ordering Methods:	Examples:
• Particles • Arrays/layers • Macromolecules • Assemblies • Networks	• Lithography – photon, electron, embossing, contract printing, dip pen • Self-assembly • Directed self-assembly • External fields • Templates • Molecular recognition	• Phase segregated block copolymers • Colloidal crystals • Layered or multilayered structures • Aligned or periodic 2-D and 3-D arrays • Nanoporous membranes • Net shape formed ceramics • High density memory (>10 $Gbit/cm^2$)

Limited tools and synthetic capability now exist (see inset). These tools provide impressive capabilities to measure, move, distribute, and assemble atoms or molecules, but are generally unsuitable for large-scale manufacturing. The resolution of photolithography, for example, is currently about 100 nanometers, and significant feature size reduction will be required to prepare the nanomaterials of the future.

Current Tools and Procedures

- Scanning tunneling microscope (STM)
- Scanning probe microscope (SPM)
- Molecular beam epitaxy (MBE)
- Dip pen lithography (DPN)
- Synthetic methods
  —Templating
  —Colloid chemistry

Methods to synthesize materials with defined properties and spatial resolution are also limited. One approach is the use of self-assembly to prepare new nanomaterials in which the primary interactions are weak covalent or noncovalent interactions. New, more powerful tools and robust synthetic methods will be needed to reveal and exploit the complex nature of the nanoscale and to manipulate atoms and molecules into nanostructures with defined structures. Thus, more robust, economical tools and synthetic processes will be required to advance the field from the laboratory to the manufacturing environment.

Manufacturing processes and application environments pose significant challenges to the successful use of nanoscale building blocks. A typical nanomaterial, for example, is more reactive than its bulk counterpart and may be more sensitive to the surrounding environment. Processing methods may be required to address this sensitivity.

E. Target Material Capabilities and Market Opportunities

The R&D strategy and priorities presented in the roadmap will promote broad commercialization of nanomaterials by emphasizing predictive development of nanomaterial building blocks, dispersions and composites, and ordered nanostructures. This section presents an un-prioritized list of important material capabilities and market opportunities for new nanomaterial-enhanced and nanomaterial-enabled materials. Many of these capabilities and opportunities have multiple uses in military, industry, and other applications. The table of Target Material Capabilities Enabled by Nanomaterials and Nanotechnologies provides examples of material properties and capabilities that could be improved and/or developed by nanoscience innovations. The table of Key Market Opportunities for Nanomaterials provides examples of markets and products/processes that could utilize targeted enabling materials. Together, these tables illustrate the far reaching impacts and benefits nanomaterials could have on the U.S. economy and society.

Targets		Key Market Opportunities												
	Target Material Capabilities Enabled by Nanomaterials and Nanotechnologies	Environment	Energy	Food and Agriculture	Medical and Health	Chemicals	Manufacturing	Housing/Construction	Transportation	Electronics and Information Technology	Personal Care	Textiles	Entertainment	Cross Cutting
1	High selectivity, high yield, nontoxic nanosize catalysts that operate at low temperatures. Applications include: Chemicals and petrochemicals Environmental applications Biotransformations (biocatalysts to utilize renewable raw materials)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
2	Efficient, low-cost solar cells	✓	✓		✓	✓		✓	✓					✓
3	High-efficiency, low-cost fuel cells and materials (including, low-cost electrolytes)	✓	✓					✓	✓					
4	High-selectivity, high-capacity sorbents *e.g.*, Hydrogen storage Removal of environmental trace toxics	✓	✓	✓	✓	✓		✓	✓	✓				✓
5	Superior barriers with novel properties *e.g.*, Molecular recognition Low permeability to oxygen Time release capabilities	✓	✓	✓	✓	✓								✓
6	Novel coatings with superior properties from ships to chips, *e.g.*, low volatile organic compounds (VOC) and/or solvent-less, multi-functional (*i.e.*, functionality without scattering light); self-healing; durable, resistant and weatherable (thermal, UV, corrosion, erosion, friction, impact and wear); anti-fouling and/or anti-microbial; containing novel dyes and pigments; energy efficient; thin coating; etc.	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

Targets		Key Market Opportunities												
	Target Material Capabilities Enabled by Nanomaterials and Nanotechnologies	Environment	Energy	Food and Agriculture	Medical and Health	Chemicals	Manufacturing	Housing/Construction	Transportation	Electronics and Information Technology	Personal Care	Textiles	Entertainment	Cross Cutting
7	Environmentally friendly, target-specific agents, *e.g.*, herbicides, pesticides, biocides	✓		✓										
8	Novel multifunctional fertilizers	✓		✓										
9	Nanopore structures for DNA sequencing			✓	✓									✓
10	Nanostructured nanoparticles and thin film coatings with quantum properties *e.g.*, Photonic bandgap materials Quantum dots	✓	✓			✓				✓				✓
11	Electron emitting devices		✓		✓			✓		✓			✓	✓
12	Photovoltaics and thermoelectrics	✓	✓				✓	✓						
13	Low-cost, ultra-pure gases					✓				✓				✓
14	Strong, lightweight industrial and construction materials	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
15	Super strong adhesives and cements			✓			✓	✓	✓			✓	✓	✓
16	Nanomaterials for net shape manufacturing of strong, ductile ceramics, metals, and cermets	✓	✓				✓	✓	✓					
17	Nanosensors and nanosensing materials *e.g.*, Biosensors Chemical and environmental sensors	✓			✓	✓								✓
18	Sensor bearing "smart" materials	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
19	High energy density batteries and supercapacitors	✓	✓				✓	✓	✓	✓				✓
20	Novel resins (strong, fire resistant, electrically and thermally conducting, etc.)	✓		✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
21	High-temperature, light weight, high-strength metals and ceramics		✓		✓				✓				✓	
22	Low-cost, high-strength nanodimensional fibers with special properties *e.g.*, Flame retardant Dirt and odor resistant							✓	✓			✓	✓	✓
23	Novel pharmaceutical and medical materials *e.g.*, Nanomaterial platforms for drug delivery Medical diagnostics and gene therapy Biomaterials				✓						✓		✓	
24	Molecular electronic materials and devices				✓		✓			✓			✓	✓
25	Magnetic nanomaterials and devices	✓	✓				✓		✓	✓			✓	
26	Optical computing		✓							✓			✓	
27	Optical displays		✓				✓			✓				✓
28	Materials to repair, enhance and protect: eyes, hair, facial and body tissue, and bone				✓						✓		✓	

Key Market Opportunities for Nanomaterials

Key Market Opportunities	Priority Products/Processes
Environment	• Chemical and biosensors • Environmental sensing (toxics) • Remediation (TiO_2 +UV, catalysts, *etc.*) • Clean water (nano-filtration, sorption, exchange) • Clean air (adsorbents) • Catalysts (hydrodesulfurization, emulsion) • Hydrogen storage for fuel cells • "Green" technologies (manufacturing) • Environmental upgrading of fuels (catalysis, separations)
Energy	• Energy conversion (Gratzel [photolytic] cell type devices-dye plus nano inorganic, solid polymer heterojunctions) • Energy storage (hydrogen storage, nanotubes) • Batteries (high performance electrodes and electrolytes) • Fuel cells • Alternative energy • Thermoelectrics • Magnetocaloric effects • Solid state lighting • Supercapacitors • Stronger pipes for distribution of natural gas • Thermal barriers for materials enabling higher temperature combustion • Materials for nuclear fusion devices • Motors (higher efficiency through better magnets) • High-performance catalysts • Low power consumption lighting and displays
Food and Agriculture	• Targeted, non-toxic bio-degradable pesticides, herbicides • Time-released fertilizers and pesticides • Packaging • Freshness, contamination and/or tampering sensors • Genetic improvement of plants and animals • Delivery of genes and drugs to plants and animals
Medical and Health	• Nanosensors for early detection • Nanomachines for therapy • Sterilization and control of superbugs in medical facilities • Rapid DNA sequencing for diagnostics and therapeutics (DNA chips) • Remote and in vivo devices • Drug discovery (miniaturization, bio arrays) • Drug delivery – directed delivery of actives to target sites • Prosthetics • Tissue engineering (biocompatible, high performance materials) • Diagnostic imaging • Minimally invasive surgery
Chemicals	• Petrochemical processing (nanocatalysts for high yields, greater energy efficiency) • Chemical separations (well structured pores, sorbents, membranes) • Chemical catalysis • Filtration systems (nanodesign) • Chemical and bio arrays, DNA sequencing, electrophoresis • Alternate feedstocks
Manufacturing	• Highly selective control sensors • Manufacturing nanostructured metals, ceramics, polymers (no machining) • Cutting tools (carbide control nanocoating) • Materials that are halogen-free, low or no heavy metals, low volatile organic compounds (VOCs)
Housing/Construction	• Improved bonding and strength/toughness (smaller materials) • Concrete (nanotubes or carbon fibers fillers) • Drill bits (stronger, longer lasting) • Steel (stronger because of nanostructure)

Key Market Opportunities	Priority Products/Processes
	• Lighter, more durable composites • Low-VOC and/or solvent-less, multi-functional coatings (paint) • High-performance insulating materials
Transportation	• Thermal barrier materials for engines • Wear resistant materials for brakes and moving parts • Nanocomposites (lighter, more durable) — Automobiles (replace steel in cars) — Aerospace (reduction in size and weight of structure and skin) • Avionics (nanoelectronics, nanosensors) • Replace carbon black in tires • Superior coatings and adhesives
Electronics and Information Technology	• Batteries • Nano electronic devices • Nanocoatings • Nanofabrication on a chip • Nanostructured microprocesses • Small mass storage devices (1000x) • Integrated nanosensor systems for massive data handling • Communication systems (higher frequencies, optical spectrum with 10^x bandwidth) • Virtual reality • Individual teaching aids • Information processing capability • Optical coatings • Optical computing
Personal Care	• Low-toxicity, high-efficiency sunscreen additives, SPF enhancers • Transparent UV absorbers, transparent hard coatings • Hair and skin care • Special effect pigments with good application properties • Dental materials with improved strength, adhesion, application properties • Deodorants (absorbents) with improved efficacy and less skin irritation • Anti-aging creams • Biodegradable materials (detergents)
Textiles	• Nanofibers – strong and durable • Functional fibers for soil resistance, detoxification, deodorizing, biostat, antistat, etc.
Entertainment	• Improved printing, digital imaging (better dyes and pigments) • Virtual reality • Optics and optical displays
Cross Cutting (*i.e.*, applicable to a diverse range of markets and products/processes)	• Coatings (thermal, fouling, corrosion, wear, friction, impact, self-healing, smart) • Barrier coatings for mass transport (control release, selective delivery) • Material separation and purification • Structural materials (light weight, high strength, durable, weather resistant) • Self-cleaning • Antimicrobial • High pressure systems • Highly selective sensors (lab-on-a-chip) • Highly selective catalysts • Highly selective sorbents and membranes • Virtual reality training • Automation and robotics • Electroactive and conductive polymers • Energy-wear coatings • Photonic band gap materials; holographic, optical and magnetic storage • Sustainable "green" chemistries

F. Summary of R&D Priorities for Nanomaterials By Design

Fundamental Understanding and Synthesis			
Rank	**Timeframe**	**R&D Priority**	**Impact**
		Develop Fundamental Understanding of the Physics and Chemistry at the Nanoscale	
Top	20 years	**Develop a fundamental understanding of structure-property-processing relationships at the nanoscale** Understand the origin of unexpected nanoscale behavior and develop the ability to predict properties such as: — Hardness and ductility — Electronic and optical properties — Mass transport — Reactivity — Catalytic properties — Thermoelectric and piezoelectric properties — Magnetic properties	• Enhanced understanding of structure-property relationships redirects R&D continuously (ongoing) • Enabling capability provided for nanomaterial development *via a priori* prediction of structure-property relationships (years 10-20) • Database details structure-property relationships at all length scales (years 10-20)
Top	15 years	**Develop models, theories and experimental validation of physics and chemistry at the nanoscale, including the kinetic and thermodynamic principles guiding synthesis and assembly** • Phase diagrams for nanostructured materials to control composition and phase of nanomaterials • Basic knowledge of self-assembly processes, particularly those governed by noncovalent forces (*e.g.*, understanding biological processes such as molecular recognition and templated synthesis, and translation of these principles to man-made systems) • Nucleation, growth and disassembly mechanisms • Mechanisms controlling interfacial interactions in the production of nanoparticles (non-agglomeration), dispersions, nanocomposites, and ordered spatially-resolved nanostructures—especially understanding defect control and placement, uniformity and control, particle size control, and integration of dissimilar materials such as organic/inorganic/biological composites • Mechanisms controlling heterogeneous integration across time and length scales • A database of key nanomaterial properties (*e.g.*, physical, chemical, mechanical) that compares performance to bulk materials. This dataset is needed to reveal unexpected similarities, differences, and unique atributes within groups of building blocks and assemblies. The database will allow the determination of the minimal set of fundamental building blocks with distinct properties so that the lowest common structural denominator for a given property may be ascertained • A toolkit of kinetic and thermodynamic rules for synthesis and assembly which researchers can use to rationally design nanomaterials from first principles	• Database of key nanomaterial properties (years 5-10) • Toolkit of kinetic and thermodynamic rules for synthesis and assembly (year 15)

		Develop Synthetic Strategies for Rational Nanomaterial Design	
Top	**15 years**	**Develop new paradigms for creating nanoscale building blocks based on understanding the physics and chemistry at the nanoscale** • New catalysts for nucleation, growth, and disassembly of nanostructures • Methods to reliably and easily functionalize surfaces to control interfacial interactions and agglomeration	• New synthetic methods available based on the understanding of nanoscale physics and chemistry (years 5-10) • New materials not previously imagined are commercially feasible and cost-effective (years 10-15)
Top	**15 years**	**Develop new design strategies and paradigms for the controlled assembly of nanocomposites and spatially resolved nanostructures with long-range order** • New bottom-up methods based upon exploitation of biological principles such as molecular recognition and templated synthesis, and supramolecular chemistry • Methods to integrate across length and time scales with dissimilar materials (hierarchical heterogeneous integration)	• Knowledge of parameters governing self-assembly (years 10-15)
Top	**10 years**	**Develop new high-throughput screening methods to determine structure-property relationships**	• New high-throughput screening methods (years 5-10) • New synthetic strategies (years 5-10) • New materials obtained via high-throughput screening (year 10) • New rapid, highly efficient, parallel methods for analysis of nanoscale properties (year 10)
Top	**20 years**	**Determine nanomaterial performance at the laboratory scale** • Screen nanomaterial performance in applications at the laboratory scale • Develop device and application design concepts and paradigms based on exploitation of the properties of the nanoscale • Develop systems approaches to enable new, paradigm-shifting applications using nanomaterials	• Total systems approach to Nanomaterials By Design is consistently employed to accelerate commercialization (years 15-20)
High	**20 years**	**Develop a compendium of methods to synthesize and assemble nanomaterials that will perform pre-determined functions in specific applications**	• Peer-reviewed compendium of synthetic methods (years 3-5) • Significant documentation of peer-reviewed synthetic methods available (year 20)
		MANUFACTURING AND PROCESSING	
Rank	**Timeframe**	**R&D Priority**	**Impact**
Top	**5 years**	**Develop unit operations and robust scale-up and scale-down methodologies for manufacturing** • Models and documented design tools to scale-up/scale-down processes quickly and effectively • Processes to engineer materials at the device level that retain properties of nanoscale (*e.g.*, retention of nanograins in sintered consolidated material) • Reliable passivation techniques to allow safe handling and preservation of nanomaterial functionality • Processes for nanomaterial emissions control • Purification and classification processes	• Nanomaterial supplies available, satisfying industry needs in various applications (year 2) • Identical materials supplied on gram or ton scale (year 5)

High	20 years	**Develop novel manufacturing techniques for hierarchical assembly** • Robust reproducible self-assembly techniques that integrate synthesis and assembly functions of manufacturing and minimize labor and energy input • Efficient modular tools for building-block assembly	• Demonstrated commercial viability of self-assembly methods in select markets (year 10) • Novel manufacturing techniques displace many traditional techniques (year 20)
High	5 years	**Develop dispersion and surface modification processes that retain functionality** • Determine how much of the current micro-scale technology is transferable to the nanoscale • Techniques for direct measurement of dispersion characteristics and surface modification in the manufacturing environment • Ability to address contamination in the process • Broad library of scalable surface functionalization and compatibilization techniques for modifying and dispersing all families of nanoparticles while retaining functionality	• Incorporation of nanomaterials into polymer or liquid matrices commercially practiced in multiple industries (year 2) • Standard, reproducible methods to tailor nanomaterial surfaces employed in manufacturing (year 5)
High	20 years	**Develop process monitoring and controls to achieve nanomaterial and product consistency** • Robust, rapid QC tests • "Smart" responsive control systems for real-time processing based on improved analytical tools that provide on-line imaging techniques	• Responsive control systems developed for key physical properties, such as particle size distribution (year 10) • First-pass yield reaches 100% (year 20) • Process control expanded to chemical parameters, such as surface functionality (year 20)
High	20 years	**Develop processes to integrate engineered materials into devices while retaining nanoscale properties** • Manufacturing methods that cross material-scale boundaries • Processes that integrate engineered materials at the device level while retaining properties of the nanoscale	• Nanoscale effects become practicable in real-world objects (year 20)
Medium	5 years	**Develop the ability to remove impurities from raw material precursors to meet application specifications** • Understand the raw material requirements (solids, liquids, and gases) to ensure the quality of nanomaterialsproduced for specific applications	• Raw material quality no longer limits nanomaterial commercialization (year 5)
CHARACTERIZATION TOOLS			
Rank	**Timeframe**	**R&D Priority**	**Impact**
Top	20 years	**Develop real-time characterization methods and tools needed for research and manufacturing** • Advanced methods and instrumentation (hardware and software) to provide chemical and physical properties and structural information in *real-time*, with 1-nm or less spatial resolution, including, but not limited to: — Spectroscopies — Scattering techniques (Fourier Space) — Microscopies (Real Space) • Integrate individual techniques into 2-D, *real-time* multi-probe systems — Improved sample handling and manipulation — Miniaturization capability	• 1-D tools provide brighter sources, improved optics, detectors with better signal/noise, lower detection limits, improved spatial resolution (years 1-15) • 2-D tools provide parallel sampling with parallel probes; advanced nanoscale machining (years 5-15) • 3-D tools provide simultaneous x,y and z sampling and processing for research and manufacturing applications (years 10-20)

		— Vibration isolation capability — Reproducible interprobe performance — Operation *in-vacuo, in-vitro,* and *in-vivo* • Complete integration of single probes and multiprobe techniques into *real-time*, 3-D imaging tomography — New data design algorithms — Assimilation of robust tools into manufacturing environments	
High	**5 years**	**Develop the infrastructure essential to tool development and manufacturing** • Provide affordable access to specialized government tools and facilities — Improved access to facilities with high-end technologies (*e.g.*, beamlines) for proprietary projects including standardized procedures — Uniform, user-friendly policies across all federal laboratories and across all federal agencies (*e.g.*, standardized forms and policies especially regarding intellectual property and access) — Additional user facilities • Build partnerships to ensure the development of high-end, next-generation analytical tools — Develop network between instrument makers (research and commercial) and users for feedback and expediting tool development — Foster multi-disciplinary collaborations for new tool development: ○ Across disciplines: analytical, modeling and processing ○ Across industries ○ Across vendors and users • Determine the facility requirements for analytical tool development and operation — Identify facility requirements — Support retrofitting existing analytical facilities to satisfy the requirements for nanoscale analytical tools so individual users (individual companies and researchers) can economically upgrade and maintain their own facilities • Foster the commercial development of affordable, robust analytical tools suitable for research and manufacturing environments — Develop a training program at user facilities — Develop robust, user-friendly tools capable of being operated in a manufacturing environment • Develop effective data acquisition and management strategies and tools — Establish a central repository for data. Identify an organization to address data management issues and establish appropriate methods for exchange of pre-competitive information	• Infrastructure available to support development of tools for research and manufacturing (years 1-5) • Increased access and uniform usage policies for national laboratory facilities (years 1-5) • Improved information technology hardware and software for data acquisition and analysis support progress in tool development and other research areas (years 1-5)

Modeling and Simulation

Rank	Timeframe	R&D Priority	Impact
Top	**20 years**	**Develop fundamental models to accurately predict nanostructure formation** • Methods for including chemistry (reaction and degradation) in force-field modeling to understand nanostructure formation • Modeling of the chemistry of deformable interfaces • Integrate chemical functionality of nanomaterials into models • Link molecular simulation output to constitutive models • Methods for comparing equilibrium, non-equilibrium, and kinetically-trapped systems	• Models provide insight into nanostructure formation for continually improved processes (year 3) • Models connect lessons learned between discrete experiments, facilitating cross-application of knowledge (year 10) • Predictive models available for multiple types of nanostructures (year 20) • Novel nanostructured materials identified from theoretical understanding (year 20)
Top	**20 years**	**Develop methods for bridging models between scales, from atoms to self-assembly to devices** • Link modeling and simulation results to experimental data • Simultaneously incorporate atomistic and mesoscale techniques in *ab initio* methods to predict properties or extract atomistic contributions from observed properties • Advance molecular dynamics (MD) simulation methods • Models of properties that apply to industry and consider unique scaling laws from nano to meso to macro scale (*e.g.*, mechanical, electrical, magnetic, optical, convective transport [heat, momentum, mass], diffusion, thermodynamic equilibria, including adsorption, surface-surface interaction, and chemical reaction) • Extend models to recognize and predict new and unexpected emergent properties of self-assembled systems • Expand models to understand and predict toxicology and environmental impact • Develop and validate extensions of continuum models from the macroscale to the nanoscale • Combine simultaneous effects (such as a flow dynamics and thermodynamic driving forces) to provide a powerful tool for evaluating potential technologies • Integrate *ab initio* and combinatorial modeling approaches to improve efficiency	• Nanomaterial use increases as new performance characteristics are discovered (year 3) • Predictive models for macroscopic performance inspire the use of new materials (year 10) • Nanostructure – macroproperty relationships predict performance *a priori* (year 20) • Nanostructures reverse engineered from desired macroscopic properties (year 20)
High	**10 years**	**Improve research infrastructure to support model advancement** • Support and integrate national centers for advancement of nanoscale modeling, simulation, and informatics to: — Develop and validate new models and simulation methods — Provide a "moon shot-like" intellectual focus for the research community (actual centers, not virtual centers, as personal interactions are vital to cross-fertilizing techniques) — Conduct multidisciplinary research with a team focus — Facilitate sabbaticals for industrial, university, and government researchers • New computational architectures for breakthrough performance in quantum mechanical simulation and calculation • Information exchange protocols and infrastructure for data acquisition, interpretation, and dissemination	• Increased production of models and simulations for nanostructured materials (year 5) • Specialized tools and techniques to facilitate nanomaterial simulation (year 10) • Highly trained workforce available in theoretical and practical modeling, simulation and informatics of nanomaterials (year 10)
		The informatics needs for modeling and simulation are presented in the Standards and Informatics section.	

Environment, Safety, and Health			
Rank	**Timeframe**	**R&D Priority**	**Impact**
High	**20 years**	**Assess human health and environmental impact hazards** • Determine the health, toxicological, and epidemiological effects and environmental impact resulting from the creation and existence of nanostructures • Determine the biological fate of nanomaterials • Identify model systems to extend findings across classes of materials • Establish and fund an accessible national ES&H database that collects peer-reviewed research from all sources. Encourage industrial researchers to to participate in the process • Encourage research investment in ES&H by all interested parties and collaboration between researchers to provide peer-reviewed analysis • Conduct independent, government-funded research to validate health and environmental impacts and to promote confidence in research findings and acceptance of nanomaterial use	• Compilation and survey of pertinent literature (year 1) • Identification of model systems to perform in-depth analysis (year 2) • Acute toxicology study on model systems completed (year 5) • Exposure protocol and relevant testing established (year 5) • Chronic and developmental toxicology on model systems completed (year 7) • Environmental impact of model systems determined (year 20)
High	**5 years**	**Determine exposure potentials for nano-sized materials** • Determine the make-up of product and waste streams needed to establish nanomaterial exposure potentials • Develop new methodologies for exposure sampling and analysis, both in the environment and in the workplace • Determine transport mechanisms for nanomaterials in various environmental media • Develop accurate real-time monitoring of environmental nanomaterials • Determine the environmental persistence and bioaccumulation potential of nanomaterials • Estimate impacts through the entire product life cycle using Responsible Care® principles • Develop science-based exposure limits from research results	• Nanomaterial product/waste streams characterized (year 1) • Real-time monitoring incorporated into control/containment systems (year 5)
Top	**5 years**	**Establish handling guidelines for operations involving nanomaterials** • Develop best practice exposure control methods for R&D and manufacturing environments involving nanoscale products • Determine effectiveness of current PPE for nanoscale materials • Manufacture affordable new PPE equipment, handling, and monitoring systems • Develop control/containment systems for nanoscale materials (filtration, fluid/powder handling) • Develop an education program to communicate appropriate safe work practices • Foster NIOSH and ACGIH® involvement and encourage completion of an independent assessment • Recommend protocols guiding nanomaterial handling	• Communication document providing safe work practices distributed (year 1) • Effectiveness of existing personal protection equipment (PPE) determined (year 2) • Best practices for exposure control of nanomaterials established (year 5)

Standards and Informatics			
Rank	**Timeframe**	**R&D Priority**	**Impact**
Top	**20 years**	**Develop standard procedures for nanomaterial synthesis** • Develop reproducible methods for synthesis of high-quality nanomaterials with agreed-upon analytical criteria • Conduct round robins to validate synthetic methods • Publish validated synthetic methods in dedicated, peer-reviewed publications	• Peer-reviewed journal dedicated to standard nanomaterial synthetic methods (now) • Documented list of standard nanomaterial synthetic methods (years 2-10) • Standard procedures to control the

			composition, size, dispersivity, and functionalization of nanomaterials (years 5-10) • Standard procedures to control dispersion of nanomaterials (years 5-10) • Standard methods for self assembly (year 20) • Source of well-characterized nanomaterials for property determination/validation (years 10-20)
Top	**20 years**	**Develop a set of reference materials for property measurement standardization** • Identify appropriate reference standards for the chemical industry • Manufacture a commercially available library of high-quality standard reference materials for property measurements and disseminate it throughout the chemical industry • Conduct round robins to calibrate reference materials and standards	• New analytical tools generate data, enabling other research areas (years 3-20) • Reliable standard reference materials available as physical standards for all desirable properties (years 3-20)
Top	**20 years**	**Develop standard methods for physical and chemical property evaluation** • Identify the best methods for obtaining any given physical or chemical property • Rapidly disseminate round robin results to tool and method developers • Ensure that certified methods possess the flexibility to adapt to novel approaches and incorporate key learnings to mainta in the most up-to-date practices • Develop statistical evaluation techniques for validation and analysis of the properties of nanomaterials • Conduct round robins to validate standard methods • Document standard methods in ASTM, IUPAC, and other publications	• Publication of various ASTM or other certified methods for measuring diverse nanoscale chemical and physical properties (years 3-20) • Analytical tools conform to certified methods (years10-20)
High	**10 years**	**Develop computational standards to improve information processing and transfer for modeling and simulation** • Develop an easily accessible and searchable National Data and Model Repository to improve information processing and transfer for modeling and simulation • Establish standards for communication between modeling modules • Define common taxonomy and units • Provide remote communication to link experimentalists to modelers to facilitate virtual collaboration • Develop library of validated modeling and simulation protocols that can be accessed by industrial users • Establish a modeling architecture that supports modeling integration	• National Data and Modeling Repository established (year 1) • Virtual community established in parallel with bio-informatics efforts (year 5) • Improved ability to utilize knowledge developed by other practitioners (ongoing) • Improved productivity of modeling and simulation efforts (faster development, cross-disciplinary application, and broader application of developed models) (ongoing)
Top	**10 years**	**Develop standards for material evaluation in applications** • Standardized and readily implemented (*i.e.*, robust and economical) quality control (QC) protocols are required to measure key physical and chemical properties of nanomaterials • Develop standard micro- and macro-scale integration platforms for measuring the properties of imbedded nanmaterials and devices	• Standard methods for characterization and QC of nanomaterials are widely accepted and uniformly practiced, enabling accurate decisions to be made on the suitability for given applications (year 10)
Top	**5 years**	**Establish internationally recognized nomenclature standards** • Define and document a common nomenclature including taxonomy and units (*e.g.*, similar to IUPAC)	• Common nomenclature and taxonomy accepted (year 3) • Common language accepted and

		• Develop a common "language" for nanotechnology practitioners (definitions, glossary of terms, *etc.*)	consistently used (year 5) • Significant increase in communication between researchers and consumers of nanotechnology information (ongoing) • Significant improvement in the reproducibility of results and speed of technology transfer (ongoing)
High	**5 years**	**Establish the organizational infrastructure and other requirements to foster standardization and development of standards** • Develop internationally recognized calibration standards, validated measurement technologies and robust protocols • Establish a journal to report standard synthetic methods verified by two or more independent research groups and procedures for synthesizing reference standards for property evaluation • Develop stable property evaluation methods; standard methods, protocols, and statistical evaluation techniques for validation; and conduct round-robins to calibrate standards, validate equipment, and determine reliability • Encourage active U.S. chemical industry participation and leadership with international organizations and professional societies that set standards, such as IUPAC, VAMAS, and ASTM • Develop commercial sources for standardized materials and instrumentation • Develop a National Data and Model Repository	• Organization dedicated to nanotechnology standardization (year 1) • Independent nanomaterial evaluation established at competent and consistent laboratories • Repository and publication of reviewed methods (ongoing)
Knowledge and Technology Transfer			
Rank	**Timeframe**	**Priority**	**Impact**
Top	**10 years**	**Establish technology transfer policies that foster nanomaterial commercialization** • Establish technology transfer protocols that promote commercialization, facilitate timely information exchange, and reduce the time and expense required for negotiating and establishing collaboration and licensing agreements • Establish a nanotechnology working group within the U.S. Patent Office to foster education and communication among patent examiners • Facilitate industry-university, industry-government, and industry-industry partnerships	• Reviewed effectiveness of policies to promote commercialization (annually)
High	**10 years**	**Build an infrastructure to encourage knowledge sharing in order to facilitate nanoscience understanding and foster near-term commercialization** • Develop a roadmap for fostering a shared-knowledge infrastructure that builds on knowledge gained from standards and informatics research • Establish knowledge-sharing protocols in funding agreements so that results from government-funded research is readily available	• Roadmap on shared-knowledge infrastructure completed (year 1) • Roadmap implementation completed (year 10)

Education and Training			
Rank	**Timeframe**	**Priority**	**Impact**
Top	**10 years**	**Implement strategies to attract and prepare a workforce for nanomaterial research and manufacturing** • Develop and implement a roadmap for nanoscience and technology education and training — Attract more bright U.S. students to science and engineering — Provide interdisciplinary education for K-12, undergraduate, and graduate students — Develop state-of-the-art nanomaterial curriculum and text books — Enable rapid and cost-effective transition of knowledge into manufactured products, including new curriculum and university-national laboratory-industry partnerships — Expand corporate and school (all levels) access to resources at government centers, national laboratories, and universities — Provide opportunities for training at Federally funded centers — Foster international collaborations in academic research and encourage U.S. students to pursue graduate degrees abroad — Develop professional accreditation for nanomaterial education and training	• Roadmap on nanomaterial education training completed (year 1) • Nanomaterial curriculum in universities (year 5) • Roadmap implementation completed (year 10)
Top	**10 years**	**Promote public awareness of nanoscience and technology** • Educate the public regarding the benefits, risks, and opportunities enabled by nanomaterials • Educate the public regarding the safety of nanomaterial technology and provide the results of Federally funded studies Include the public in discussions of nanomaterial safety	• Awareness-raising publication available on opportunities, benefits, and risks of nanomaterials (update annually) • Education implementation strategies in place, ready when research results are available (year 2)

Infrastructure and Enabling Resources			
Rank	**Timeframe**	**Priority**	**Impact**
		Priorities to support R&D are addressed in the following areas of this roadmap: • Modeling and Simulation – to support model advancement • Characterization Tools – to support tool development and use • Standards and Informatics – to foster development of standards • Knowledge and Technology Transfer – to encourage knowledge sharing	• See other sections

G. Acronyms and Professional Organizations

Acronyms

ACGIH	American Conference of Governmental Industrial Hygienists
ACS	American Chemical Society
AIChE	American Institute for Chemical Engineers
APS	American Physical Society
ASTM	American Society for Testing and Materials
CCR	Council for Chemical Research
DHS	Department of Homeland Security
DOA	Department of Agriculture
DOC	Department of Commerce
DOD	Department of Defense
DOE	Department of Energy
DOJ	Department of Justice
EPA	Environmental Protection Agency
ESH	Environment, Safety, and Health
HHS	Department of Health and Human Services
IP	Intellectual Property
IUPAC	International Union of Pure and Applied Chemistry
MRS	Materials Research Society
NASA	National Aeronautics and Space Administration
NIOSH	National Institute for Occupational Safety and Health
NIST	National Institute of Science and Technology
NNCO	National Nanotechnology Coordinating Office
NNI	National Nanotechnology Initiative
NSET	Nanoscale Science, Engineering, and Technology Subcommittee
NSF	National Science Foundation
NSTC	National Science and Technology Council
OECD	Organization for Economic Co-operation and Development
OSHA	Occupational Safety and Health Administration
PCAST	President's Council of Advisors on Science and Technology
VAMAS	Versailles Project on Advanced Materials and Standards
Vision2020	Chemical Industry Vision2020 Technology Partnership

Professional Organizations

The following chemical industry organizations have important activities dedicated to advancing the development of nanotechnology:

American Institute for Chemical Engineers (AIChE)
American Chemical Society (ACS)
American Physical Society (APS)
Council for Chemical Research (CCR)
Chemical Industry Vision 2020 Technology Partnership (Vision 2020)
Materials Research Society (MRS)

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Comments

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