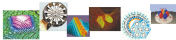


# ***National Nanotechnology Initiative***

LEADING TO THE NEXT  
INDUSTRIAL REVOLUTION



Supplement to the President's FY 2002 Budget

National Science and Technology Council

Committee on Technology

Interagency Working Group on Nanoscience, Engineering and Technology

# **NATIONAL NANOTECHNOLOGY INITIATIVE:**

## **Leading to the Next Industrial Revolution**

**A Report by the Interagency Working Group on  
Nanoscience, Engineering and Technology**

**Committee on Technology  
National Science and Technology Council**

February 2000  
Washington, D.C.



# THE WHITE HOUSE

**February 7, 2000**

MEMBERS OF CONGRESS:

I am pleased to forward with this letter *National Nanotechnology Initiative: Leading to the Next Industrial Revolution*, a report prepared by the Interagency Working Group on Nanoscience, Engineering and Technology (IWGN) of the National Science and Technology Council's Committee on Technology. This report supplements the President's FY 2001 budget request and highlights the nanotechnology funding mechanisms developed for this new initiative, as well as the funding allocations by each participating Federal agency.

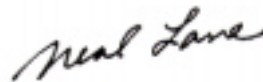
The President is making the National Nanotechnology Initiative (NNI) a top priority. Nanotechnology thrives from modern advances in chemistry, physics, biology, engineering, medical, and materials research and contributes to cross-disciplinary training of the 21<sup>st</sup> century science and technology workforce. The Administration believes that nanotechnology will have a profound impact on our economy and society in the early 21<sup>st</sup> century, perhaps comparable to that of information technology or of cellular, genetic, and molecular biology.

In the FY 2001 budget, the President proposes to expand the Federal nanotechnology investment portfolio with this \$495 million initiative, nearly doubling the current Federal research in nanotechnology. The NNI incorporates fundamental research, Grand Challenges, centers and networks of excellence and research infrastructure, as well as ethical, legal and social implications and workforce.

The President's Committee of Advisers on Science and Technology (PCAST) strongly endorses the establishment of the NNI, beginning in FY 2001, as proposed by the IWGN. PCAST's endorsement is based on a technical and budgetary review of this report. With PCAST's recommendation, the President is taking the vital first step to increase funding for long-term, high-risk R&D that will allow our nation to move to the forefront of the nanotechnology frontier.

The Administration looks forward to working with Congress to strengthen investments in nanotechnology research. Only by working in a bipartisan manner can we further solidify the technological base that lies at the heart of America's scientific and economic leadership.

Sincerely,



Neal Lane  
Assistant to the President  
for Science and Technology



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## **EXECUTIVE SUMMARY**

“My budget supports a major new National Nanotechnology Initiative, worth \$500 million. ... the ability to manipulate matter at the atomic and molecular level. Imagine the possibilities: materials with ten times the strength of steel and only a small fraction of the weight -- shrinking all the information housed at the Library of Congress into a device the size of a sugar cube -- detecting cancerous tumors when they are only a few cells in size. Some of our research goals may take 20 or more years to achieve, but that is precisely why there is an important role for the federal government.”

**--President William J. Clinton  
January 21, 2000  
California Institute Of Technology**

President Clinton’s FY 2001 budget request includes a \$225 million (83%) increase in the federal government’s investment in nanotechnology research and development. The Administration is making this major new initiative, called the National Nanotechnology Initiative (NNI), a top science and technology priority. The emerging fields of nanoscience and nanoengineering – the ability to precisely move matter - are leading to unprecedented understanding and control over the fundamental building blocks of all physical things. These developments are likely to change the way almost everything – from vaccines to computers to automobile tires to objects not yet imagined – is designed and made.

The initiative, which nearly doubles the investment over FY 2000, strengthens scientific disciplines and creates critical interdisciplinary opportunities. Agencies participating in NNI include the National Science Foundation (NSF), the Department of Defense (DOD), the Department of Energy (DOE), National Institutes of Health (NIH), National Aeronautics and Space Administration (NASA), and Department of Commerce’s National Institute of Standards and Technology (NIST). Roughly 70% of the new funding proposed under the NNI will go to university-based research, which will help meet the growing demand for workers with nanoscale science and engineering skills. Many of these research goals may take 20 or more years to achieve, but that is precisely why there is an important role for the Federal government.

### **Nanotechnology Research and Development Funding by Agency:**

	FY 2000 (\$M)	FY 2001 (\$M)	Percent Increase
National Science Foundation	\$97M	\$217M	124%
Department of Defense	\$70M	\$110M	57%
Department of Energy	\$58M	\$94M	66%
NASA	\$5M	\$20M	300%
Department of Commerce	\$8M	\$18M	125%
National Institutes of Health	\$32M	\$36M	13%
TOTAL	\$270M	\$495M	83%

**Nanotechnology is the builder's new frontier and its potential impact is compelling:** In April 1998, Dr. Neal Lane, the Assistant to the President for Science and Technology remarked, "If I were asked for an area of science and engineering that will most likely produce the breakthroughs of tomorrow, I would point to nanoscale science and engineering."

This initiative establishes Grand Challenges to fund interdisciplinary research and education teams, including centers and networks, that work for major, long-term objectives. Some of the potential breakthroughs that may be possible include:

- Shrinking the entire contents of the Library of Congress in a device the size of a sugar cube through the expansion of mass storage electronics to multi-terabit memory capacity that will increase the memory storage per unit surface a thousand fold;
- Making materials and products from the bottom-up, that is, by building them up from atoms and molecules. Bottom-up manufacturing should require less material and pollute less;
- Developing materials that are 10 times stronger than steel, but a fraction of the weight for making all kinds of land, sea, air and space vehicles lighter and more fuel efficient;
- Improving the computer speed and efficiency of minuscule transistors and memory chips by factors of millions making today's Pentium IIIs seem slow;
- Using gene and drug delivery to detect cancerous cells by nanoengineered MRI contrast agents or target organs in the human body;
- Removing the finest contaminants from water and air and to promote a cleaner environment and potable water;
- Doubling the energy efficiency of solar cells.

### **The NNI Investment Strategy:**

The President's Committee of Advisers on Science and Technology (PCAST) established a PCAST Nanotechnology Panel comprised of leading experts from academia and industry to provide a technical and budgetary review of the NNI which is detailed in this document. Upon review of this initiative, PCAST strongly endorsed the establishment of the NNI, beginning in Fiscal Year 2001, saying that 'now is the time to act.' In PCAST's December 14, 1999 letter to President Clinton, PCAST described the NNI as a top Administration priority and an excellent multi-agency framework to ensure U.S. leadership in this emerging field that will be essential for economic and national security leadership in the first half of the next century.

This initiative builds upon previous and current nanotechnology programs, including some early investment from some of the participating agencies. The research strategy listed below is balanced across the following funding mechanisms: fundamental research, Grand Challenges, centers and networks of excellence, research infrastructure, as well as ethical, legal and social implications and workforce programs. This strategy has been endorsed by PCAST. This initiative initially supports five kinds of activities:

- **Long-term fundamental nanoscience and engineering research** that will build upon a fundamental understanding and synthesis of nanometer-size building blocks with potential breakthroughs in areas such as materials and manufacturing, nanoelectronics, medicine

and healthcare, environment and energy, chemical and pharmaceutical industries, biotechnology and agriculture, computation and information technology, and national security. This investment will provide sustained support to individual investigators and small groups doing fundamental, innovative research and will promote university-industry-federal laboratory and interagency partnerships.

- **Grand Challenges that are listed above.**
- **Centers and Networks of Excellence** that will encourage research networking and shared academic users' facilities. These nanotechnology research centers will play an important role in development and utilization of specific tools and in promoting partnerships in the coming years.
- **Research Infrastructures** will be funded for metrology, instrumentation, modeling and simulation, and user facilities. The goal is to develop a flexible enabling infrastructure so that new discoveries and innovations can be rapidly commercialized by the U.S. industry.
- **Ethical, Legal, Societal Implications and Workforce Education and Training** efforts will be undertaken to promote a new generation of skilled workers in the multidisciplinary perspectives necessary for rapid progress in nanotechnology. The impact nanotechnology has on society from legal, ethical, social, economic, and workforce preparation perspectives will be studied. The research will help us identify potential problems and teach us how to intervene efficiently in the future on measures that may need to be taken.

**Funding by NNI Research Portfolio:**

	Fundamental Research	Grand Challenges	Centers And Networks of Excellence	Research Infrastructure	Ethical, Legal, and Social Implications and Workforce	<b>Total</b>
FY 2000	\$87M	\$71M	\$47M	\$50M	\$15M	\$270M
FY 2001	\$170M	\$140M	\$77M	\$80M	\$28M	\$495M

**Next Steps:**

The Administration is currently evaluating the mechanisms to establish a coordination office that would support the NNI and an external review board of experts that would annually monitor the NNI goals. These issues will be detailed in an implementation plan to be published latter this Spring.

## NATIONAL NANOTECHNOLOGY INITIATIVE – LEADING TO THE NEXT INDUSTRIAL REVOLUTION

### **1. Initiative Overview**

The President's budget proposes a "National Nanotechnology Initiative (NNI) – Leading to the Next Industrial Revolution," as part of the fiscal year (FY) 2001 Federal budget. The initiative will support long-term nanoscale research and development leading to potential breakthroughs in areas such as materials and manufacturing, nanoelectronics, medicine and healthcare, environment and energy, chemical and pharmaceutical industries, biotechnology and agriculture, computation and information technology, and national security. The impact of nanotechnology on the health, wealth, and lives of people could be at least as significant as the combined influences of microelectronics, medical imaging, computer-aided engineering, and man-made polymers developed in this century. The proposed level of additional annual funding for FY 2001 nearly doubles the current level of effort of \$270 million in FY 2000. The NNI incorporates fundamental research, Grand Challenges, centers and networks of excellence, research infrastructure that are high risk, high payoff, and broadly enabling. This initiative also addresses development of a balanced infrastructure, novel approaches to the education and training of future nanotechnology workers, the ethical, legal and social implications of nanotechnology, and rapid transfer of knowledge and technology gained from the research and development efforts. The interplay between fundamental research and technology development will be supported for synergistic results. The National Science and Technology Council Committee on Technology's Interagency Working Group on Nanoscience, Engineering and Technology (IWGN) prepared a few publications, as listed in Appendix C, that form the foundation for the evolution of the NNI.

The President's Committee of Advisers on Science and Technology (PCAST) established a PCAST Nanotechnology Panel comprised of leading experts from academia and industry to provide a technical and budgetary review of the NNI which is detailed in this document. Upon review of this initiative, PCAST strongly endorsed the establishment of the NNI, beginning in Fiscal Year 2001, saying that "now is the time to act". In PCAST's December 14, 1999 letter to President Clinton, PCAST described the NNI as a top Administration priority and an excellent multi-agency framework to ensure U.S. leadership in this emerging field that will be essential for economic and national security leadership in the first half of the next century. PCAST's endorsement to the President is attached in Appendix D for your review.

The Administration is currently evaluating the mechanisms to establish a coordination office that would support the NNI and an external review board of experts that would annually monitor the NNI goals. These issues will be detailed in an implementation plan to be published later this Spring.

## **2. Definition of Nanotechnology**

The essence of nanotechnology is the ability to work at the molecular level, atom by atom, to create large structures with fundamentally new molecular organization. Compared to the behavior of isolated molecules of about 1 nm ( $10^{-9}$  m) or of bulk materials, behavior of structural features in the range of about  $10^{-9}$  to  $10^{-7}$  m (1 to 100 nm - a typical dimension of 10 nm is 1,000 times smaller than the diameter of a human hair) exhibit important changes. Nanotechnology is concerned with materials and systems whose structures and components exhibit novel and significantly improved physical, chemical, and biological properties, phenomena, and processes due to their nanoscale size. The aim is to exploit these properties by gaining control of structures and devices at atomic, molecular, and supramolecular levels and to learn to efficiently manufacture and use these devices. Maintaining the stability of interfaces, and the integration of these “nanostructures” at the micron-length scale and macroscopic scale is another objective.

New behavior at the nanoscale is not necessarily predictable from that observed at large size scales. The most important changes in behavior are caused not by the order of magnitude size reduction, but by newly observed phenomena intrinsic to or becoming predominant at the nanoscale, such as size confinement, predominance of interfacial phenomena and quantum mechanics. Once it is possible to control feature size, it is also possible to enhance material properties and device functions beyond those that we currently know or even consider as feasible. Reducing the dimensions of structures leads to entities, such as carbon nanotubes, quantum wires and dots, thin films, DNA-based structures, and laser emitters, which have unique properties. Such new forms of materials and devices herald a revolutionary age for science and technology, provided we can discover and fully utilize the underlying principles.

## **3. A Revolution in the Making: Driving Forces**

In 1959 Richard Feynman delivered his now famous lecture, “There is Plenty of Room at the Bottom.” He stimulated his audience with the vision of exciting new discoveries if one could fabricate materials and devices at the atomic/molecular scale. He pointed out that, for this to happen, a new class of miniaturized instrumentation would be needed to manipulate and measure the properties of these small—”nano”—structures.

It was not until the 1980s that instruments were invented with the capabilities Feynman envisioned. These instruments, including scanning tunneling microscopes, atomic force microscopes, and near-field microscopes, provide the “eyes” and “fingers” required for nanostructure measurement and manipulation. In a parallel development, expansion of computational capability now enables sophisticated simulations of material behavior at the nanoscale. These new tools and techniques have sparked excitement throughout the scientific community. Traditional models and theories for material properties and device operations involve assumptions based on “critical scale lengths” that are generally larger than 100 nanometers. When at least one dimension of a material structure is under this critical length, distinct behavior often emerges that cannot be explained by traditional models and theories. Thus, scientists from many disciplines are avidly fabricating and analyzing nanostructures to



discover novel phenomena at the intermediate scale between individual atoms/molecules and hundred of thousand of molecules where the novel phenomena develop. Nanostructures offer a new paradigm for materials manufacture by submicron-scale assembly (ideally, utilizing self-organization and self-assembly) to create entities from the “bottom up” rather than the “top down” ultraminiaturization method of chiseling smaller structures from larger ones. However, we are just beginning to understand some of the principles to use to create “by design” nanostructures and how to economically fabricate nanodevices and systems. Second, even when fabricated, the physical/chemical properties of those nanostructured devices are just beginning to be uncovered; the present micro- and larger devices are based on models working only at scale lengths over the 100+ nm range. Each significant advance in understanding the physical/chemical/bio properties and fabrication principles, as well as in development of predictive methods to control them, is likely to lead to major advances in our ability to design, fabricate and assemble the nanostructures and nanodevices into a working system.

This proposal for strong financial support for nanoscale research and development is motivated by the impressive potential for economic return and social benefit, including continued improvement in electronics/electrooptics for information technology; higher-performance, lower-maintenance materials for manufacturing, defense, space, and environmental applications; and accelerated biotechnology advances in medical, health care, and agriculture. John Armstrong, formerly Chief Scientist of IBM, wrote in 1991, “I believe nanoscience and nanotechnology will be central to the next epoch of the information age, and will be as revolutionary as science and technology at the micron scale have been since the early ‘70s.” More recently, industry leaders including those at the January 27-29, 1999, IWGN workshop have extended his vision by concluding that nanoscience and technology will change the nature of almost every human-made object in the next century. Such significant improvements in materials performance and changes in manufacturing paradigms will spark an industrial revolution.

Federal support of the nanotechnology infrastructure is necessary to enable the United States to compete in the global marketplace and take advantage of this strategic technology. Focused research programs on nanotechnology have been initiated in almost all industrialized countries in the last five years. Currently, the United States has a lead on synthesis, chemicals, and biological aspects; it lags in research on nanodevices, production of nano-instruments, ultraprecision engineering, ceramics, and other structural materials. Japan has an advantage in nanodevices and consolidated nanostructures; Europe is strong in dispersions, coatings, and new instrumentation. Japan, Germany, U.K., Sweden, Switzerland, and EU all are creating centers of excellence in specific areas of nanotechnology.

#### **4. Nanotechnology’s Impact**

The potential benefits of nanotechnology are pervasive, as illustrated in the fields outlined below:

**Materials and Manufacturing.** Nanotechnology is fundamentally changing the way materials and devices will be produced in the future. The ability to synthesize nanoscale building blocks with precisely controlled size and composition and then to assemble them into larger structures with unique properties and functions will revolutionize segments of the materials manufacturing industry. At present we perceive only the tip of the iceberg in terms of the benefits that nanostructuring can bring: lighter, stronger, and programmable materials; reductions in life-cycle costs through lower failure rates; innovative devices based on new principles and architectures; and use of molecular/cluster manufacturing, which takes advantage of assembly at the nanoscale level for a given purpose. We will be able to develop structures not previously observed in nature. Challenges include synthesis of materials by design, development of bio- and bio-inspired materials, development of cost-effective and scalable production techniques, and determination of the nanoscale initiators of materials failure. Applications include (a) manufacturing of nanostructured metals, ceramics and polymers at exact shapes without machining; (b) improved printing brought about by nanometer-scale particles that have the best properties of both dyes and pigments; (c) nanoscale cemented and plated carbides and nanocoatings for cutting tools, electronic, chemical, and structural applications; (d) new standards for measurements at nanoscale, and (d) nanofabrication on a chip with high levels of complexity and functionality.

**Nanoelectronics and Computer Technology.** The Semiconductor Industry Association (SIA) has developed a roadmap for continued improvements in miniaturization, speed, and power reduction in information processing devices—sensors for signal acquisition, logic devices for processing, storage devices for memory, displays for visualization, and transmission devices for communication. The SIA roadmap projects the future to approximately 2010 and to 0.1 micron (100 nm) structures, just short of fully nanostructured devices. The roadmap ends just short of true nanostructure devices because the principles, fabrication methods, and the way to integrate devices into systems are generally unknown. The SIA roadmap explicitly calls for “sustained government support if this industry is to continue to provide for strong economic growth in the U.S.” The lead time for science maturing into technology is approximately 10 to 15 years; now is the critical time for government investment in the science and technology of nanostructures for the hardware necessary to satisfy continuing demands in information technology. Further, the investment will have spin-offs that enable the attainment (or acceleration) of other SIA roadmap goals. The area of magnetic information storage is illustrative. Within ten years of the fundamental discovery of the new phenomenon of giant magnetoresistance, this nanotechnology completely replaced older technologies for disk computer heads in a market worth \$34 billion in 1998. Other potential breakthroughs include (a) nanostructured microprocessor devices that continue the trend in lower energy use and cost per gate, thereby improving the efficacy of computers by a factor of millions; (b) communications systems with higher transmission frequencies and more efficient utilization of the optical spectrum to provide at least ten times more bandwidth, with consequences in business, education, entertainment, and defense; (c) small mass storage devices with capacities at multi-terabit levels, a thousand times better than today; and (d) integrated nanosensor systems capable of collecting, processing, and communicating massive amounts of data with minimal size, weight, and power consumption. Potential applications of nanoelectronics also include affordable virtual reality stations that provide individualized teaching aids (and entertainment); computational capability sufficient

to enable unmanned combat and civilian vehicles; and communication capability that obviates much commuting and other business travel in an era of increasingly expensive transport fuels.

**Medicine and Health.** Living systems are governed by molecular behavior at nanometer scales where the disciplines of chemistry, physics, biology, and computer simulation all now converge. Such multidisciplinary insights will stimulate progress in nanobiotechnology. The molecular building blocks of life—proteins, nucleic acids, lipids, carbohydrates and their non-biological mimics—are examples of materials that possess unique properties determined by their size, folding, and patterns at the nanoscale. Recent insights into the uses of nanofabricated devices and systems suggest that today’s laborious process of genome sequencing and detecting the genes’ expression can be made dramatically more efficient through utilization of nanofabricated surfaces and devices. Expanding our ability to characterize an individual’s genetic makeup will revolutionize the specificity of diagnostics and therapeutics. Beyond facilitating optimal drug usage, nanotechnology can provide new formulations and routes for drug delivery, enormously broadening their therapeutic potential. Increasing nanotechnological capabilities will also markedly benefit basic studies of cell biology and pathology. As a result of the development of new analytical tools capable of probing the world of the nanometer, it is becoming increasingly possible to characterize the chemical and mechanical properties of cells (including processes such as cell division and locomotion) and to measure properties of single molecules. These capabilities thus complement (and largely supplant) the ensemble average techniques presently used in the life sciences. Moreover, biocompatible, high-performance materials will result from controlling their nanostructure. Proteins, nucleic acids, and lipids, or their nonbiological mimics, are example of materials that have been shown to possess unique properties as a function of their size, folding, and patterns. Based on these biological principles, bio-inspired nanosystems and materials are currently being formed by self-assembly or other patterning methods. Artificial inorganic and organic nanoscale materials can be introduced into cells to play roles in diagnostics (e.g., quantum dots in visualization), but also potentially as active components. Finally, nanotechnology-enabled increases in computational power will permit the characterization of macromolecular networks in realistic environments. Such simulations will be essential in developing biocompatible implants and in the drug discovery process. Potential applications include (a) rapid, more efficient genome sequencing enabling a revolution in diagnostics and therapeutics; (b) effective and less expensive health care using remote and in-vivo devices; (c) new formulations and routes for drug delivery that enormously broaden their therapeutic potential by targeting the delivery of new types of medicine to previously inaccessible sites in the body; (d) more durable rejection-resistant artificial tissues and organs; (e) enable vision and hearing aids; and (f) sensor systems that detect emerging disease in the body, which will ultimately shift the focus of patient care from disease treatment to early detection and prevention.

**Aeronautics and Space Exploration.** The stringent fuel constraints for lifting payloads into earth orbit and beyond, and the desire to send spacecraft away from the sun (diminished solar power) for extended missions, compel continued reduction in size, weight, and power consumption of payloads. Nanostructured materials and devices promise solutions to these challenges. Nanostructuring is also critical to design and manufacture of lightweight, high-strength, thermally stable materials for planes, rockets, space stations, and planetary/solar

exploratory platforms. Moreover, the low-gravity, high-vacuum space environment may aid development of nanostructures and nanoscale systems that cannot be created on Earth. Applications include (a) low-power, radiation-tolerant, high performance computers; (b) nanoinstrumentation for microspacecraft; (c) avionics made possible by nanostructured sensors and nanoelectronics; and (d) thermal barrier and wear-resistant nanostructured coatings.

**Environment and Energy.** Nanotechnology has the potential to significantly impact energy efficiency, storage, and production. It can be used to monitor and remediate environmental problems; curb emissions from a wide range of sources; and develop new, “green” processing technologies that minimize the generation of undesirable by-product effluents. The impact on industrial control, manufacturing, and processing will be impressive and result in energy savings especially through market driven practices as opposed to regulations. Several new technologies that utilize the power of nanostructuring but developed without benefit of the new nanoscale analytical capabilities, illustrate this potential: (a) a long-term research program in the chemical industry into the use of crystalline materials as catalyst supports has yielded catalysts with well-defined pore sizes in the range of 1 nm; their use is now the basis of an industry that exceeds \$30 billion/year; (b) the discovery of the ordered mesoporous material MCM-41 produced by oil industry, with pore sizes in the range of 10-100 nm, is now widely applied in removal of ultrafine contaminants; (c) several chemical manufacturing companies are developing a nanoparticle-reinforced polymeric material that can replace structural metallic components in the auto industry; widespread use of those nanocomposites could lead to a reduction of 1.5 billion liters of gasoline consumption over the life of one year’s production of vehicles and reduce related carbon dioxide emissions annually by more than 5 billion kilograms; and (d) the replacement of carbon black in tires by nanometer-scale particles of inorganic clays and polymers is a new technology that is leading to the production of environmentally friendly, wear-resistant tires. Potential future breakthroughs also include use of nanorobotics and intelligent systems for environmental and nuclear waste management, use of nanofilters to separate isotopes in nuclear fuel processing, of nanofluids for increased cooling efficiency of nuclear reactors, of nanopowders for decontamination, and of computer simulation at nanoscale for nuclear safety.

**Biotechnology and Agriculture.** The molecular building blocks of life - proteins, nucleic acids, lipids, carbohydrates and their non-biological mimics - are examples of materials that possess unique properties determined by their size, folding and patterns at the nanoscale. Biosynthesis and bioprocessing offer fundamentally new ways to manufacture new chemicals and pharmaceutical products. Integration of biological building blocks into synthetic materials and devices will allow to combine biological functions with otherwise desirable materials properties. Imitation of biological systems provides a major area of research in several disciplines. For example, the active area of bio-mimetic chemistry is based on this approach. Nanoscience will contribute directly to advancements in agriculture in a number of ways: molecular-engineered biodegradable chemicals for nourishing the plants and protecting against insects; genetic improvement for animals and plants; delivery of genes and drugs to animals; and nanoarray-based testing technologies for DNA testing. For example, such array-base technologies will allow a plant scientist to know which genes are expressed in a plant

when its is exposed to salt or drought stress. The application of nanotechnology in agriculture has only begun to be appreciated.

**National Security.** The Department of Defense recognized the importance of nanostructures over a decade ago and has played a significant role in nurturing the field. Critical defense applications include (a) continued information dominance through advanced nanoelectronics, identified as an important capability for the military; (b) more sophisticated virtual reality systems based on nanostructured electronics that enable more affordable, effective training; (c) increased use of enhanced automation and robotics to offset reductions in military manpower, reduce risks to troops, and improve vehicle performance; for example, several thousand pounds could be stripped from a pilotless fighter aircraft, resulting in longer missions, and fighter agility could be dramatically improved without the necessity to limit g-forces on the pilot, thus increasing combat effectiveness; (d) achievement of the higher performance (lighter weight, higher strength) needed in military platforms while simultaneously providing diminished failure rates and lower life-cycle costs; (e) badly needed improvements in chemical/biological/nuclear sensing and in casualty care; (f) design improvements of systems used for nuclear non-proliferation monitoring and management; and (g) combined nano and micromechanical devices for control of nuclear defense systems.

**Other Government Applications.** Nanoscience and technology can benefit other Government agency missions, including (a) lighter and safer equipment in transportation systems (Department of Transportation, DOT); (b) measurement, control, and remediation of contaminants (Environmental Protection Agency, EPA); (c) enhanced forensic research (Department of Justice, DOJ); and (d) printing and engraving of high quality, forgery-proof documents and currency (Bureau of Engraving and Printing, BEP).

**Science and Education.** The science, engineering, and technology of nanostructures will require and enable advances in many disciplines: physics, chemistry, biology, materials, mathematics, and engineering. In their evolution as disciplines, each area is now strengthened and simultaneously equipped to address nanostructures providing a fortuitous opportunity to revitalize their interconnections. The dynamics of interdisciplinary nanostructure efforts will reinforce educational connections among disciplines and give birth to new fields that are only envisioned at this moment. Further development of the field requires changes in the laboratory and human resource infrastructure in universities and in the education of nanotechnology professionals, especially for industrial careers.

**Global Trade and Competitiveness.** Technology is the major driving factor for growth at every level of the U.S. economy. Nanotechnology is expected to be pervasive in its applications across nearly all technologies. Investment in nanotechnology research and development is necessary to maintain and improve our position in the world marketplace. A national nanotechnology initiative will allow the development of critical enabling technologies with broad commercial potential, such as nanoelectronics, nanostructured materials and nanoscale-based manufacturing processes. These are necessary for U.S. industry to take advantage of nanotechnology innovations.

## 5. Investment Opportunities

**Need for Investment.** Made possible by the availability of new investigative tools and a new interdisciplinary synergism, and driven by emerging technologies and their applications, nanoscale science and engineering knowledge is exploding worldwide. The number of revolutionary discoveries reported in nanotechnology can be expected to accelerate in the next decade; these are likely to profoundly affect existing and emerging technologies in almost all industry sectors and application areas, including computing and communications, pharmaceuticals and chemicals, environmental technologies, energy conservation, manufacturing, and diagnostics and treatment in healthcare. As a result of the highly competitive and dynamic nature of nanotechnology, of the clear need to create a balanced infrastructure for nanoscale science, engineering, technology and human resources development, and of the potentially immense return on investment, the time appears right for the nation to establish a significant R&D initiative to support nanotechnology.

Federal Government expenditure for nanotechnology in FY 1997 was approximately \$116 million, according to the 1998 WTEC report “*R&D Status and Trends in Nanoparticles, Nanostructured Materials, and Nanodevices in the United States*” (NTIS Report PB98-117914). Nanotechnology as defined there only included work to generate and use nanostructures and nanodevices; it did not include the simple observation and description of phenomena at the nanoscale. Utilizing the broader definition, the Federal Government expenditure is estimated to be about \$270 million for FY 2000. A much greater investment could be utilized effectively. Funding agencies and professional societies are experiencing a flurry of new results in nanotechnology, and there is exploding interest within the research community. The funding success rate for the small-group interdisciplinary research program, FY 1998 NSF “Functional Nanostructures” initiative, was about 13% (lower, if one considers the limitation of two proposals per university). The success rate for the DOD 1998 MURI initiative on nanostructures was 17% (5%, if one starts with the number of white papers submitted to guide proposal development).

The promises of nanotechnology can best be realized through long term and balanced investment in U.S. infrastructure and human resources in five R&D categories in particular: (1) *Nanostructure properties*: Develop and extend our understanding of biological, chemical, materials science, electronic, magnetic, optical, and structural properties in nanostructures; (2) *Synthesis and processing*: Enable the atomic and molecular control of material building blocks and develop engineering tools to provide the means to assemble and utilize these tailored building blocks for new processes and devices in a wide variety of applications. Extend the traditional approaches to patterning and microfabrication to include parallel processing with proximal probes, self-assembling, stamping, and templating. Pay particular attention to the interface with bionanostructures and bio-inspired structures, multifunctional and adaptive nanostructures, scaling approaches, and commercial affordability; (3) *Characterization and manipulation*: Discover and develop new experimental tools to broaden the capability to measure and control nanostructured matter, including developing new standards of measurement. Pay particular attention to tools capable of measuring/manipulating single macro- and supra-molecules of biological interest; (4) *Modeling and simulation*: Accelerate the application of novel concepts and high-performance

computation to the prediction of nanostructured properties, phenomena, and processes; (5) *Device and system concepts*: Stimulate the innovative application of nanostructure properties in ways that might be exploited in new technologies.

**International Perspective.** The United States does not dominate nanotechnology research. There is strong international interest, with nearly twice as much ongoing research overseas as in the United States (see the worldwide study *Nanostructure Science and Engineering*, NSTC 1999). Other regions, particularly Japan and Europe, are supporting work that is equal to the quality and breadth of the science done in the United States because there, too, scientists and national leaders have determined that nanotechnology has the potential to be a major economic factor during the next several decades. This situation is unlike the other post-war technological revolutions, where the United States enjoyed earlier leads. The international dimensions of nanotechnology research and its potential applications implies that the United States must put in place an infrastructure that is equal to that which exists anywhere in the world. This emerging field also creates a unique opportunity for the United States to partner with other countries in ways that are mutually beneficial through information sharing, cooperative research, and study by young U.S. researchers at foreign centers of excellence. A suitable U.S. infrastructure is also needed to compete and collaborate with those groups.

## **6. High-Level Recognition of Nanotechnology's Potential**

The promise of nanoscience and engineering has not passed unnoticed. Dr. Neal Lane, currently the President's Advisor for Science and Technology and former NSF director, stated at a Congressional hearing in April 1998, "If I were asked for an area of science and engineering that will most likely produce the breakthroughs of tomorrow, I would point to nanoscale science and engineering." In March 1998, Dr. John H. Gibbons, the former President's Science Advisor identified nanotechnology as one of the five technologies that will determine economical development in the next century. Several federal agencies have been actively investigating nanoscience R&D. NSF started the National Nanofabrication User Network in 1994, the Nanoparticle Synthesis and Processing initiative in 1991, has highlighted nanoscale science and engineering in its FY 1998 budget. The Defense Department identified nanotechnology as a strategic research objective in 1997. NIH identified nanobiotechnology as a topic of interest in its 1999 Bioengineering Consortium (BECON) program.

More recently, on May 12, 1999, Richard Smalley, Nobel Laureate, concluded in his testimony to the Senate Subcommittee on Science, Technology, and Space that "We are about to be able to build things that work on the smallest possible length scales. It is in our Nation's best interest to move boldly into this new field." On June 22, 1999, the Subcommittee on Basic Research of the Committee on Science organized the hearing on "Nanotechnology: The State of Nano-Science and Its Prospects for the Next Decade". The Subcommittee Chairman Nick Smith, Michigan, concluded the hearings stating that "Nanotechnology holds promise for breakthroughs in health, manufacturing, agriculture, energy use and national security. It is sufficient information to aggressively address funding of this field."

## **7. Proposed Federal Contribution to the NNI**

**Government's role in nanoscience and technology.** While nanotechnology research is in an early stage, it already has several promising results. It is clear that it can have a substantial impact on industry and on our standard of living by improving healthcare, environment and economy. But investments must be made in the science and engineering that will enable scientists and engineers to invent totally new technologies and enable industry to produce cost-competitive products. Since many of the findings on nanostructures and nanoprocesses are not yet fully measurable, replicable, or understood, it will take many years to develop corresponding technologies. Industry needs to know what are the principles of operation and how to economically fabricate, operate, and integrate nanostructured materials and devices. Private industry is unable in the usual 3-5 year industrial product time frame to effectively develop cost-competitive products based on current knowledge. Further, the necessary fundamental nanotechnology research and development is too broad, complex, expensive, long-term, and risky for industry to undertake. Thus, industry is not able to fund or is significantly underfunding critical areas of long-term fundamental research and development and is not building a balanced nanoscience infrastructure needed to realize nanotechnology's potential.

As for Federal and academic investments in nanotechnology R&D, U.S. nanotechnology research has developed thus far in open competition with other research topics within various disciplines. This dynamics is one reason that U.S. nanotechnology research efforts tend to be fragmented and overlap among disciplines, areas of relevance, and sources of funding. It is important to develop a strategic research and development and implementation plan. A coordinated national effort could focus resources on stimulating cooperation, avoid unwanted duplication of efforts, capture the imagination of young people, and support of basic sciences. The government should support expansion of university and government laboratory facilities, help to build the workforce skills necessary to staff future industries based on nanotechnology and future academic institutions, encourage cross-disciplinary networks and partnerships, ensure the dissemination of information, and encourage small businesses to exploit the nanotechnology opportunities.

**Nanotechnology R&D require long-term Federal investment.** Nano-science and engineering R&D will need a long-term investment commitment because of their interdisciplinary characteristics, the limitations of the existing experimental and modeling tools in the intermediate range between individual molecules and microstructure, and the need for technological infrastructure. The time from fundamental discovery to market is typically 10-15 years (see for instance the application of magnetoresistance, and of mesoporous silicate for environmental and chemical industry applications). Historically, industry becomes a major player only in the last 3-5 years, when their investments are much larger than in the previous period, but the economic return is more certain. Industry is frequently reluctant to invest in risky research that takes many years to develop into a product. In the United States, the government and university research system can effectively fill this niche.

Government leadership and funds are needed to help implement policies and establish the nanotechnology infrastructure and research support in the next decade. Since major industrial



markets are not yet established for nanotechnology products, it is proposed that the government support technology transfer activities to private industry to accelerate the long-term benefits. The enabling infrastructure and technologies must be in place for industry to take advantage of nanotechnology innovations and discoveries. The increasing pace of technological commercialization requires a compression of past time scales, parallel development of research and commercial products, and a synergy among industry, university, and government partners. The government role will be on crosscutting, long-term research and development nanotechnology areas identified in this report.

**Budget summaries for participating departments and agencies** are as follows:

- **Current level of support:** The estimated nanotechnology funding in FY 1999 is approximately \$255 million, and for FY 2000 is \$270 million.
- **The proposed investments in FY 2001:** The total proposed increase in Federal expenditures for all participating departments and agencies for FY 2001 is \$225 million. Table I illustrates the Federal agency investments from 1999 onward.

Table I. National Nanotechnology Initiative funding (in \$ millions)

Agency	FY 1999 (\$ M)	FY 2000 (\$ M)	FY 2001 (+from FY 2000) (\$ M)	Percentage Increase (%)
DOC/NIST	16 (with ATP)	8	18 (+10)	125%
DOD	70	70	110 (+40)	57%
DOE	58	58	94 (+36)	62%
NASA	5	5	20 (+15)	300%
NIH	21	32	36 (+4)	13%
NSF	85	97	217 (+120)	124%
Total	255	270	495 (+225)	83%

**Funding themes and modes of research proposed for Funding Agencies in FY 2001:** Below is an outline of the funding mechanisms (for more details on specific plans for each theme – please see Appendices A1 to A5).

1. Fundamental research (total FY 2001 is \$170 million, \$83 million above FY 2000). Fund single investigators and small groups with awards of \$200-500K each. This investment will provide sustained support to individual investigators and small groups conducting fundamental, innovative research; larger investment should be given at the beginning to funding fundamental research, as well as to development of university-industry-laboratory and interagency partnerships.
2. Grand Challenges (total FY 2001 is \$140 million, \$69 million above FY 2000). Fund interdisciplinary research and education teams, that aim to achieve major, long-term objectives, as outlined below:

- a. *Nanomaterials ‘by design’ –stronger, lighter, harder, self-repairing and safer:* Structural carbon and ceramic materials ten times stronger than steel for use in industry, transportation, and construction; polymeric materials three times stronger than present materials, melting at 100°C higher temperature, for use in cars and appliances; and “smart” multifunctional materials;
  - b. *Nano-electronics, optoelectronics and magnetics:* Nanometer structures for minuscule transistors and memory chips that will improve the computer speed and efficiency by factors of millions; expansion of mass storage electronics to multi-terabit memory capacity that will increase the memory storage per unit surface a thousand fold and make data available on a pinhead; changes in communication paradigms by increasing bandwidth a hundred times, which will reduce business travel and commuting;
  - c. *Healthcare:* Effective and less expensive health care by remote and in-vivo diagnostics and treatment devices; diagnostics and therapeutics using rapid genome sequencing and intracellular sensors; gene and drug delivery to targeted cancer cells and organs in the human body; earlier detection of cancer by nanoengineered MRI contrast agents; biosensors that will allow earlier detection of diseases, 50 percent reduction in rejection rate of artificial organs; and use of tiny medical devices that will minimize collateral damage of human tissues;
  - d. *Nanoscale processes and environment:* Removal of the finest contaminants from water (under 300 nm) and air (under 50 nm), and continuous measurement in large areas of the environment; Water purification and desalination desalting seawater with at least 10 times less energy than state-of-the art reverse osmosis.
  - e. *Energy:* Dramatic improvement in the efficiency of energy conversion and storage; double the efficiency of solar cells;
  - f. *Microspacecraft:* Continuous presence in space outside of the solar system with low-powered microspacecraft;
  - g. *Bio-nanodevices for detection and mitigation of threats to humans:* Efficient and rapid bio-chemical detection and mitigation in situ for chemical-biowarfare, HIV, and tuberculosis; Miniaturized electrical/mechanical/chemical devices will extend human performance, protect health, and repair cellular/tissue damage; The research into these basic devices will be coordinated with the Healthcare Grand Challenges;
  - h. *Economical and safe transportation:* Adoption of novel materials, electronics, energy, and environmental concepts;
  - i. *National security: Maintain* defense superiority, with special attention to the nanoelectronics, multifunctional materials and bionanodevices Grand Challenges.
3. Centers and networks of excellence (total FY 2001 is \$77 million, \$30 million above FY 2000). Fund ten new centers at about \$3 million each for five years with opportunity of one renewal after the review. Encourage research networking and shared academic users’ facilities. Establish nanotechnology research centers similar to supercomputer centers that will play an important role in reaching other initiative priorities (fundamental research, Grand Challenges and education), in development and utilization of the specific tools, and in promoting partnerships in the next decade.
  4. Research infrastructure (total FY 2001 is \$80 million, \$30 million above FY 2000). Increase funding for metrology (\$7 million), instrumentation (\$8 million), modeling and simulation (\$6 million), and user facilities (\$9 million). Encourage university-industry-

national laboratory and international collaborations as well as knowledge and technology transfer between universities and industry. Develop a flexible enabling infrastructure so that new discoveries and innovations can be rapidly commercialized by U.S. industry.

5. Societal implications of nanotechnology and workforce education and training (total \$28 million, \$13 million above FY 2000). Fund student fellowships/traineeships and curriculum development on nanotechnology; and change the general teaching paradigms with new teaching tools. Focused research on societal implications of nanotechnology, including social, ethical, legal, economic and workforce implications will be undertaken.

**Priority research areas for increases in nanotechnology funding in FY 2001 over FY 2000:**

- A. *Long-term fundamental nanoscience and engineering research.* The goal is to build fundamental understanding and to discover novel phenomena, processes, and tools for nanotechnology. Tools refer to measurement, modeling, simulation, and manipulation. This commitment will lead to potential breakthroughs and accelerated development in areas such as medicine and healthcare, materials and advanced manufacturing, computer technology, environment and energy. It will refocus the Government's investment that led to today's computer technology and biotechnology.
- B. *Synthesis and processing "by design"* of engineered, nanometer-size, material building blocks and system components, fully exploiting molecular self-organization concepts. This commitment will generate new classes of high-performance materials and bio-inspired systems; changes in device design paradigms; and efficient, affordable manufacturing of high-performance products. Novel properties and phenomena will be enabled as control of structures of atoms, molecules, and clusters become possible.
- C. *Research in nanodevice concepts and system architecture.* The goal is to exploit properties of new nanodevice principles in operational systems and combine building-up of molecular structures with ultra-miniaturization. Nanodevices will cause fundamental changes such as orders-of-magnitude improvements in microprocessors and mass storage, widespread use of selective drug and gene delivery systems, tiny medical tools that minimize collateral human tissue damage, and unmanned combat vehicles in fully imaged battlefields. There will be dramatic payback to other programs with National priority in fields such as information technology, nanobiotechnology, and medical technology.
- D. *Application of nanostructured materials and systems* to manufacturing, power systems, energy, environment, national security, and health care. Research is needed in advanced dispersions, catalysts, separation methods, and consolidated nanostructures. Also needed is development of core enabling technologies such as fundamental molecular scale measurement and manipulation tools and standard methods, materials, and data that can be applied to many commercial sectors.
- E. *Education and training* of a new generation of skilled workers in the multidisciplinary perspectives necessary for rapid progress in nanotechnology. Study the impact of nanotechnology on the society at large, including economic, social, ethical and legal considerations.

Table II illustrates the NNI research portfolio by themes in FY 2001, as well as the FY 2001 increment above FY 2000 by each agency.

Table II. Funding by NNI Research Portfolio in FY 2001.  
The data in parenthesis are FY 2001 increments above FY 2000. All budgets are in \$ millions.

Agency	Fundamental Research	Grand Challenges	Centers and Networks of Excellence	Research Infrastructure	Societal Implications and Workforce	Total
DOC/NIST		10 (+5)		6 (+4)	2 (+1)	18 (+10)
DOD	10 (+4)	54 (+23)	24 (+8)	19 (+5)	3 (+0)	110 (+40)
DOE	27 (+10)	36 (+23)	15 (+0)	16 (+3)		94 (+36)
NASA	4 (+3)	11 (+8)		5 (+4)		20 (+15)
NIH	7 (+1)	17 (+1)	1 (+1)	9 (+1)	2 (+0)	36 (+4)
NSF	122 (+65)	12 (+9)	37 (+21)	25 (+13)	21 (+12)	217 (+120)
Total	170 (+83)	140 (+69)	77 (+30)	80 (+30)	28 (+13)	495 (+225)

**Individual Agencies' Activities in the Initiative.** A preliminary inventory of activities assembled by the IWGN is outlined below. The participating agencies are DOC, DOD, DOE, NASA, NIH, and NSF. Other agencies with nanotechnology-related activities included in other programs may be added in the future such as DOJ (with interest in forensic research, high performance computing, and data base management), DOT (with interest in nanostructured materials and sensors for physical transportation infrastructure), EPA (with interest in measurement and remediation of nanoparticles in air, water, and soil), and the Treasury Department (with interest in special colloidal suspensions at BEP). The following topics are addressed for each of the participating agencies (Note that all dollar figures are estimates):

*Department of Commerce (DOC, NIST, TA)*

- a. Total FY 2001 request is \$18 million, \$10 million above FY 2000. Requested increment increase is for measurement, standards, and economic and foreign assessment studies.
- b. Major interests in nanotechnology: measurement science and standards, including methods, materials, and data; development and acceleration of enabling commercial technologies through industry-led joint ventures.
- c. Estimated funding in FY 1999: \$8.4 million for measurement and standards research, and approximately \$8 million in FY 1998 ATP cost-shared awards to U.S. industry in FY 1998; Estimated funding in FY 2000: \$8.4 million for measurement and standards research.
- d. Modes of R&D support: Development of measurement and standards infrastructure to support U.S. industry development and commercialization of nanotechnology; conduct of economic and foreign assessment studies.
- e. Major themes and new programs in FY 2001 include
  - Nanodevices and biotechnology for quantum level measurement and calibration (This corresponds to the priority research areas A, B, C, D listed on page 25)
  - Magnetic measurements and standards research (priorities A, C, D)

- Nanoscale characterization: measurement systems, approaches and algorithms; standard data and materials (priorities A, C, D)
- Nanoscale manipulation for synthesis and fabrication of measurement systems and standards (priorities A, B, D)
- Study the economical, social and legal aspects (priority E)

*Department of Defense (DOD)*

- a. Total FY 2001 request is \$110 million, \$40 million over FY 2000.
- b. Major interests in nanotechnology: Information acquisition, processing, storage and display; materials performance and affordability; chemical and biological warfare defense.
- c. Estimated funding in FY 1999 and FY 2000: \$70 million in mainstream nanotechnology. The main topics are: novel phenomena, processes, and tools for characterization and manipulation (\$19 million); nanoelectronics (\$40 million), bio-chemical sensing (\$1 million), and materials (\$10 million).
- d. Modes of R&D support: Principally university-based programs for individual investigators (\$22 million) and centers (\$8 million), some programs at the DOD laboratories (\$5 million); and infrastructure (equipment, high performance computing, \$5 million).
- e. Major themes and new programs in FY 2001 include:
  - Advanced processes and tools (priority research areas A to D listed on page 25)
  - Nanostructured materials and systems (priority C)
  - Multifunctional electronics and materials “by design” (priorities A to D)
  - University centers focused on nanotechnology (priorities A-E)

*Department of Energy (DOE)*

- a. Total FY 2001 request is \$94 million, \$36 million over FY 2000. Requested increment increase in FY 2001 is for \$23 million to national laboratories, \$10 million to academic support, and \$3 million for SBIR.
- b. Major interests in nanotechnology: Basic energy science and engineering, with research relevant to energy efficiency, defense, environment, and nuclear nonproliferation.
- c. Estimated funding in FY 1999 and FY 2000: Approximately \$58 million (\$35 million materials, \$11 million chemistry; \$7 million defense, \$1 million engineering).
- d. Modes of R&D support: Capital development at national labs; secondary funding of universities for collaboration with DOE labs; support of national labs to work with other government agencies and industry; 2-3 laboratory user facilities.
- e. Major themes and new programs in FY 2001 include
  - Research user facilities at four national laboratories, with a different focus (priority research areas A to E listed on page 25)
  - Academic support for energy and environment related topics (priorities A, B, D, E)

*National Aeronautics and Space Agency (NASA)*

- a. Total FY 2001 request is \$20 million, \$15 million above FY 2000.
- b. Major interests in nanotechnology: Lighter and smaller spacecraft, biomedical sensors and medical devices, powerful computers that are smaller and consume less power, radiation-tolerant electronics, thin film materials for solar sails.

- c. Estimated funding: \$5.3 million in FY 1999 (additional \$13 million are spent in other targeted programs), and \$5 million in FY 2000.
- d. Modes of R&D support: Fund laboratories JPL (Pasadena), NASA (Ames) and JSC (Houston); academic research.
- e. Major themes and new programs in FY 2001 include: – Manufacturing techniques of single walled carbon nanotubes for structural reinforcement; electronic, magnetic, lubricating, and optical devices; chemical sensors and biosensors (priority research areas B, C, D listed on page 25)
  - Tools to develop autonomous devices that articulate, sense, communicate, and function as a network, extending human presence beyond the normal senses (priorities C, D)
  - Robotics using nanoelectronics, biological sensors and artificial neural systems (priorities C, D)

*National Institutes of Health (NIH)*

- a. Total FY 2001 request is \$36 million, \$4 million above FY 2000. Additional \$20-30 million will be spent in other targeted programs.
- b. Major interests in nanotechnology: Biomaterials (e.g., material-tissue interfaces, biocompatible materials); devices (e.g., biosensors, research tools); therapeutics (e.g., drug and genetic material delivery); infrastructure and training.
- c. Estimated funding: approximately \$21 million in FY 1999, and \$32 million in FY 2000.
- d. Modes of R&D support: Academic research; small business research; in-house studies
- e. Major themes and new programs in FY 2001 include: – Biomaterials (priority research areas A, B, D listed on page 25)
  - Clinical diagnostic sensors (priorities B, D)
  - Genomics sensors (priorities A, B, D)
  - Nanoparticles and nanospheres for drug and gene delivery (priorities B, D)
  - Multidisciplinary training (priority E)
  - Study social, ethical and legal aspects (priority E)

*National Science Foundation (NSF)*

- a. Total FY 2001 request is \$217 million, \$120 million above FY 2000.
- b. Major interests in nanotechnology: Fundamental research on novel phenomena, synthesis, processing, and assembly at nanoscale; instrumentation, modeling; materials by design; biostructures and bio-inspired systems; nanosystem architecture; infrastructure and education;
- c. Estimated funding: \$85 million in FY 1999 (\$40 million, materials; \$14 million, chemistry; \$3 million, biology; \$25 million, engineering; \$1 million, physics; \$2 million, information systems); \$97 million in FY 2000.
- d. Modes of R&D support FY 2001 increment: Individual academic research: \$65 million; Grand Challenges \$9 million; group and center awards for ERC/MRSEC/STC/National Nanofabrication Users Network including infrastructure: \$34 million; Education, training and studies on societal impact: \$12 million.
- e. Major themes and new programs in FY 2001 include :
  - Nano-biotechnology: biosystems, bio-mimetics and composites (priority research area A listed on page 25)

- Nanoscale processes in environment: small length scale/ long time scale processes; functional interfaces between biological/inorganic, inorganic, and biological structures (priority A)
- New paradigms of operation, synthesis and fabrication: nanostructures “by design”; quantum realm; exploratory computational principles: quantum, DNA, etc. (priorities A, B)
- Integration of systems and architectures at the nanoscale: integration at nanoscale and with other scales; multiscale and multiphenomenal modeling and simulations (priorities A, B, C)
- Multiscale/multi-phenomena at nanoscale (priorities A, B and C)
- Education and training of the new generation of professionals for nanotechnology (priority E)
- Study the impact of nanotechnology on the society at large, including economic, social, ethical and legal considerations (priority E)

**Collaborative Activities in the FY 2001 National Nanotechnology Initiative.** The IWGN will coordinate joint activities that synergize the individual agencies’ activities in a variety of topics and modalities of collaboration. The main collaborative activities planned for FY 2001 are:

- *University-based centers* on simulation at nanoscale, integration at nanoscale, interaction processes at nanoscale, nanofabrication, nanotechnology and bio-robotics, and nano-biomedicine (Participants: NSF/centers and DOD and NIH)
- *Coordinated research and education activities in all five priority areas listed on page 9. The agency participation to different priorities is shown under each agency on pages 10 to 12.*
- *National laboratory-based user facilities and research networks.* Four facilities are recommended, to be developed at Oak Ridge National Laboratory, Argonne National Laboratory, Lawrence Berkeley National Laboratory, and Sandia National Laboratory (Participants: DOE, other agencies, state and private organizations)
- *Focused joint programs* on bioengineering (NIH, NSF and DOD); unmanned missions (NASA and DOD); lab-on-a chip (NIH, DOE, DOD, and NSF); quantum computing (DOD, NASA and NSF); and environmental monitoring (DOE and NASA)
- *An education and training network on nanoscience and engineering* (Participants: all agencies)
- *National facility at NIST for calibration and standards at the nanoscale* (Participants: all agencies)
- *National information center for nanotechnology* (Participants: all agencies)
- *Societal implications of nanotechnology* (Participants: NSF, NIH, DOC and other agencies)

Research topics of interest for joint funding include

- Nanoelectronics and information technology
- Multi-scale, hierarchical modeling and simulation of nanostructures and nanoprocesses
- Development of experimental methods and devices to measure various properties and phenomena at nanoscale; combine measurement, manipulation, and manufacturing tools
- Connection to biology (biostructures and bio-inspired systems)

- Synthesis, assembly, and processing of nanostructured materials “by design”
- System architecture and devices
- Focus on fundamentals that are broadly enabling of many technology areas and that help industry to develop new competitive, profitable products that it would not develop on its own

Partnerships will be encouraged

- Among disciplines (small group research)
- Among institutions and types of institutions (e.g., universities, industry, government labs)
- Among U.S. Federal government and state funding agencies (support for complementary activities)
- Among expensive equipment users (joint funding and use of facilities in centers)
- Among countries (international collaborations to promote access to centers of excellence abroad, visits by young researchers abroad, and bilateral and multilateral agreements)

**Infrastructure Needs for Nanotechnology.** A major objective is to create a balanced, predictable, strong, and flexible U.S. infrastructure in nanoscale science, engineering, and technology. This kind of infrastructure is required for the nanotechnology initiative to stimulate further rapid growth of the field. Ideas, concepts, and techniques are developing at an exceedingly rapid pace, such that the field needs coordination and focus with a national perspective. Demands are being made on universities and government to continue to evolve this science and to bring forth the changes in technology that are expected from the field. Even greater demands are on industry to exploit new ideas, protect intellectual property, and develop appropriate products. This field has major transdisciplinary aspects that will be difficult to coordinate without a strategic R&D plan. It is imperative to address these kinds of issues; the future economic strength, quality of life, and national security of the United States may be at stake.

Tools must be provided to investigators in nanotechnology for them to carry out competitive, state-of-the-art research. Tools will include but not be limited to ion, neutron and photon sources, instruments for manipulation, new forms of lithographies, computational capabilities, and other systems to characterize the nanoscale systems. Centers involving multiple grantees or laboratories where these tools would be available should be established at a level of several million dollars annually. These centers should also have diverse research teams that will be effective in different scientific disciplines. Means should be investigated to achieve remote use of these facilities. Funding mechanisms should be emphasized that encourage collaboration between centers, university, laboratories, and industry, as well as single investigators who are tied into these networks. A major potential barrier to cooperative efforts is the issue of intellectual property rights, which must be addressed in a national framework.

Support to single investigators for their competence and imaginative programs should provide a corresponding level of personnel and equipment support. University grants should encourage work among research groups to make maximum use of concepts and ideas being developed in other disciplines. The infrastructure must support building of links between researchers, developers, and users of nanotechnology innovations and development of critical enabling technologies that have significant value added in many industries. The focus should



be on development of new profitable products that maintain and improve global competitiveness, both short-term (3-5 years) and long-term.

It will be necessary to fund training of students and support of postdocs under fellowships that will attract some of the best students available. This is extremely important, considering the rapid changes in the knowledge base. Students should receive multidisciplinary training in various nanotechnology fields. Both organizational attention and funding should also be devoted to ensuring the open exchange of information in multidisciplinary meetings and to rapid publication of results, through, for example, workshops and widely disseminated summaries of research.

Because of the rapidly evolving nature of nanotechnology and its importance to society, program management must be flexible, with the capability of making changes as necessary. Working groups should be supported to make recommendations to modify the program as it evolves.

## Appendix A. Statements for the Proposed Funding Themes and Modes of Research in FY 2001

### National Nanotechnology Initiative, Appendix A1

#### **A1. Fundamental Research** (total FY 2001 is \$170 million, \$83 million above FY 2000)

The National Nanotechnology Initiative identifies five “high priority” research areas for additional funding beginning in FY2001. The first and largest of these is “long-term science and engineering research leading to new fundamental understanding and discoveries of phenomena, processes, and tools for nanotechnology”. The investment will provide sustained support to individual investigators and small-groups, with a typical award of \$200K to \$500K. Sustained and larger funding for fundamental research in the early years of the Initiative is critical for its success.

##### *Vision*

The Initiative will develop the capacity to create affordable products with dramatically improved performance through **basic understanding of ways to control and manipulate matter at the ultimate frontier – the nanometer** – and through the incorporation of nanostructures and nanoprocesses into technological innovations. In addition to producing new technologies, the study of nanoscale systems also promises to lead to fundamentally new advances in our understanding of biological, environmental, and planetary systems.

Nanoscience is still in its infancy, and only rudimentary nanostructures can be created with some control. The science of atoms and simple molecules, on one end, and the science of matter from microstructures to larger scales, on the other end, are generally established. The remaining size-related challenge is at the nanoscale, roughly between 1 and 100 molecular diameters, where the fundamental properties of materials are determined and can be engineered. A revolution has been occurring in science and technology, based on the recently developed ability to measure, organize, and manipulate matter on a scale of 1 to 100 nanometers ( $10^{-9}$  to  $10^{-7}$  m) and on the importance of controlling matter at nanoscale on almost all human-made products. Recently discovered organized structures of matter (such as carbon nanotubes, molecular motors, DNA-based assemblies, quantum dots and molecular switches) and new phenomena (such as magnetoresistance and size confinement) are scientific breakthroughs that merely indicate future potential developments. Nanotechnology creates and utilizes functional materials, devices, and systems by controlling matter on this scale.

Nanotechnology promises to be a dominant force in our society in the coming decades. The few commercial inroads in the hard disk, coating, photographic, and pharmaceutical industries have already shown how new scientific breakthroughs at this scale can change production paradigms and revolutionize multibillion dollar businesses. Formidable challenges remain,

however, in fundamental understanding of systems on this scale before the potential of nanotechnology can be realized. An acceleration of the pace of fundamental research in nanoscale science and engineering will allow for development of the necessary knowledge and human and technological base. Currently, Federal agencies are not able to support many research requests in nanosystems, nano-bioengineering, quantum control, nanosimulations, and nanoscale processes in the environment. Also, there is a need for interdisciplinary consortia that will integrate various disciplines and university/industry/national laboratories' efforts in nanoscience and engineering.

There are several reasons why the nanoscale is so interesting and important:

- Electronic and atomic interactions inside matter are influenced by variations at the nanometer scale. Patterning matter at a nanometer length scale will make it possible to control the fundamental properties of materials (such as magnetization, charge capacity, catalytic activity) without having to change their chemical composition. For instance, nanoparticles of different sizes emit light at different frequencies so they can be used for different color, and nanoparticle are of the size of single magnetic domains so vastly improved magnetic devices can be made.
- Because systematic organization of matter at nanoscale is a key feature of biological systems, nanoscience and technology will allow us to place artificial components and assemblies inside cells and to make new structurally organized materials by mimicking the self-assembly methods of nature. These materials and components will be more biocompatible.
- Nanoscale components have very high surface areas, making them ideal for use as catalysts and other reacting systems, adsorbents, drug delivery, energy storage, and even cosmetics.
- Many nanostructured materials can be harder, yet less brittle than comparable bulk materials with the same composition because of certain interface and confinement effects. Nanoparticles are too small to have defects and are harder because of the surface energy so they can be used to make very strong composite materials.
- The speed of interacting nanostructures is much faster than that of microstructures because the dimensions involved are orders of magnitude smaller. Much faster and energy efficient systems are envisioned.

As Feynman sagely pointed out in 1959, nanoscience is one of the unexplored frontiers of science. It offers one of the most exciting opportunities for innovation in technology. It will be a center of fierce international competition when it lives up to its promise as a generator of technology.

#### *Special Research Opportunities*

The nanoscale is not just another step towards miniaturization, but a qualitatively new scale. The new behavior is dominated by quantum mechanics, material confinement in small structures, large interfaces, and other specific properties and phenomena because of the size. Many present theories of matter at microscale have critical length of nanometer dimensions; these theories will be inadequate to describe the new phenomena at nanoscale.

*Long-term, basic research opportunities arise in*

- developing scaling laws, and threshold length and time scales for the properties and phenomena manifested in nanostructures.
- linking biology, chemistry, and physics to accelerate progress in understanding the fundamental principles behind living systems and the environment.
- discovering and eventually tailoring the novel chemical, physical, and biological properties and phenomena associated with individual and ensembled nanostructures being anticipated.
- creating new instruments with the sensitivity and spatial localization to measure, manipulate, and able to *in-situ* monitor processing of nanostructures; utilizing the new ability to measure and manipulate supramolecules to complement and extend prior measurements derived from ensemble averages.
- addressing the synthesis and processing of engineered, nanometer-scale building blocks for materials and system components, including the potential for self-organization and self-assembly.
- exploiting the potential for both modeling/simulation and experiment to understand, create and test nanostructures quantitatively.
- developing new device concepts and system architecture appropriate to the unique features and demands of nanoscale engineering.

*Priorities and Modes of Support*

Long-term nanoscale research should be focused on understanding basic processes for the new ranges of length and time scales, on development of new measurement and manipulation tools, and on development of the processes necessary to fabricate quality nanostructures in areas of maximum potential impact on technology, health, national security, and the environment. Areas of focus include the following:

- *Biosystems at the nanoscale*: Study of biologically based or inspired nanoscale systems that exhibit novel properties and potential applications will include study of the relationship, on this scale, among chemical composition, physical shape, and function. Potential applications include improved drug and gene delivery, biocompatible nanostructured materials for implantation, artificial photosynthesis for clean energy, and nanoscale sensory systems, such as miniature sensors for early detection of ovarian cancer.
- *Nanoscale structures and quantum control*: Computing, communications, and information storage technologies will approach physical limits of miniaturization as feature sizes in electronic devices reach the nanoscale level. Novel phenomena at the quantum limit that must be explored, understood, and exploited in order to overcome barriers will appear on this scale. New tools will be needed for molecular scale synthesis and processing, fabrication, manipulation, and control. Potential applications include the development of new processes across the entire range of communications and information technology, including ‘quantum computing’.
- *Device and system architecture*: Research is needed to develop new concepts and investigative tools for nanostructured device concepts and system architectures, to understand the interfaces and dynamics of interacting nanostructures, to control complexity, and to simulate nanostructure assemblies like sensors and nano-motors.

Potential applications include integrated devices to monitor health, interconnected nanoscale mechanical and electronic circuits, and multifunctional ‘smart’ devices that can change physical properties in response to external stimuli for safety, space, and national security applications.

- *Nanoscale processes in the environment*: The role and impact of nanoscale phenomena in the environment is only beginning to be realized. Research is needed to develop and adapt new experimental, theoretical, and computational approaches for characterizing nanostructures in the environment and to develop an integrated understanding of the role of nanoscale phenomena in ecosystems. Potential applications include pollution control and understanding the origins of biodiversity. Because natural and artificial nanoparticles can be trapped in lungs, the nanoparticle generation and transport need to be investigated.
- *Multiscale/multiphenomena modeling and simulation*: The emergence of genuinely new phenomena at the nanoscale creates a great need for theory, modeling, and large-scale computer simulation in order to understand new nanoscale phenomena and regimes. The links between the electronic, optical, mechanical, and magnetic properties of nanostructures and their size, shape, topology, and composition are not understood well, although for the simplest semiconductor systems, carbon nanotubes, and similar “elementary” systems, considerable progress has been made. However, for more complex materials and hybrid structures, even the basic outline of a theory describing these connections remains to be written. In nanoscale systems, thermal energy fluctuations and quantum fluctuations are comparable to the activation energy scale of materials and devices, so that statistical and thermodynamic methods must include these effects more fully. Thus, the performance of nanoscale devices depends on stochastic simulation methods, as well as computational models incorporating quantum and semi-classical methods for evaluation. Consequently, computer simulations, both electronic-structure-based and atomistic, will play a major role in understanding materials at the nanometer scale and in the development “by design” of new nanoscale materials and devices. The greatest challenge and opportunity will be in those transitional regions where nanoscale phenomena are just beginning to emerge from macroscopic and microscale regimes that are describable by bulk property theories combined with the effects of interfaces and lattice defects.

Nanoscale science and engineering is inherently interdisciplinary. A focus on interdisciplinary teams of researchers and on exploratory research projects is recommended. Active collaboration between academic and industrial scientists and engineers, and integration of research and education will be encouraged. Interagency partnerships will play a synergistic role in these activities.

#### *Impact on Infrastructure*

The research activities will use and help develop a laboratory and human resource infrastructure for nanotechnology. A skilled workforce familiar with the tools and concepts of nanoscience will be established for moving scientific breakthroughs from the laboratory to practical application.

*Budget request for FY 2001* is \$170 million, a \$83 million increase above FY 2000.

*Agency Participation and Partnerships*

NSF will contribute the largest investment to this generic fundamental research topic. While DOD, DOE, NASA, and NIH will primarily address the fundamental research issues inherent in their Grand Challenges, they will also contribute to generic fundamental research as a way to retain flexibility. Both academic institutions and government research laboratories will conduct fundamental research.

## **A2. Grand Challenges** (total FY 2001 is \$140 million, \$69 million above FY 2000)

The following Grand Challenges have been identified as essential for the advancement of the field: nanostructured materials "by design"; nanoelectronics, optoelectronics and magnetics; advanced healthcare, therapeutics and diagnostics; nanoscale processes for environmental improvement; efficient energy conversion and storage; microcraft space exploration and industrialization; bio-nanosensors for communicable disease and biological threat detection; economical and safe transportation, and national security.

### **Nanostructured Materials "by Design" — Stronger, Lighter, Harder, Self-Repairing, and Safer**

#### *Vision*

The initiative will support new generations of innovative materials that exploit the organization of matter at nanoscale and that are high performance yet affordable, able to adapt, and more environmentally benign. The novel materials will be created for given purposes and may be multifunctional, may sense and respond to changes in surroundings, may be ten times stronger than steel, may be ten times lighter than paper, may be paramagnetic or superconducting, optically transparent, and may have a higher melting point. The new materials may combine best properties of two or more known structures.

#### *Special Research Opportunities*

Nanostructured materials have smaller structures than most of current materials, and this has an important qualitatively effect under a threshold small size. A typical current structure is composed of groups of many trillions of molecules. Nanotechnology involves groups of a few or even single molecules. This difference fundamentally changes the way nanostructured materials behave and opens entirely new and radically different applications. Major differences between the ways nanostructured materials and conventional materials behave result from nanostructured materials' much larger surface area per unit volume and the confinement effects within each material entity. Since many important chemical and physical interactions are governed by surfaces, a nanostructured material can have substantially different properties than a larger material of the same composition. Compared to conventional materials, nanostructured materials yield extraordinary differences in rates and control of chemical reactions, electrical conductivity (nanostructured materials can be highly conductive, highly insulating, or semiconducting), magnetic properties, thermal conductivity, strength of bulk substance made of nanoparticles (resistance to fracture or deformation, elasticity, ductility, etc.), and fire safety.

To make nanostructures, we must learn to design and manufacture structures that are correct at the atomic and single molecule level. The synthesis and formation of individual nanostructures have many promising opportunities, including dendritic polymers, block copolymers, sol-gel chemistry and controlled crystallization, aerosol nucleation, modified

condensation, and nanotube growth. Research into self-assembly, net-shape forming, templating, and other manufacturing approaches will allow for a high level of control over the basic building blocks of all materials. An important challenge is to scale up the laboratory processes and develop commercially viable production methods to manufacture stable nanostructures. The creation of new materials will make extensive use of molecular modeling and simulation. High performance computing now permits simulations based on first physico-chemical principles with few molecules, and these capabilities are expanding rapidly. Another challenge is to develop a single simulation that includes multiple length scales.

The properties of individual nanostructures must be quantitatively measured to establish differences from bulk properties. But the real challenge is to investigate the properties of percolating structures (nanostructure networks) and matrix isolated nanostructures where the impact of neighboring grain interactions begins to modify nanostructure properties. As we move from the individual nanostructure to networks, composites, and coatings, the admixtures of different nanostructures into an integrated entity will benefit from the unique contributions of the different components.

Compacting nanostructures offers another opportunity. The properties of nanostructure interfaces can be unique in themselves. For instance, nanopowder compacts offer high strength simultaneously with ductility. Techniques to make these compacts in bulk and coating forms are necessary; control of the interface composition/structure is crucial. This opportunity could yield coatings for reduced life-cycle-cost, net-shape forming structures for reduced manufacturing costs, and many other improvements.

High surface area materials provide another perspective on nanostructures — controlled porosity where the nanostructure is open space enveloped in a thin material structure. Aerogels and zeolites offer two examples. These materials offer important opportunities in chemical synthesis (hetero-catalytic reactions), clean-up (adsorbents), and separation (controlled porosity membranes) with expected applications in the chemical industry, environmental clean up, and biotechnology.

### *Relevance*

Performance advances of materials have impact on broad commercial, standard of living and national security aspects. Nanostructuring leads to the next generation of high performance materials. Areas of impact include:

- Materials that are much *harder, stronger, more reliable, and safer* so that they last many times longer than our current technology allows will make bridges, roads, road signs, and traffic control systems — helping our tax dollars go farther. The means of transportation by ground, water and air spacecraft need lightweight, long-lived, yet strong materials: strength for function and safety, low weight for fuel economy and agility, and low failure rates (wear, corrosion, fracture, and fatigue) for life-cycle cost and waste reduction. Present military/space platforms have material limitations on their duration and performance that are clearly deleterious to mission success. The importance of better gas mileage will increase with the diminution in oil supply, expected in 10-20 years. Safety requirements in transportation will lead to introduce smart furniture fabrics with



nanodesign and high strength nanostructured plastics that do not burn. New polymer and nanocomposite materials will not only be many times stronger, but they will prevent fires from spreading and dramatically reduce the production of toxic fumes.

- With the incorporation of sense/response functions directly into materials, these *smart materials* will have condition-based maintenance (reducing the enormous cost of multibillion \$/year associated with materials replacement) and will provide new materials capabilities. One military application would be stealthy materials that can recognize probing radar or sonar beams and initiate an action that gives no return signal. Automobile and aircraft materials could also be made to sense incipient failure and warn the user well in advance, rather than stranding him on the highway or plunging her from the air. Paints that change color with temperature — white when hot (solar reflective) and black when cold (solar absorptive) — could provide home heating or cooling adjustments. *Smart windows* in the home and workplace will create huge energy savings.
- Nanotechnology will potentially lead to long lasting, self-cleaning surface finishes; reducing friction, wear, and corrosion; and providing multispectral camouflage (visible, infrared, millimeter wave, radar, sonar).
- In medical applications, nanomaterials will make self-regulating pharmaceutical dispensers compatible with biosystems so that they will not be rejected by the human body and will last many times longer in the corrosive and mechanically harsh environment of the human body.

Materials manufacture and disposal contribute substantially to environmental problems. Nanotechnology offers new biodegradable structures that can be designed for chosen functions. Self-assembly and/or final shape forming *of* manufactured nanostructures will have less waste by-product than the cutting operations presently used in manufacturing. Longer-lived materials — reduced wear corrosion, fatigue, and fracture through nanostructure control — will reduce the amount of material to dispose.

#### *Priorities and Modes of Support*

Nanostructured materials offer a wide range of investment opportunities, with the following expecting to lead to good future return on investment:

- Develop synthesis, processing, and fabrication methods for nanostructures like nanoparticle powders and nanotubes from inorganic and organic materials, and scale up these methods for industrial uses
- Develop models and simulations that incorporate all size scales from nano to macro and that predict materials performance
- Extend the range and sensitivity of analytical tools that measure the composition, structure, and properties of individual nanostructures and their various aggregated forms (networks, composites, coatings, compacts)
- Measure the properties of individual nanostructures, percolating structures (nanostructure networks), and matrix isolated nanostructures. The latter two provide a high degree of

design freedom for potential applications such as dielectrics for electromagnetic absorbers, sensors, detectors, and converters

- Develop nanostructured fillers embedded in a matrix; for instance, nanotubes for strength, nanoclay for fire, nanocarbons for wear resistance, tailored “pigment” incorporation for multispectral low observable structures and materials, including a focus on interfacial properties between filler and matrix
- Develop nanostructured nanoparticles consolidated into composites and nanoporous materials where control of porosity holds promise for chemical selectivity in adsorption, permeation, and chromatographic applications
- Understand the physics and control of nanoscale failure initiation mechanisms

Single investigator projects will dominate the investment portfolio, but selected centers will be necessary to fund expensive equipment.

#### *Infrastructure*

Centers and networks will be crucial for nanostructure characterization. The National Laboratory synchrotron and neutron facilities will be important for the range of wavelengths (sub-nanometer to thousands of nanometers) since they provide diffraction/scattering characterization for various length scales. Academic centers with high-resolution electron microscopes (HREM) and other high cost analytical tools will be necessary.

#### *Agency Participation and Partnerships*

All agencies, with larger contributions from DOC, DOD, DOE, and NASA, will move toward materials issues that address their mission needs and will partner with NSF to establish the generic science base.

## **Nano- Electronics, Optoelectronics and Magnetics**

#### *Vision*

Nanometer structures will foster a revolution in information technology hardware rivaling the microelectronics revolution begun about 30 years ago that displaced vacuum tube electronics. Minuscule transistors and memory chips will improve computer speed and efficiency by factors of millions, expand mass storage electronics to multi-terabit memory capacity that will increase the memory storage per unit surface a thousand-fold and make data available on a pinhead, and reduce power consumption tens of thousands of times. Communication paradigms will change by increasing bandwidth a hundred times — which will reduce business travel and commuting — and by developing foldable panel displays that are also ten times brighter. Merging biological and non-biological objects into interacting systems will create new generations of sensors, processors, and nanodevices.

#### *Special Research Opportunities*

The cost of a single fabrication plant for 70 nm nanometer microelectronics is estimated at over \$10B. It is necessary to identify synthesis, processing, and manufacturing approaches for commercially affordable nanostructures, such as printing and stamping approaches to pattern transfer, innovations in surface processing, controlled nucleation, directional growth,

and directional etching. Other approaches under consideration are individual atom and molecule manipulation, batch formation of precursor nanostructures (powder, cluster, colloid, nanowires, nanodots, fullerene/nanotubules), directed self-assembly whereby individual nanostructures aggregate, and parallel processing via arrays of microfabricated proximal probes.

An investment must be made to accelerate progress in measurement capabilities — electronic, optic, magnetic, and other properties essential to device design; chemical and structural analysis for fundamental understanding and control; the integration of tools for simultaneous, multiple property measurements on the same structure; and techniques compatible with *in situ* fabrication processes.

Novel device concepts must be established. Nanodevices require understanding fundamental phenomena, the synthesis of appropriate materials, the use of those materials to fabricate functioning components, and the integration of these components into working systems. For this reason, success will require a substantial funding level over a long period of time. Exploratory research is necessary on quantum size effects, tunneling, exchange coupling, and other phenomena where present physical models have critical scale lengths larger than the size of the structure. The desirability of room temperature operation will be a severe constraint, but nanostructures promise stable, manipulable state at room temperature. Examples of innovative device concepts include single electron devices, spin-electronics, resonant tunneling devices, quantum dots, molecular electronics, and vertical cavity lasers.

The new properties of nanostructures and the requirements for quality control for large numbers of small nanodevices in a system will necessitate innovative approaches to information system architectures. Examples include cellular automata, quantum computers, cellular parallel computers, neural networks, photonic crystals, computation using DNA, and mechanical molecular memory.

Our ability to control materials in one dimension to build nanometer scale structures with atomic scale precision in now-commercial giant magnetoresistance devices comes from a decade of basic and applied research on thin film growth, surfaces, and interfaces. The extension from one nanodimension to two or three is not straightforward, but the payoffs can be enormous.

In all of the above opportunities, modeling and simulation will play an essential role. As one gains control of matter at the nanometer scale, the possible combinations and permutations of structures become far too great for only experimental approaches to progress.

### *Relevance*

Nanodevices will extend the U.S. lead into hardware for information technology and other nanodevice use. For example, the goal of microspacecraft guarantees strong attention by the space community. Revolutionary advances in medicine for disease control and in defense for combat knowledge superiority fields are envisioned.

The Semiconductor Industry Association (SIA) roadmap projects nanotechnology to 0.1 micron by approximately 2010, then terminates; it states that new materials, new technologies, affordable scaling, and new approaches must be invented and that these required inventions constitute a Grand Challenge. The year 2010 is only ten years away; now is the time for government investment in the nanoscience base that will enable information nanotechnology.

#### *Priorities and Modes of Support*

The research interests should be focused on the following:

- New approaches to nanostructure synthesis and processing that will lead to affordable commercial fabrication
- The physics of innovative device concepts
- New systems and architectures for given functions
- Multiscale/multiphenomena modeling and simulation of complex systems with focus on information technologies
- New optical properties achieved by fabricating photonic band gap superlattices to guide and switch optical signals with nearly 100% transmission, in very compact architectures

A strong, single investigator program is essential to introduce the broad range of innovations necessary to this Grand Challenge. But there is also the need for multidisciplinary centers — combining physics, chemistry, electrical engineering, computational science, and other traditional academic departments. The centers should be charged with integrating industrial and academic interests.

#### *Infrastructure*

Instrumentation and facility centers — incorporating not only the expensive items such as high voltage, high-resolution electron microscopes, but also suites of proximal probes — will be necessary for full characterization capability. These centers must provide competent, affordable assistance to visiting users. They must also develop new instrumentation that eliminates the many deficiencies in the present capability. The National Nanofabrication Network will need expansion and enhancement.

#### *Agency Participation and Partnerships*

All agencies, with particular attention by DOD, DOE and NASA for mission driven projects and NSF for fundamental aspects. Partnerships between university/government/industry will be essential to the rapid transition of nanostructure science into new information technology hardware. The DOD/MARCO and DoD/EPRI Government-Industry-Cosponsorship of University Research (GICUR) research center programs are an example of this needed partnership.

## **Advanced Healthcare, Therapeutics and Diagnostics**

#### *Vision*

Nanotechnology will contribute to major advances in healthcare through the development of biosensors and new imaging technologies that will allow earlier detection of cancer and other

diseases; more effective, less expensive diagnostics and therapeutics using rapid gene sequencing; novel biocompatible materials that will double the retention time of artificial organs; targeted gene and drug delivery systems; enable vision and hearing aids; and use of tiny “smart” medical devices for treatment modes that will minimize collateral damage of human tissues.

#### **a. Earlier Detection and Treatment of Disease**

##### *Special Research Opportunities*

Nanotechnology will play a central role in the development of new technologies to detect and treat disease much earlier. Current approaches to healthcare for most diseases depend on the appearance of substantial symptoms before medical professionals can recognize that the patient has the disease. By the time those symptoms have appeared, effective treatment may be difficult or impossible. Earlier detection of incipient disease will greatly enhance the success rate of existing treatment strategies and would significantly advance our ability to employ prevention strategies that could arrest or delay the onset of clinical symptoms that may require chronic treatment and/or intervention. Nanoscience and technology will play a central role in the development of novel methods for detecting the biological and structural evidence of incipient disease.

##### *Priorities*

- ***Improved medical imaging technology***

Medical imaging today uses X-rays, magnetic resonance, and ultrasound imaging. These technologies have an impressive ability to report, non-invasively, on structures within the body. However, they have not yet reached the speed, low cost, resolution, and sensitivity that their practitioners strive for; and as a result, most diseases and conditions must be relatively advanced before they can be detected. Advances that nanotechnology will bring to other fields such as electronics and computing will directly benefit medical imaging. Nanotechnology will also result in improved contrast agents for use in conjunction with imaging systems. Delivery of conventional contrast agent molecules to sites in the body that are currently inaccessible to those molecules will be achieved through the use of small particles designed to have the physical and chemical properties consistent with delivery to their target organ. New chemical and particulate formulations will also be created to enhance the images created by such imaging modalities as MRI and ultrasound.

As a result of these improvements, diseases will be detectable earlier than they are today: Tumors consisting of just a few cells, or subtle perturbations to blood flow that signal a warning of impending heart disease, will be detectable, making earlier treatment possible.

- ***Sensors***

Implantable sensors or ‘smart’ patches will be developed that can monitor patients who are at risk for specific conditions. Such sensors might monitor, for example, blood chemistry, local electric signals, or pressures. The sensors would communicate with devices outside the body to report results, such as early signals that a tumor, heart damage, or infection is developing. Or these sensors could be incorporated into “closed loop” systems that would dispense a drug or other agent that would counteract the detected

anomaly. For chronic conditions like diabetes, this would constitute a great leap forward. Nanotechnology will contribute critical technologies needed to make possible the development of these sensors and dispensers.

- ***Susceptibility Testing***

Sensor systems that can rapidly process patient samples and detect an array of medically relevant signals at high sensitivity and selectivity will also be developed for the clinical laboratory or doctor's office. Some of these tests will be based on nucleic acids like DNA or RNA and will be used, for example, to rapidly determine a patient's susceptibility to certain diseases, infections, toxins, etc. Knowledge of this information will help the patient make lifestyle and employment decisions and watch for those diseases likely to affect them. More effective, more personalized treatments will come with the ability to use DNA profiles to classify patients according to their responsiveness to certain pharmaceutical drugs or to their potential for having adverse reactions to particular pharmaceuticals. Current technology leads toward such tests/devices, but nanotechnology will expand the options leading to greater sensitivity and far better efficiency and economy.

### **b. Improved Implants**

#### *Special Research Opportunities*

Artificial organs or organ-assist devices require implantable materials both compatible with the biological environment and resilient to the chemistry of that environment. Better materials and understanding of their interactions with the body may lead to implants that the body will not only accept but will actually become integrated into the body. Nanometer scale surface modifications offer potential for creating novel structures that will allow scientists to control interactions between materials and biological systems.

It is clear that effective manipulation of biological interactions at the nanometer level can dramatically improve the functionality and longevity of implanted materials. For example, titanium implants used today for orthopedics and in dentistry become encapsulated with dense fibrous tissue. This tissue creates an uneven stress distribution at the implant-bone interface, which can result in implant loosening and failure, and even fracture the adjacent bone. By applying "bioactive" thin (nanoparticle) coatings on the surface of the implants, it will be possible to bond the implant more naturally to the adjoining bone and significantly improve the implant lifetime. Future fundamental discoveries in nanoscience, biology, chemistry, and instrumentation will provide the basis for the development of materials that will overcome the challenges implicit in the design and creation of novel biocompatible materials with broad biomedical applications.

### **c. Nanotechnology for Therapeutic Delivery**

#### *Special Research Opportunities*

The challenge is to develop and deploy nanoparticles for delivering drugs, gene therapies, and other therapeutics. These technologies will deliver drugs or other molecules that are hard to dissolve and may even deliver them directly to their site of action. Such nanoparticles will be used to treat cancer and a wide range of other diseases.

Many drugs that work well in the test tube fail in the body because they will only dissolve in fluids that cause undesirable side effects or become trapped in other parts of the body than where they are needed. Evidence has shown that drugs whose chemical structure must today be modified to improve their solubility (potentially compromising those chemical features that are responsible for their desired pharmacological effect) could be used without those changes by using nanoparticle delivery instead of chemical dissolution.

Furthermore, most drugs are delivered throughout the body, rather than to the specific area where they are meant to have an effect. As a result, side effects on other tissues are unavoidable. Nanoparticles are showing promise for the delivery of drugs to specific tissues (e.g., a tumor) where they are needed. By directing drugs primarily to their desired sites of action, lower overall doses of drugs will be given because these will concentrate where they are needed and exposure of other body tissues to the drugs will be reduced. This, in turn, will reduce undesirable side effects of the drugs.

In gene therapy, specific targeting by nanoparticle design will be extremely useful. Some current attempts at gene therapy use viral particles to aim therapy at a particular type of cell and, once there, at the appropriate location within the cell, in order for the gene therapy to have its desired effect. To date, however, the effectiveness of using viral vectors to introduce DNA into cells is quite variable. Nanoparticles may be able to deliver nucleic acids to specific cells and even to the specific compartment (cytoplasm or nucleus) within those cells — wherever their action is required.

#### *Agency Participation and Partnerships*

NIH in collaboration with other agencies, including NSF and DoD.

### **Nanoscale Processes for Environmental Improvement**

#### *Vision*

Nanoscience and engineering could significantly affect molecular understanding of nanoscale processes that take place in the environment; of the generation and remediation of environmental problems through control of emissions from a wide range of sources; of the development of new, “green” technologies that minimize the production of undesirable by-products; and of the remediation of existing waste sites and streams. Removal of the smallest contaminants from water supply (less than 200 nm) and contaminated air (under 20 nm) and continuous measurement and mitigation of pollution in large areas of the environment will be achieved.

Other Grand Challenges related to energy, materials, electronic, and biodevices address the environmental technologies needed to reduce the pollution at its source.

#### *Special Research Opportunities*

Physical and chemical processes involving nanoscale structures are essential to phenomena that govern the trapping and release of nutrients and contaminants in nature. The aerosol and colloidal structures provide sites for complicated interactions with microbes that control or

mediate the bioavailability of a wide variety of organic and inorganic compounds. Nanoparticles have large and active lateral surfaces that can absorb and transport pollutants in the form of colloidal suspensions and aerosols. Also, such particles are involved in complex chemical processes in the atmosphere and in soils, and can catalyze adverse reactions. An increased knowledge of the dynamics of processes specific to nanoscale structures in natural systems can improve understanding of complex processes occurring in the environment and can lead to the development of approaches for mitigating environmental harm.

In order to understand the environmental consequences of processing and transporting contaminants in the environment, interdisciplinary research is needed on molecular and nanoscale processes that take place at one or more of the interfaces or within nanoscale structures in natural systems. Such research includes studies of the interfaces between inorganic/inorganic, inorganic/organic, and organic/organic structures focused on the specific processes characterized by small-length scale.

Interdisciplinary research that involves novel approaches and that adapts newly developed experimental, theoretical, and computational methods for characterizing nanostructures is needed. The intention is to bring the community of scientists and engineers studying the fundamental properties of nanostructures together with the community attempting to understand complex processes in the environment in order to hasten the integrated understanding of the environmental role of nanoscale phenomena. Model nanostructures can be studied, but in all cases the research must be justified by its connection to naturally occurring systems or to environmentally beneficial uses. Environments for investigations are not limited and might include terrestrial locations such as acid mines, subsurface aquifers, or polar environments.

#### *Priorities*

- Study of the effects of finite size, reduced dimensions, or special geometrical arrangements of atoms or molecules on the interaction of nanoscale particles with substrates
- Development of an understanding of how structures peculiar to surfaces or interfaces influence environmentally relevant reactions
- Use of modern experimental techniques such as optical traps, laser tweezers, or synchrotron radiation to examine model environmental processes that occur within nanoparticles or at surface nanostructures
- Study of the role of nanostructures in important processes such as protein precipitation, desorption of pollutants, stability of colloidal dispersion, micelle aggregation, or microbe mobility
- Development of experimental, theoretical, and computational techniques to examine the role of nanoparticles in atmospheric and water resources processes
- Meso-porous structures integrated with micromachined components that are used to produce high-sensitivity and highly selective chip-based detectors of pollutants

#### *Agency Participation and Partnerships:*

DOE, NSF and other collaborating agencies.



## Efficient Energy Conversion and Storage

### *Vision*

Nanoscale synthesis and assembly methods will result in more energy-efficient lighting, stronger light-weight materials that will improve efficiency in transportation, use of low-energy chemical pathways to break down toxic substances for environmental remediation and restoration, better sensors and controls to increase efficiency in processing and manufacturing, and significant improvements in solar energy conversion and storage. The efficiency of solar energy conversion and of fuel cells is expected to double.

### *Special Research Opportunities*

A key challenge is to understand how deliberate tailoring of materials at the nanoscale can lead to novel and enhanced functionalities of relevance in energy conversion, storage and conservation. The enhanced properties of nanocrystals for novel catalysts, tailored light emission and propagation, and supercapacitors for energy storage are being explored, as are nanocomposite structures for chemical separations, adaptive/responsive behavior and impurity. Nanocrystals and layered structures offer unique opportunities for tailoring the optical, magnetic, electronic, mechanical and chemical properties of materials.

### *Relevance and Research Priorities*

This work has significant potential for energy technologies. For example, nanocrystalline semiconductors in the form of fractal films of particles, isolated colloidal quantum dots, ordered and disordered arrays of close-packed colloidal quantum dots, and two- and three-dimensional arrays of self-organized epitaxially grown quantum dots have many potential and existing applications in renewable energy systems. These include very inexpensive and color tunable (from clear to colored to black) photovoltaic solar cells based on the dye-sensitization of nanocrystalline wide bandgap oxides (like  $\text{TiO}_2$ ) operating in a photoelectrochemical cell, and novel solar cells with extremely high conversion efficiency. Nanocrystals could also be used as efficient photocatalysts for photodetoxification of polluted or toxic water and air streams. Semiconductor nanocrystals and nanostructures may be used as efficient photoactive materials for solar-photon conversion of simple molecules to fuels and chemicals, for instance photolytic water splitting to produce hydrogen, photoreduction of carbon dioxide to alcohol and hydrocarbon fuels, and photoreduction of molecular nitrogen to ammonia for fertilizer production.

A deeper understanding of the physics of phonon transport in nanostructured materials may facilitate production of practical all-solid-state and environmentally clean thermoelectric energy-conversion devices with performances far superior to current vapor-based refrigerators and combustion-based engines. The pervasive role of hard and soft magnets in electric-power production and utilization is another arena in which new nanoscale magnetic materials may yield substantial energy savings by reducing losses and conserving natural resources consumed in the generation and use of electricity.

Nanostructured carbon-based nanotubes have the potential to act as a hydrogen storage medium that could exhibit very high storage density per unit weight, which is critical for

hydrogen-based transportation systems. A crucial issue is whether or not the hydrogen could be extracted efficiently from such a storage medium at relatively low temperatures.

Opportunities exist for increasing thermal transport rates in fluids by suspending nanocrystalline particles in them. These “nanofluids” have recently been shown to exhibit substantially increased thermal conductivities and heat transfer rates compared to fluids that do not contain suspended particles. However, there is no real understanding of the mechanisms by which nanoparticles alter thermal transport in liquids. Multibillion-dollar industries, including transportation, energy, electronics, textiles, and paper, employ heat exchangers that require fluids for efficient heat transfer. If researchers can improve these fluids, there can be significant gains in efficiency.

Nanostructured materials also promise greatly improved structural properties in comparison with conventional metal alloys. For example, small-diameter bundles of single-walled carbon nanotubes are predicted and observed to have the largest strength-to-weight ratio of any known material, which is approximately *one hundred times that of steel but with only one-sixth its weight*. Such materials offer opportunities for reducing the weight of automobiles and increasing fuel economy, if they can be made by an economically competitive process that is compatible with other manufacturing technologies.

Other examples of new or enhanced properties from nanostructured materials that can improve energy technologies include:

- Nanoscale layered materials that can yield a four-fold increase in the performance of permanent magnets
- Addition of aluminum oxide nanoparticles that converts aluminum metal into a material with wear resistance equal to that of the best bearing steel
- Layered quantum well structures to produce highly efficient, low-power light sources and photovoltaic cells
- Novel chemical properties of nanocrystals that show promise as photocatalysts for more energy efficient breakdown of toxic wastes
- Meso-porous inorganic hosts with self-assembled organic monolayers that are used to trap and remove heavy metals from the environment

While microsystems and microdevices are built on the dimensional scale of microns to centimeters, their functionality and performance depend on the understanding and control of materials properties on the nanoscale. Some of the nanoscale science and technology issues that are relevant for micro-electro-mechanical devices are lubrication, friction, wear, and micro-mechanical properties. Examples of current research include the science of self-assembled nanolayers to reduce adhesion and friction, and the development and use of new interfacial force microscopies to study lubrication at the nanoscale. Areas of interest in the area of micro-electro-mechanical devices include an understanding of materials performance and aging under operational conditions, including mechanical stresses and atmospheric environments; methods of surface preparation/passivation/lubrication for the purpose of minimizing adhesion, friction, wear and corrosion; novel analytical techniques and diagnostics to probe performance and degradation phenomena at molecular size scales (particularly spatially resolved techniques), polymer or other silicon-compatible optical

components and sensors; studies to relate operating lifetime of the integrated microsystems, and any of their component nanotechnologies, to details of the fabrication process, and investigations of the operation of these systems in extreme environments, including shock, vibration, extreme temperature excursions and radiation. Investigations of these phenomena with nanostructures holds the promise for understanding the initiation mechanisms of friction, wear, fatigue and other causes of materials failure.

#### *Research Priorities*

- For future generations of energy systems, nanotechnology can provide significant advances in terms of functionality, speed and capacity.
- Innovative approaches to improved conversion of solar energy into electricity.
- Catalysts for improved conversion of hydrocarbon energy into thermal energy; Catalysts and membranes that enable effective, commercially viable fuel cells that utilize a range of materials as fuels.
- Nanostructured materials for thermoelectricity, magnetic refrigeration and other innovations in efficient energy conversion.
- Improved materials and coatings for reduced materials failure rates and lower friction (wasted energy dissipation)
- Nanostructures that will selectively bind and concentrate radionucleotides, thereby sequestering them from benign waste material and lowering waste disposal costs for nuclear energy.
- Nanostructured materials that are more radiation tolerant for greater nuclear reactor lifetimes.
- Advances in nanoelectronics development could enable new generations of high speed, low power circuits for special purpose high performance needs.

#### *Agency Participation and Partnerships*

DOE (the Department's Office of Science for fundamental research, and the Department's Technology Offices for research focused on useful technological solutions) and other collaborating agencies including DOC and NSF.

## **Microcraft Space Exploration and Industrialization**

#### *Vision*

Continuous presence in space outside of the solar system with nanotechnology enabled low powered microspacecraft. Reduce the size and energy consumption ten fold.

### *Special research opportunities*

Microspacecraft development is a key thrust for the exploration of space. Motivators for this demand include the high cost of launching into space, the desire to reach ever more remote and hostile environments in our solar system, and the unique capabilities of missions involving large numbers of cooperative spacecraft. To fulfill the promise that microspacecraft hold for exploring space, these spacecraft cannot be scaled down versions of larger spacecraft, limited in capability. This new breed of spacecraft must surpass the current state of technology in today's fleets of vehicles. Long duration missions (decades) to the outer reaches of the solar system; exploration into the interiors of planets, comets, and moons, searching for the subtle clues of the presence of life; fleets of telescopes, acting in concert, imaging Earthly planets around other stars; all these long range goals for space exploration in the 21<sup>st</sup> century will be enabled through the development of advanced nanoscale technology.

### *Priorities*

The key challenge for NASA is identifying, developing, and exploiting nanotechnology advances that offer unique advantages for space exploration. Research areas that are promising in achieving the nation's space goals include:

- 1- *Nanostructured materials*: one key enabling technology for future NASA missions is the development of ultralight weight and ultrastrong materials that can survive the space environment. These materials are necessary for the creation of very large structures (telescopes, antennas, solar sails, to name a few) whose mass will be a only a small fraction of current systems. The utilization of these materials in deployable and inflatable systems permits very small spacecraft to undertake missions that were otherwise deemed far too costly or simply undoable. Beyond the mass and strength advantages of nanoscale materials lie unique optical, piezoelectric, and other material properties that will allow the creation of truly smart and agile structures. Active control of mirror surfaces, adjustable thermal properties, and self-repairing materials represent a partial list of developments that will change how space missions will be done.
- 2- *Nanoelectronics*: Processing, sensing and information management technologies are critical for space systems. Strong pushes for much more capable spacecraft electronics come from the following:
  - greater autonomy and on board decision making,
  - the large, diverse data sets to be collected by future missions,
  - greater sensitivities of the scientific instruments,
  - Sophisticated fault management and self-repair capability.

However, these requirements are colliding with the realities of the limitations of microelectronics, with space applications putting extreme demands on the electronics for ultralow power consumption, radiation tolerance, and safety. The development of transistors and other circuit elements utilizing single quantum excitations (electrons, Cooper pairs, photons) enable spacecraft to collect, process and then transmit information that will far surpass the capabilities of current missions. Specific examples include:

- detectors capable of detecting and measuring single photons, which will fully utilize the large area apertures enabled by nanoscale materials
- non volatile, radiation resistant, high density memory systems

- ultrahigh speed computation, for s/c decision making and data set reduction
  - rugged, miniaturized spacecraft avionics systems utilizing microwatts of power
- 3- *Biomimetic systems*: Micro systems based on biological principles, or on biological building blocks, is a key future area for space exploration. Ultra long duration missions, or missions in hazardous environments, will benefit greatly from adopting strategies and architectures from the biological world. Also, in the search for life outside the earth, understanding and controlling processes at the molecular level is necessary for enabling in situ systems to carry out advanced laboratory analyses. Self replicating systems, utilization of in situ resources to create complex structures in space, spacecraft that can adapt and react to changing environmental or mission needs are examples of the kinds of advances that NASA is pushing to be enabled through applying nanotechnology and molecular biology methods to spacecraft.

*Agency Participation and Partnerships*

NASA and other collaborating agencies including DOD, DARPA, NSF, and NIH/NCI.

**Bio-nanosensor Devices for Communicable Disease  
and Biological Threat Detection**

*Vision*

Nanoscience and technology will foster efficient and rapid biochemical detection and mitigation in situ for chemical-biowarfare, HIV, and tuberculosis. Miniaturized electrical/mechanical/chemical devices will extend human performance, protect health, and repair cellular/tissue damage.

*Special Research Opportunities*

Minimally intrusive devices for human tissue and vasculature will benefit from nanoscale manufacturing. As the structures are reduced to nanometer scale size, molecular structures will begin to compete with inorganic structures, and new device functions will be made possible. The opportunities for molecular mechanical systems are compelling. Living systems depend on a variety of molecular motors. Molecular motors derive their power from body chemistry; it is possible that an *in vivo* bionanodevice could be powered by that same body chemistry.

For *ex situ* applications, the bionanodevices must be able to sense and identify pathogenic chemical/biological species and then initiate action to neutralize the pathogen. Most chemical/biological detectors select for a known threat. It is important to develop detectors that can sense distress in living cell/tissue and alarm the organism to the presence of an unknown threat. Such a detector will require attention to interactions between inanimate silicon devices and living organic devices. Microfluidics, wall adsorption, fouling will be critical issues for attention. Nanometer-sized clusters can have novel properties and can provide new approaches to the difficult problem of species neutralization without hazard to personnel and machinery. *Ex situ* size constraints will be less severe on Bionanodevices. This application will be a stepping stone toward *in situ* application.

As *in vivo* systems, bionanodevices will initiate appropriate biochemical and biophysical responses by stimulating biomolecular systems. Highly specific, functional biomolecules — poly-nucleic, peptide, and saccharide — can be synthesized by chemical/biological techniques. These molecules hold promise as highly selective sensors (DNA pairing, antibody and antigen, receptor recognition) and actuators (molecular motors from flagella and muscle, ion channel activation) to interact with body chemistry and physics. This Grand Challenge will require those biomolecules to be isolated, their structure and properties relationships understood, their coupling to inorganic substrates without loss of function determined, the mechanisms for communication between biomolecules and semiconductor electronics ascertained, and the extent of power that can be derived from body chemistry ascertained. Better techniques for single molecule manipulation and measurement must be developed using proximal probes and optical tweezers.

### *Relevance*

Miniaturized, low power, sensitive, and selective detection/remediation of biological and chemical threats is a recognized problem with immediate significance because of concern over weapons of mass destruction. Mother Nature has produced some of the worst threats to humans — HIV, TB, and the Ebola virus, to name a few. Public health, military and police forces are in desperate need of the improvements expected from bionanodevices. These sensors will revolutionize medical diagnostics, making sophisticated blood/urine/saliva tests inexpensive and routine operations at the doctor's office. Many professions require sustained human performance under demanding conditions — pilots, the military, police — even so simple a task as long-distance driving. Bionanodevices will monitor body chemistry and physics, provide alerts to mental or physical deterioration, and take appropriate countermeasures. As miniaturization progresses, bionanodevices will be inserted into the body with the ability to recognize locations in distress (like cancer sites, infections, calcification, and bleeding) and take localized, measured remedial action. Whole body infusion of a prophylactic drug won't be necessary. Cancerous tissue can be treated directly without disturbing healthy tissue. In addition to general health care, the casualty care of special concern to police, trauma, and military operations will benefit.

### *Priorities and Modes of Support*

- Development and measurement of single supramolecular chemical, biological, and physical properties
- Development of nanomechanical systems, miniaturization of microelectromechanical systems (MEMS) by a thousand-fold, and incorporation of molecular activation and motility
- Sense and actuate information transfer between inorganic electronics and biomolecular systems

### *Infrastructure*

Bionanodevices will require extremely close coupling among various disciplines, especially biology and the physical/engineering sciences and the microelectronics communities. Centers facilitating such interaction will be essential. The fabrication of nanometer-sized electromechanical devices will need the equivalent of the Microelectronics Center of North

Carolina's Multi-User MEMS Processes (MUMPS) facility that presently enables affordable manufacture of MEMS devices for research purposes.

*Agency Participation and Partnerships*

NSF – fundamental science base

NIH – bionanotechnology approaches to body chemistry intervention

DOD – development of nanoelectromechanical systems (NEMS) and chemical-bio agent detection

DOE – laboratory on a chip concepts

## **Application to Economical and Safe Transportation**

*Vision*

Nanotechnology will be the building tool for advances in transportation in the 21<sup>st</sup> century. It's potential benefits are broad and pervasive, including lighter and more efficient cars using nanostructured materials, corrosion-free bridges and no-maintenance roads, and tiny "traps" that remove pollutants from vehicle emissions.

Among the **breakthrough applications** that we may see in transportation are the following:

- Nanotechnology will yield advanced materials that will allow for longer service life and lower failure rates. Among the key applications are: nanocoating of metallic surfaces to achieve super-hardening, low friction, and enhanced corrosion protection; "tailored" materials for infrastructure and vehicles; and "smart" materials that monitor and assess their own status and health and repair any defects including fire-resistant materials in vehicles and aircraft.
- Applications of nanoelectronics for transportation include: advanced communications that maximize the benefits of intelligent transportation systems and obviate the need for some travel altogether; sensors that continuously monitor the condition and performance of roads, bridges, and other infrastructure; and "brilliant" vehicles that can avoid crashes and improve operator performance.
- New materials developed through nanotechnology will permit the ultra-miniaturization of space systems and equipment, including the development of smart, compact sensors; miniscule probes; and microspacecraft. Applications include: economical supersonic aircraft; low-power, radiation-hard computing systems for autonomous space vehicles; and advanced aircraft avionics.
- Nanotechnology has the potential to reduce transportation energy use and its impacts on the environment. Applications include nanosensors used to monitor vehicle emissions and to trap any pollutants; nanoparticle-reinforced materials that replace metallic components in cars; replacement of carbon black in tires with nanoparticles of inorganic clays and polymers, leading to tires that are environmentally friendly and wear-resistant; and carbon-based nanostructures that serve as "hydrogen supersponges" in vehicle fuel cells.

### *Agency Participation and Partnerships*

Various agencies including, DOE, DOD, NIST and NASA, developing materials and manufacturing for transportation.

## **National Security**

### *Vision*

Retain and extend technology to enable rapid military dominance simultaneously with reduced manpower, lower human exposure to risk, and more affordable systems. DOD investment in nanoscience is essential to meet its stated goals of knowledge superiority, full spectrum dominance, and warrior protection in the 21<sup>st</sup> century.

### *Relevance*

The 1998 Defense Science Board study “Joint Operations Superiority in the 21<sup>st</sup> Century” states that: “Perhaps the most pervasive operational challenge enabling early and continuous combat effectiveness is knowledge superiority.” Nanoscience and technology will enable us to achieve knowledge superiority at all levels, in the 2020 time frame. It can lead to incredible gains: in sensor suites with 1000 times smaller size/power embedded in autonomous microsystems; in processors with 100 times faster speed, 100 times higher density, and 1000 times less power per function; in nonvolatile, radiation-resistant static memory with 100 times higher density and 50 times faster access speed; in flat, foldable displays with 10 times greater brightness (nanophosphors) without a concomitant increase in power requirements; and in communications with 100 times greater bandwidth. The Network Centric Warfare, Information Warfare, and Simulation/Modeling operations — already accelerated by the previous improvements in information technology hardware — will be revolutionized once again through these additional breakthroughs in hardware capability.

The new capability will include worldwide, instantaneous communication, threat identification, secure encryption, speech recognition/language translation for joint operations, and combat ID. The huge datastreams from multispectral imaging (visible, infrared, mm-wave, microwave, and acoustic) will be transmitted, processed, correlated, and presented in millisecond time frames. The enhancements will enable the service goals of smarter weapons for surgical strikes and uninhabited combat vehicles, with special value for aircraft whose agility will improve significantly without human g-force limitations. The automation stemming from greater information processing coupled with nanofabricated sensing suites and nanoelectromechanical actuation will result in a reduced workforce. The greater training requirements imposed by the reduction in manpower will be met by affordable personal virtual reality trainers. The realization of these new concepts will require all these advances in sensing/processing/storage/display transmission.

The central theme of Joint Vision 2010 is full spectrum dominance, including dominant maneuver, precision engagement and full dimensional protection. These requirements translate into high performance platforms — satellite, aircraft, surface ship, submarine, armored vehicle — all needing premiere materials at affordable costs. Nanostructures have



novel properties not otherwise available. Their small size also permits their selective incorporation into composites with tailored performance characteristics. Expected improvements include the following: reduced manufacturing costs by self-assembly of smaller units into larger structures rather than costly machining down from bulk and by net-shape formation of ceramics through novel nanostructure interface mechanics; organic composites with high strength-to-weight made by including nanotubules (whose measured strengths are among the highest known) or with fire resistance created by including nanoclays (enabling the use of organic composites in surface ships and submarines); multispectral (visible, infrared, mm-wave, microwave, acoustic) low observable materials made by incorporating quantum dots and nanocrystal networks; lowered maintenance costs by nanostructured coatings with reduced wear/corrosion/thermal transport; higher efficiency energy conversion technology with nanostructured fuel cells, solar cells, and batteries; and smart materials that detect and respond to the environment through embedded nanosensors and nanoactuators (e.g., to sense a sonar or radar ping and squelch any echo).

Defense ultimately relies on the warrior; information and platforms are aids, not ends. We must protect the warrior from weapons of mass destruction; sense and aid his performance, especially under the extreme operating demands placed on him; and provide the casualty care he deserves. Bionanodevices will revolutionize these capabilities. The techniques and tools of nanoscience will detect single pathogens, providing the ultimate in sensitivity for chemical and biological agents packaged in fast, low-power, affordable systems no bigger than badges. Nanostructures show promise for the catalytic degradation of pathogens/chemical agents with less damage to the environment. The marriage of nanoelectronics with molecular biology will enable in-situ, body powered sensors (for pathogens, alertness, fatigue) with the ability to take action to protect the individual or enhance his performance (augmented sensory capability — hearing, vision, smell, touch).

### *Priorities*

The DOD Basic Research Plan has designated a Special Research Area — Nanoscience — with the following goal: “to achieve dramatic, innovative enhancements in the properties and performance of structures, materials, and devices that have ultra-small — but controllable — features on the nanoscale....” In the last fifty years, DOD funding has been a principal federal source of research support for the next generation of electronic/optoelectronic devices, affordable, high performance materials, and defense against weapons of mass destruction. The pending DOD-relevant nanotechnology investment has several common objectives with other Grand Challenges addressed to civilian use:

The priorities in nanoelectronics/optoelectronics are as follows:

- Synthesis/processing of quality nanostructures that can translate to commercially affordable processing technology: self-assembly, parallel processing via proximal probes, and in-situ processing controls
- Measurement of nanostructure properties: quantum effects, tunneling, exchange coupling, molecular electron transport, and terahertz response
- Innovative device concepts: single electron devices, spin-electronics, quantum dots, and molecular electronics

- Potential system architectures: cellular automata, quantum computers, cellular parallel computers, and multiple function integration
- Modeling/simulation for accelerated device/system progress
- Advanced optical components: photonic crystals, and novel phosphors
- Autonomous microsystems coupling sensing, processing, storage, actuation, communication, and the power to facilitate a complete tactical picture

The priorities in affordable, high-performance nanostructured materials are as follows:

- High volume manufacture of high quality clusters, nanotubes, and dendrimers
- New materials fabrication paradigms: superplasticity and self-assembly
- Formation and properties of high surface area materials, nanocrystal networks, and aerogels
- Measurement of individual nanostructure properties and of the interfacial properties in nanostructured materials
- Physics of the nanometer-scale initiation events of materials failure
- Tailored coatings for affordability — wear, corrosion, thermal barrier, and energy harvesting
- Smart materials for condition based maintenance, and for low observable signatures
- Models/simulations incorporating multi-scale (atomic to nanostructure to microstructure to macroscopic) computation and leading to materials by design

The priorities in bionanodevices are as follows:

- Measurements of single supramolecular properties to define the events of molecular recognition and dynamics
- Design and implement molecules to interface between nanodevices and body chemistry
- Nanoelectromechanical systems (NEMS), especially utilizing molecular motors as potential actuators

*Budget request for FY 2001* is \$140 million, a \$69 million increase above FY 2000.

#### *Agency Participation and Partnerships*

The DOD programs in nanoelectronics/electrooptics and materials are in partnership with NSF Centers, DOE facilities, and industry. The DOD expects to build on NIH investment in bionanodevices, focusing the vast opportunities there on specific DOD needs.

**A3. Centers and Networks of Excellence** (total FY 2001 is \$77 million, \$30 million above FY 2000)

*Vision*

Fund ten nanoscience and technology centers and networks at about \$3 million/yr for approximately five years with opportunity of one renewal after the review. A focus on research networking and shared academic user facilities is recommended. The establishment of nanoscience and technology research centers similar to the supercomputer centers will play a critical role in attaining other initiative priorities (fundamental research, Grand Challenges, and education), development and utilization of the specific tools, and in promoting partnerships. Collaboration with academic networks (such as NNUN for nanotechnology equipment and DesCArtES for nanoelectronics software), and with national users facilities (such as synchrotron radiation facilities and neutron sources at national laboratories) is envisioned.

*Special opportunities*

The science of nanostructures has become a theme common to many disciplines, from nanoelectronics and molecular biology to catalysis, filtration and materials science. Each of these disciplines has evolved its own independent view of nanoscience; the opportunity to integrate these views and to share the tools and techniques developed separately by each field, is one of the most exciting in all of science and brings with it enormous potential for technological innovation. Centers for nanoscience and technology will be a major component of the spectrum of support for this increasingly interdisciplinary field, with potential impact beyond that of single investigator programs.

A related need is for adequate advanced facilities to do the research demanded by nanoscience and technology. As George Whitesides and Paul Alivisatos have pointed out, to make rabbit stew, you must first catch a rabbit. In order to work in nanoscience, one must be able to fabricate and characterize nanostructures. In many cases the requisite fabrication and characterization facilities are beyond the scope of individual-investigator laboratories – it takes the scope and infrastructure of a center or ‘shared facility’ to equip and maintain them. Access to sophisticated and well-maintained facilities and instrumentation together with support for instrument development will be essential to the success of research and education nanoscience and technology.

The proposed centers will be critical to support and accomplish the core objectives of the initiative: interdisciplinary fundamental research (budget request for FY 2001: \$40 million, a \$15M/yr increase over FY 2000), Grand Challenges (\$20 million, a \$8M/yr increase), laboratory infrastructure (\$17 million, a \$7M/yr increase), and education and training.

*Priorities and Modes of Support*

Nanoscience and Technology Centers and Networks (NTCs) will catalyze the integration of research and education in nanoscience and technology across disciplines and among sectors including universities, government laboratories and the private sector. They will also help to

provide the sophisticated tools needed to do the work.. NSF's Science and Technology Centers (STCs), Engineering Research Centers (ERCs), and Materials Research Science and Engineering Centers (MRSECs) provide successful models for this process over a very wide range of science and engineering. DOD's Multidisciplinary University Research Initiative (MURI), and DOE's and NASA's university-based research centers provide successful patterns for mission oriented centers. The NTCs will include partnership among academic institutions and between academia, government laboratories and the private sector as needed. They will address interdisciplinary areas such as simulation at the nanoscale, device and systems architecture at the nanoscale, nanomaterials, nanoscale structures and quantum control, nanofabrication, hierarchical linking across multiple length and complexity scales, nanotechnology and biorobotics, nature and bio-inspired materials and systems, nanoscience for health care, and molecular nanostructures.

NTCs will:

- Address major fundamental problems in nanoscience and technology, bringing to bear the entire spectrum of disciplines including engineering, mathematics and computer science, physical sciences, earth science, and biological and medical sciences as needed. Exploratory research, and vertical integration from fundamental research to innovative technological outcomes will be encouraged. Stimulate and support interagency partnerships to foster emerging areas of nanoscience and technology at interdisciplinary frontiers.
- Support interdisciplinary research groups comprising strongly coupled groups of investigators - the whole must be greater than the sum of the parts. Provide incentives to enable interdisciplinary research and education to prosper;
- Develop and sustain strong links between experiment, theory, modeling and simulation to advance nanoscience and engineering;
- Integrate research and education from pre-college through postdoctoral;
- Provide and maintain state of the art instrumentation and shared user facilities that are beyond the reach of benchtop science, including fabrication and characterization equipment, for the benefit of users both within and outside the centers;
- Foster intensive cooperation, collaboration and partnerships among investigators from universities, government laboratories and industry involved in nanotechnology. Programs for visitors from industry and other research centers will be established.
- Promote exchange programs for students and faculty with other centers of excellence in the US and from abroad;
- Include effective collaboration with and access to unique capabilities offered by existing facilities at such as synchrotron x-ray, neutron sources, the National High Magnetic Field Laboratory, the National Nanofabrication User Network, and advanced computational facilities and resources, through partnership with national laboratories and other institutions and centers as needed;
- Provide access to databases, remote access to instrumentation, and links from research and education to producers and users of nanotechnology;
- Allow investigators flexibility to pursue promising new lines of high-risk research within the overall scope of the Center's goals, without agency 'micromanagement'.

### *Infrastructure*

Physical laboratory infrastructure will be created in the emerging areas of nanoscience and technology, including expensive equipment that can not be obtained or adequately maintained by individual academic researchers. This will contribute to an advanced and balanced infrastructure.

The educational value of NTCs and their role in workforce development deserves special mention. They will provide both a horizontal and vertical integration of education, with students interacting at all levels of their training: precollege, undergraduate, graduate students, postdocs, junior and senior faculty and investigators from industry and government labs. They will also provide a platform for outreach to generate and maintain public support for nanoscience and technology, and for curriculum development in critical cross-disciplinary areas involving engineering, the physical sciences and biology.

*Budget Request for FY 2001: \$77 million, a \$30 million increase.* Establish approximately ten new nanoscience and technology centers/networks by competitive review, each at about \$3M total funding over approximately 5 years, renewable for a further 5 years. Each NTC will address a major topical area in nanoscience and technology, and will support about 10-20 core researchers plus students and postdocs and support for instrumentation, access to facilities, materials and supplies, partnership with industry and national laboratories as appropriate, and programs for education and outreach. The new centers will be integrated in the existing group of about 15 large university-based and national laboratory-based centers with research on nanoscale science and engineering.

### *Agency Participation and Partnerships*

All participating agencies. NSF will focus on university-based centers and networks, while other agencies will support a combination of government research laboratories and academic institutions. Vertical integration from fundamental research to technological innovation will be supported by joint funding from NSF and mission oriented agencies, DOD, DOE, NASA and NIH, respectively.

**A4. Research Infrastructure** (total FY 2001 is \$80 million, \$30 million above FY 2000)

One of the IWGN “high priority” themes for additional funding beginning in FY2001 is ‘research infrastructure’ that includes metrology (budget request for FY 2001: \$10 million, a \$6 million increase over FY 2000), instrumentation (\$30 million, a \$8 million increase), modeling and simulation (\$15 million, a \$6 million increase), and user facilities (\$25 million, a \$10 million).

*Vision*

A balanced, strong, but flexible infrastructure will be developed to stimulate new discoveries and innovations that can be rapidly commercialized by U.S. industry. The focus will be on developing measurements and standards, research instrumentation, modeling and simulation capabilities, and R&D user facilities.

The potential is great for universities and government to transition this science and technology, bringing forth fundamental changes. There are great demands in industry to attract new ideas, protect intellectual property, and develop high performance products. The transition will require a sustained and timely investment. If the issues associated with research infrastructure and transition from knowledge-driven to product-driven efforts are not satisfactorily addressed, the United States will not remain internationally competitive and, therefore, have difficulty maintaining the economy and quality of life and security that exist today.

**Metrology (Measurement Technology)**

*Challenges and Opportunities*

Nanotechnology offers an outstanding challenge to measurement technology by requiring three-dimensional, atomic-scale measurement capabilities over large areas. To design, observe, test, and understand the next generation of nanodevices, we must be able to measure all the important physical, chemical and at times biological parameters associated with the devices. These measurements are not currently possible because the necessary tools and theories are only rudimentary, but must be developed through this Federal Initiative. .

While nanoscale measurement is challenging, nanotechnology offers totally new mechanisms and instruments for measurements of new phenomena at subatomic spatial scales. Those measurements are currently out of our reach. Also, exquisitely accurate measurements of macroscopic physical, chemical and biological properties are possible through nanotechnology.

*Priorities*

The research supported by this federal nanotechnology initiative will:

- Develop new measurement systems with intrinsic, atomic-scale accuracy for length, mass, chemical composition, electricity, magnetism and other properties;

- Develop a fundamental understanding of the interactions of matter at the single atom, and molecule level allowing the design of new measurement approaches and instruments; and
- Create new standard materials, standard data, analytical methods, and standard tools to assure the quality of the new nano-based commercial products.
- Rapid transfer of the new measuring techniques and standards to industry.

The new measurement capabilities developed through this initiative will impact all industrial sectors and the everyday lives of each American. For example, new health related measurements will improve the accuracy, availability, and cost of diagnostic tests and allow more diseases to be diagnosed in a timely fashion. The reliability, cost, and function of cars, planes, telephones, computers and many other devices will improve through manufacturing improvements enabled by these measurements. For example, nanometer accuracy has made possible the giant magnetoresistance layers to be manufactured and the most advanced NASA spacecraft to be built.

#### *Agency Participation and Partnerships*

DOC/NIST in collaboration with other agencies as a function of the area of relevance.

### **Instrumentation**

#### *Challenges and Opportunities*

Availability of instrumentation in university, government laboratories and industry will be a determining factor in the advancement of the field. This initiative will provide tools to investigators in nano-science and engineering to carry out state-of-the-art research, to achieve the nanotechnology potential, and to remain competitive. Funding support will include the continuous development and advancement of the instrumentation for nanotechnology in partnership with the private sector.

In the last few years there has been continually increasing interest in nanotechnology here in the United States as well as in Japan and Europe. It is critical that we have the state-of-the-art instrumentation for development of materials at the nano-scale and processing of nanostructures and devices, development of nano-scale systems, and for testing, measurements, and characterization. Progress is being made in the instrumentation - such as the scanning tunneling microscope (STM), the atomic force microscope (AFM) and near-field microscopy (NFM) - which has been developed, for the observation, characterization and analysis of nanostructures. These instruments and the development of relevant technologies are helping scientists and engineers in making scientific advances in the area of nanotechnology. At the same time these tools are being modified and improved to increase the capabilities available for manipulation and manufacturing of nanostructures.

It is possible to make nanomaterials and nanostructures using the existing facilities and capabilities available in many of the above mentioned disciplines. However, to make significant progress and impact in nanotechnology, we will have to extend those capabilities and to develop more interdisciplinary facilities that have the appropriate instrumentation.

### *Priorities*

- Development of new instruments for research, development and processing in nanotechnology. Instrumentation for the characterization of individual and ensembled nanostructures will be required. For example, the development, detection, and manipulation of biological structures, semiconductor technology and polymeric materials will require instrumentation that is capable of handling all these materials in one facility and without the danger of cross-contamination.
- Fund the purchase of instrumentation enhancing the capabilities of the existing research centers, networks and consortiums. This includes funding of industry/university/government collaboration to develop the tools and technology. The major R&D instrumentation and facilities will be made available to users not only from the institution that houses the facilities, but also for users from other institutions, industries and government.
- Provide computer network capabilities and a nanotechnology database for the management and dissemination of information to the nanotechnology science and engineering community in order to promote collaborations.

### *Agency Participation and Partnerships*

The development of the instrumentation and capabilities for research and development in nanotechnology will require cooperation and collaboration of scientists and engineers from universities, industries, and the funding support of all government agencies. NSF, DOD, DOE and NASA will develop the instrumentation infrastructure in universities.

## **Modeling and Simulation Infrastructure**

### *Challenges and Opportunities*

Experimentation and modeling/simulation capabilities will be equally important to advances in understanding, each testing and stimulating the other, compelling the development of new computational methods, algorithms and high performance computing resources.

Modeling and simulation at nanoscale will enable new synthesis and processing methods of nanostructures, control of nano-manipulators such as atomic force microscopes, development of scale-up techniques, and creation of complex systems and architecture based on nanostructures. Control of nano-manufacturing requires the development of manipulation strategies and associated software, using either known or new robotics techniques. Nanoassembly must be automated because the number of elementary operations required in most assemblies would be enormous. Research is needed into the programming languages suitable for assembly, into the techniques for path planning and other high-level control, and into the real-time control of single manipulators and arrays of manipulators.

Simulation and design software will *depend upon high-speed scientific computation*. Research will be needed in information technology that creates new specialized software, algorithms, and hardware that enable more effective scientific and engineering computations at nanoscale. In particular, nanodesign will need programming tools to enable more effective use of available computational resources. Software for *visualization* and for large-scale



scientific computation will be necessary to designers for an accurate view of material properties.

*The ab-initio prediction* of fundamental physicochemical and engineering properties of extended molecular systems is becoming feasible. This is being made possible by advances in atomic and electronic structure calculation, molecular dynamics simulation, and software and hardware design. Realistic predictions still rely heavily on adjustments to theory suggested by experimental verification.

#### *Relevance*

In the future, molecular modeling and simulation and high-throughput experimentation *will affect most products and processes* that depend on chemical, biological, and materials properties. This knowledge will generate new competitive advantages for modern industries, such as electronics and optoelectronics, biotechnology, environmental technology, medical engineering, sensing and automation.

Computational modeling should provide a better understanding of the parameters and constraints for these nano-devices and create a framework for *interpreting experiments*. Modeling may even reduce the need for costly experimentation. Conceivably, modeling also could give new information about nanodevices that is not evident through experimentation alone.

Applications to be considered include drug design, high performance materials, catalysis, environmental processes, energy conversion, biotechnology, nanoelectronics, and nanomagnetism and the related field of nanotechnology. Affected industries include chemicals, pharmaceuticals and other biochemicals, paper, textile, electronics, and advanced materials.

#### *Priorities*

- Develop computational facilities and human resources to facilitate development of interdisciplinary centers and network to serve nanotechnology R&D activities. Collaboration among groups working in different disciplines and areas of relevance (chemistry, thermodynamics, mechanics, electronics, biological processes, others) will be encouraged.
- Multiscale and coupled phenomena modeling and simulation of nanostructures at the atomic and molecular level in order to further fundamental understanding, explore new phenomena, and improve design predictions, will be supported with priority.
- Develop new simulation and design software to systematically create new materials and systems for given properties and functions. Computational thrusts could focus on the modern advances of quantum chemistry, molecular mechanics, molecular dynamics and device modeling and prediction applied to the chemical, energy, environmental, and advanced materials technologies. The methods may include Quantum Mechanics (QM), Force Fields (FF), Molecular Dynamics (MD), Coarse Graining (CG), Statistical Mechanics (SM), and Continuum Parameters (CP). Simulations that incorporate multiscale/multiphenomena descriptions need to be developed.

- Development of software, computational approaches, and simulation tools for process control and molecular manufacturing. This area is a very timely topic as it focuses on the regime between atomistic simulations (quantum theory, molecular dynamics) and physicochemical engineering practice (process simulation and design). The idea here is to use the results of atomistic calculations to supplement experimental data in determining the parameters of the coarse grain, phenomenological models required for process simulation and design. The use of new data on structural correlations from the atomistic simulations should provide more detailed information not available from experiment and would lead to much more detailed and accurate predictions.

*Agency Participation and Partnerships:* All agencies. A network for multiscale/multiphenomena simulation at nanoscale will be developed by NSF, DOD, DOE and NASA.

## **User Facilities**

### *Special Opportunities*

The research scientists and engineers working in the area of nanotechnology will need access to state-of-the-art instrumentation and facilities for observation, characterization, manipulation and manufacturing. University-based and national laboratory-based centers will provide access to expensive equipment with rapid state-of-the-art changes.

The most common instruments will probably be various types of scanning probe, electron and ion microscopes. On the one hand, there has to be an understanding that a single research group can easily have need for several different scanning probe microscopes, since there are now many different types each optimized for a different task. On the other, the best electron and ion microscopes are very expensive and costly to maintain, and means should be provided for universities either to acquire, maintain and operate such systems, or have access to users facilities. There will also be a need for a wide range of facilities and instruments, ranging from synchrotron radiation and neutron sources, electron-beam and ion-beam manufacturing, all types of spectrometers and computational facilities to both handle the processing of massive amounts of data and carry out the crucial modeling/simulation work needed to advance the field rapidly. Since the emphasis for most of groups performing nanotechnology research needs to be on the science and not the equipment, the existing facilities (such as the National Nanofabrication Users Network) will be extended and a number of shared laboratories and regional facilities need to be funded and staffed.

The national laboratories have the capability to develop and maintain large-scale and multi-user neutron and photon facilities. Argonne National Laboratory is the site of the Advanced Photon Source and the Intense Pulsed Neutron Source; Brookhaven National Laboratory is the home of the National Synchrotron Light Source and the High Flux Brookhaven Reactor; Oak Ridge National Laboratory houses the High Flux Isotope Reactor and will be the location of the Spallation Neutron Source; the Los Alamos Neutron Scattering Center, LANSCE, is located at the Los Alamos National Laboratory; the Lawrence Berkeley National Laboratory is the home of the Advanced Light Source; and the Stanford Synchrotron Radiation Laboratory is situated at the Stanford Linear Accelerator Center.

*Priorities*

- Multiple-user national centers and networks equipped with nanotechnology-specific equipment (type of measurement, industry, etc.) need to be funded and staffed; the centers may be based in universities or at national laboratories.
- Vertical integration of fundamental and technological research within the multiple-user centers will be encouraged for synergistic purposes. Multi-technology engineering demonstration facilities funded by mission-oriented agencies and industry should be included in the centers.
- Development and use of regional university-national laboratory-industry facilities will be encouraged.
- The issue of *information sharing* is paramount; an agency and specific funding might be identified to foster communication of ideas and results among the various subfields within nanotechnology. One approach would be for an agency such as NIST to sponsor a nanotechnology-specific information facility agreed by participating agencies.

*Budget request for FY 2001* is \$80 million, a \$30 million increase above FY 2000.

*Agency Participation and Partnerships*

DOE's national laboratories and NSF's university-based user facilities, in collaboration with other agencies and industry, will develop a national system for key facilities in the U.S..

## **A5. Societal Implications of Nanotechnology and Workforce Education and Training** (total \$28 million, \$13 million above FY 2000)

### *Vision*

A university-based program is designed to provide effective education and training of nanotechnology professionals, especially for industrial careers. Focused research on social, economic, ethical, legal and workforce implications of nanotechnology will be undertaken.

The science, engineering, and technology of nanostructures will require and enable advances in a fabric of disciplines: physics, chemistry, biology, materials, mathematics, engineering and education. In their evolution as disciplines, they all find themselves simultaneously ready to address nanoscale phenomena and nanostructures. The dynamics of interdisciplinary nanostructure efforts will reinforce educational connections between disciplines and give birth to new fields that are only envisioned at this moment. Rapid development of nanotechnology will require changes in the laboratory and human resource infrastructure in universities, and in the education of nanotechnology professionals.

A main objective of the national initiative is to provide new types of education and training that lead to a new generation of skilled workers in the multidisciplinary perspectives necessary for rapid progress in nanotechnology. The proposed initiative will leverage the existing strong foundation of nanoscience and engineering in the U.S., and will address the formidable challenges that remain.

When radically new technologies are developed, social, economical, ethical, legal, environmental and workforce development issues can rise. Those issues would require specific research activities and measures to take advantage of opportunities or reduce potential risks. NNI will address these issues in a research program.

### *Special Educational Opportunities*

Nanotechnology offers unprecedented opportunities to revitalize connection between disciplines and promote education at the interfaces between physics, mathematics, chemistry, biology and engineering. Although change is occurring in a relatively rapid fashion, there still exist many elements in the culture of our research universities that do not encourage multidisciplinary research. Specific suggestions to address these opportunities and needs are:

- *Introduce nanoscience and engineering in existing and new courses.* Courses on surface science, molecular dynamics, quantum effects, and manufacturing at molecular scale are necessary in curricula at the undergraduate and graduate levels. An integrative science and engineering approach is suggested. Technology programs cannot be developed without strong supporting science programs because of the scale and complexity of the nanosystems.
- Nanotechnology will help *integration of research and education into a new paradigm of learning based on molecular models* instead of microscopic approach. The recommended nanotechnology centers will provide an environment with facilities and interdisciplinary research teams that will enable educating a new generation of young scientists.

- *Educating and training a new generation of skilled workers* in the multidisciplinary perspectives necessary for rapid progress in nanotechnology is necessary. This represents a grand experiment in integration - integration of a multiplicity of disciplines and expertise, and integration of education and research into a true partnership. There should be a broader range of educational opportunities for students coming into nanotechnology areas. The students must become deep in one subject, but they also need to develop breadth by being able to transcend geographical location, institution and discipline. The problem with this goal is that most graduate students in technical areas are funded by the grants to their research advisors, and thus they are tied to a specific discipline and location because their mentors cannot afford to pay for students who are not in their labs. Thus, there should be a significant number of nanotechnology fellowships and training grants, which will give the best students the ability to craft their own education by specializing in one area but having the opportunity to work with one or more other mentors. This will further encourage a practice that is already occurring, since much of the current transdisciplinary nanotechnology research efforts are actually initiated by students who realize the benefits of working with more than one advisor. An emphasis on educational outreach is recommended for involving people at all levels.
- *Programs that encourage intermingling among science, engineering and business disciplines* should also be supported strongly, since grooming future technically competent entrepreneurs is at least as important as future professors and researchers. Nanotechnology workshops focused on graduate students should be held that allows them to see and understand the bigger picture, and encourage them to communicate across disciplinary boundaries.
- *Program to investigate societal impact of nanotechnology*, which will include focused research on social, economic, ethical, legal and workforce implications of nanotechnology.

### *Relevance*

Education will need to address the fast development of nano-science and nano-industries. An entirely new generation will need to be trained in the sciences underpinning nanotechnology. The centers to be created in response to this initiative will strengthen the environment in which we train our young scientists and engineers, thereby helping to ensure that the United States will lead the technologically developed nations into the 21st Century. The creation of the intellectual capital is probably the most important long-term investment for science and technology.

The funding profile for university grants and national labs in nanotechnology must increase at a rate that will encourage the best young researchers to stay in the field and allow them to build up their own research programs. The first two products to come out of the early stages of government funding will be trained people and scientific knowledge. There must be a critical mass of these two before the development of a technology and intellectual property can occur. Once these become compelling, then actual products, the manufacturing infrastructure and the high paying jobs will arise that will repay the investments that have been made in this area.

*Priorities and Modes of Support*

To most effectively respond to the opportunities discussed above, several specific priorities are:

- Introduce nano-science and engineering in existing and new courses.
- Nanotechnology centers and networks, with facilities and interdisciplinary research teams, that will enable educating a new generation of young scientists.
- Create “regional coalitions” that involve industry-tech generation that include educational and training programs.
- Support student and post-doctoral fellowships for interdisciplinary work.
- Support student and young scientist internships at centers of excellence abroad.

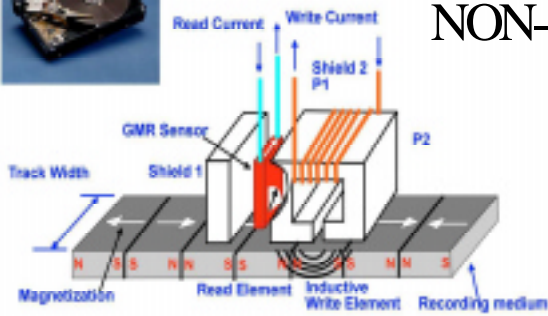
*Budget Request FY 2001:* \$28 million, a \$13 million increase over FY 2000. Indirect contributions are from other funding themes, such as fundamental research and centers.

*Agency Participation and Partnerships:* NSF in collaboration with NIH, DOC and DOD and other agencies will establish an education and training program for the critical areas in nanoscience and engineering. An education and training network with the participation of all interested agencies is envisioned. University based centers will be co-funded by various agencies.

**Appendix B. Examples of nanotechnology applications and partnerships**

(Additional examples are provided in the attached volume “Nanotechnology Research Directions – IWGN Workshop Report”, 1999)

**B6. Giant Magnetoresistance in Magnetic Storage Applications**



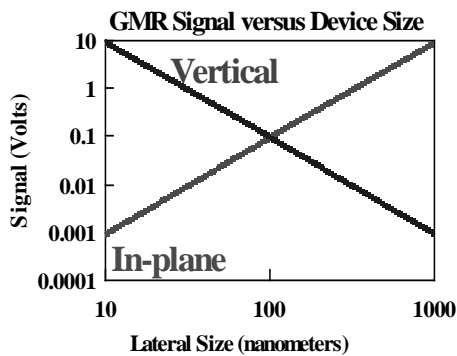
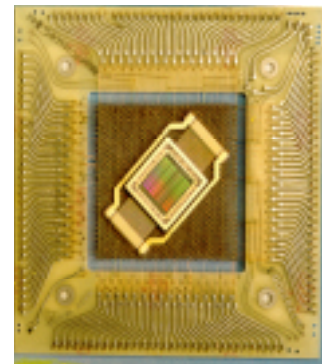
Magnetic recording process.

INFORMATION TECHNOLOGY

NON-VOLATILE HIGH DENSITY MEMORY

*IN 1999:* Within ten years from the fundamental discovery, the giant magnetoresistance (GMR) effect in nanostructured (one dimension) magnetic multilayers has demonstrated its utility in magnetic sensors for magnetic disk read heads, **the key component in a \$34B/year hard disk market in 1998**. The new read head has extended magnetic disk information storage **from 1 to ~20Gbits**. Because of this technology, most of hard disk production is done by U.S.-based companies.

*IN 5-7 YEARS:* A future application of GMR is nonvolatile magnetic random access memory (MRAM) that will compete in the **\$100B RAM market**. In-plane GMR promises 1Mbit memory chips in 1999; at the right, the size of this chip (center of image) is contrasted to an earlier 1Kbit ferrite core memory. Not only has the size per bit been dramatically reduced, but the memory access time has dropped **from milliseconds to 10 nanoseconds**. The in-plane approach will likely provide 10-100Mbit chips by 2002. Since the GMR effect resists radiation damage, these memories will be important to space and defense applications.



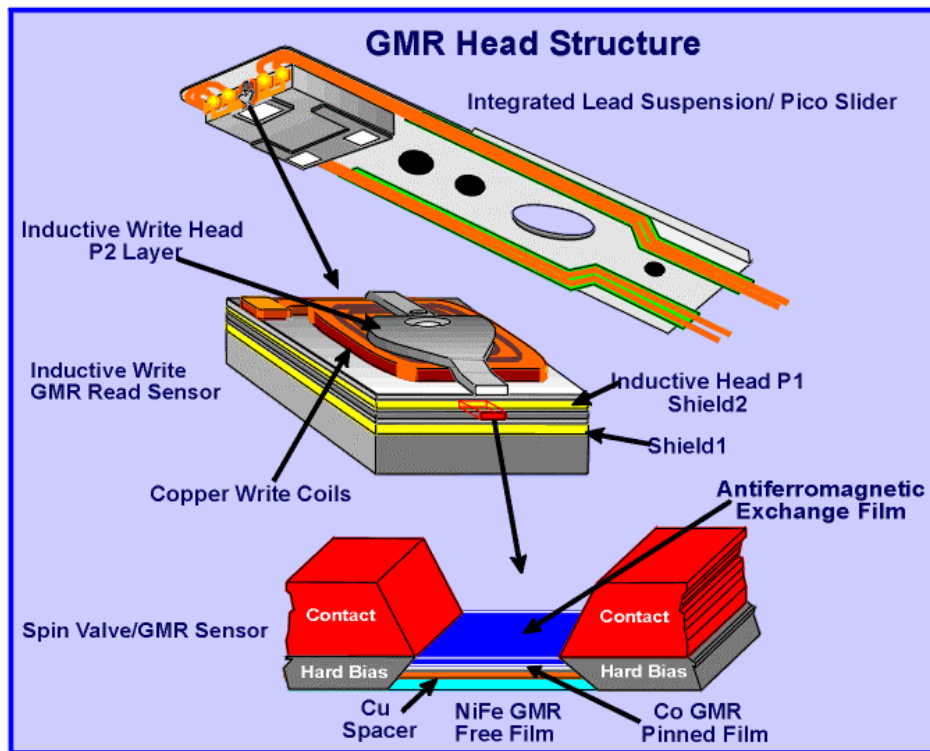
*AFTER 5 YEARS:* The in-plane GMR device performance (signal to noise) suffers as the device lateral dimensions get smaller than 1 micron. Government and industry are funding work on a vertical GMR device that gives larger signals as the device dimensions shrink. At 10 nanometer lateral size, these devices could provide signals in excess of 1 volt and memory densities of 10 Gbit on a chip, comparable to that stored on magnetic disks. If successful, this chip would eliminate the need for magneto-mechanical disk storage with its slow access time in msec, large size, weight and power requirements (**paradigm changes**)

Additional information:

## A Commercial IBM Giant Magnetoresistance Read Head

Contact person: E. Grochowski, IBM

When certain kinds of materials systems are exposed to a magnetic field, their electrical resistance changes. This effect, called the magnetoresistive effect, is useful for sensing magnetic fields such as those in the magnetic bits of data stored on a computer hard drive. In 1988, the giant magnetoresistance effect was discovered in specially prepared layers of nanometer-thick magnetic and nonmagnetic films. By 1991, work at the IBM Almaden research center demonstrated that the GMR effect could be observed in easily made samples and that a special kind of GMR structure, a spin valve, could sense very small magnetic fields. This opened the door to the use of GMR in the read heads for magnetic disk drives. A commercial product based on this design was first announced by IBM in December 1997. In the spin valve GMR head shown in the figure below, the copper spacer layer is about 2 nm thick and the Co GMR pinned layer is about 2.5 nm thick. The thickness of these layers must be controlled with atomic precision.



Commercial IBM giant magnetoresistance read head.



## B7. Nanostructured Catalysts

Researchers at Mobil Oil Co. have revolutionized hydrocarbon catalysis by the development of innovative nanostructured crystalline materials. Their program focused on zeolites, porous materials with well-defined shapes, surface chemistry and pore sizes smaller than 1 nanometer. A new zeolite class, ZSM-5 (see schematic in Figure 1) was discovered in the late 1960s. ZSM-5 has a 10 atom ring structure that contributes pore sizes in the range 0.45 – 0.6 nm (smaller than in zeolites X, Y and larger than in A) and enables shape selected chemistries not previously available.

Zeolite catalysts now are used to process over 7 billion barrels of petroleum and chemicals annually. New Zealand is using the same catalyst to produce 1/3 of its oil fuel requirement by converting it from natural gas via methanol and then high-octane fuels. ZSM-5, along with zeolite Y, now provide the basis for hydrocarbon cracking and reforming processes with a commercial value that exceeds \$30B in 1999 (J. Wise, Vice President Exxon, ret.). Another example at Mobil Oil Co. is the aluminosilicate 10 nm shaped cylindrical pores (Figure 2), which has been applied in both catalysis and filtration of fine dispersants in the environment (Liu and Mou, 1996). Further systematic advances in nanotechnology are expected to increase its share of an overall world catalyst market that exceeds \$210B in 1999.

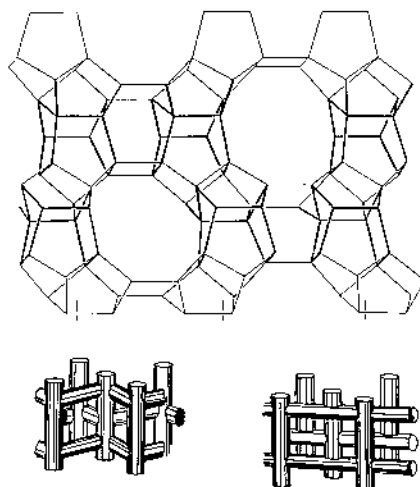


Figure 1. Schematic of the three dimensional channel structure of ZSM-5

Solid catalysts with one, two or three dimensions in the nanometer range can exhibit unique, tailorable activities. For instance, catalytic behavior of gold particles is turned on only after the particle diameter is smaller than 3-5 nm because those crystals have a special structure (icosahedral) that is different from bulk structure. A key objective of nanoscale catalyst research is increase of specificity, selectivity and yield in chemical reactors. Because of the

improvements in nanostructured catalysts, desired product yields have increased significantly in the last decade.

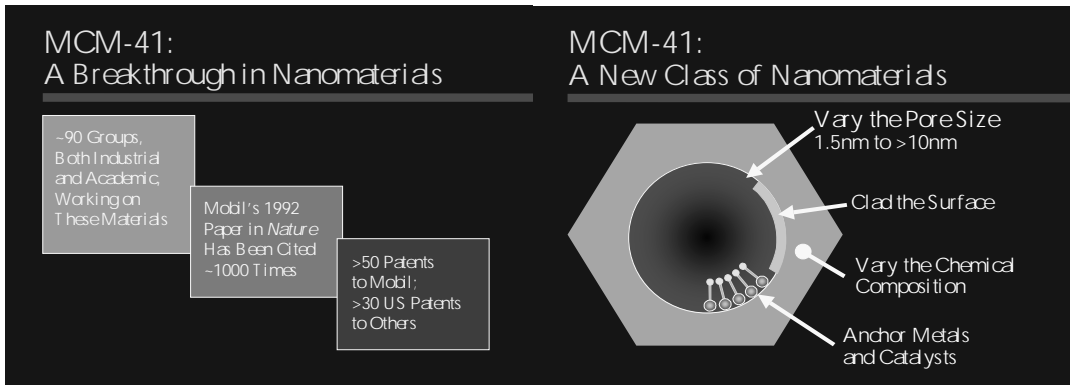


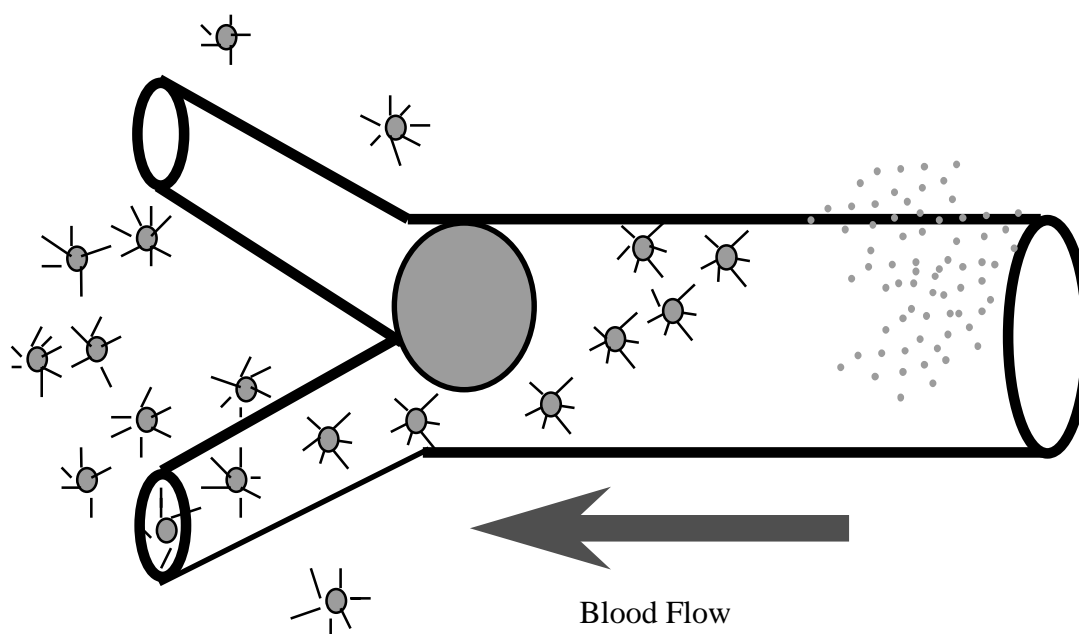
Figure 2. From discovery to application: a nanostructured material (MCM-41)

## B8. Drug Delivery Systems

By using nanotechnology fundamental changes in drug production and delivery are expected to affect about half of the \$380 billion worldwide drug production in the next decade. The U.S. company market share is about 40%. Nanotechnology will be used in various ways:

- Nanosizing will make possible the use of low solubility substances as drugs. This will approximately double the number of chemical substances available for pharmaceuticals (where particle size ranges from 100 to 200 nm).
- Dendrimer polymers have several properties (high solubility in aqueous solvent, defined structure, high monodispersity, low systemic toxicity) that make them attractive components of so-called nanobiological drug carrying devices.
- Targeting of tumors with nanoparticles in the range 50 to 100 nm. Larger particles cannot enter the tumor pores while nanoparticles can move easily into the tumor (Figure 1)
- Active targeting by adding ligands as target receptors on a nanoparticle surface. The receptors will recognize damaged tissue, attach to it and release a therapeutic drug.
- Increase the degree of localized drug retention by increasing the adhesion of finer particles on tissues
- Nanosized markers will allow for cancer detection in the incipient phase when only a few cancer cells are present .

An example of current commercialization is liposome encapsulated drugs produced by Nexstar (doxorubicin for cancer treatment and amphotericin B for fungal infection) with sales over \$20 million in 1999.



In the 1980s, academic researchers proposed using polymers to embed nanoparticles carrying drugs (Douglas and Davis, 1987, “Nanoparticles in drug delivery”). This approach did not prove practical because of the difficulties in disposing of the polymeric blends after their use. In 1992, industry researchers proposed using nanocrystals without polymeric support (U.S. Patent 5,145,682, “Surface modified drug nanoparticles”). This solution has been adopted in the current applications.

An example of industry-government partnerships in this area is the project “Using nanosized particles for more effective cancer therapy” (NIST-ATP, NIH-NCI, CytImmune Sciences Inc., and EntreMed, Inc.). The partnership seeks to develop novel cancer therapeutics, using colloidal gold to effectively deliver biologics and gene therapies to targeted cells, thereby greatly improving the efficacy of the agents while reducing toxic side effects. Most drugs and other therapeutics have a systemic effect on healthy and unhealthy cells. There are often toxic side effects. The unique chemical properties of colloidal gold (tiny gold particles that remain evenly distributed in a solution) make it a promising vehicle for delivering drugs or genes to specifically targeted cells. Colloidal gold is already used as a protein marker by chemists and is also used for medical purposes. However, its therapeutic mechanisms are not completely understood. CytImmune Sciences, Inc. proposes to develop a novel cancer treatment using colloidal gold to deliver cytokines (which modulate the body's immune system) such as tumor necrosis factor. The company will evaluate the optimum size of the gold particles, study the pharmacokinetics and safety issues, and determine whether and how gold-cytokine complexes affect tumors. Studies evaluating colloidal gold for gene therapy to replace defective or missing genetic material also are envisaged. In the gene therapy research, the company will exploit the capability of a colloidal gold particle to bind and deliver genetic materials to target cells. CytImmune hopes to demonstrate cytokine treatment and gene therapy with enhanced safety and efficacy, enabling these cancer treatments to achieve their full potential. If successfully developed and commercialized, the technology could reduce the toxicity of many drugs and potentially enable therapies that harness the body's natural defenses. Colloidal gold is inexpensive to manufacture and therefore should be a cost-effective way of improving health. The ATP program will accelerate the collection of convincing preclinical data thus making it more probable that CytImmune can find a private-sector partner for conducting clinical trials. The research will be carried out in collaboration with the National Cancer Institute (Bethesda, Md.) and EntreMed, Inc. (Rockville, Md.). This 3-year project has received joint funding with \$2 million from ATP/NIST and \$1.7 million from industry.

## B9. Nanocomposites: Nanoparticle Reinforced Polymers

### - Low-Cost, High-Strength Materials for Automotive Parts –

Requirements for increased fuel economy in motor vehicles demand the use of new, lightweight materials - typically plastics - that can replace metal. The best of these plastics are expensive and have not been adopted widely by U.S. vehicle manufacturers. Nanocomposites, a new class of materials under study internationally, consist of traditional polymers reinforced by nanometer-scale particles dispersed throughout (Figure 1). These reinforced polymers may present an economical solution to metal replacement. In theory, the nanocomposite can be easily extruded or molded to near-final shape, provide stiffness and strength approaching that of metals, and reduce weight. Corrosion resistance, noise dampening, parts consolidation, and recyclability all would be improved. However, producing nanocomposites requires the development of methods for dispersing the particles throughout the plastic, as well as means to efficiently manufacture parts from such composites.

Dow Chemical Company and Magna International of America (in Troy, MI) have a joint Advanced Technology Program (ATP) sponsored by the National Institute of Science and Technology (NIST) to develop practical synthesis and manufacturing technologies to enable the use of new high-performance, low-weight “nanocomposite” materials in automobiles (NIST 1997). The weight reduction from proposed potential applications would save 15 billion liters of gasoline over the life of one year’s production of vehicles by the American automotive industry and thereby reduce carbon dioxide emissions by more than 5 billion kilograms. These materials are also likely to find use in non-automotive applications such as pipes and fittings for the building and construction industry; refrigerator liners; business, medical, and consumer equipment housings; recreational vehicles; and appliances.

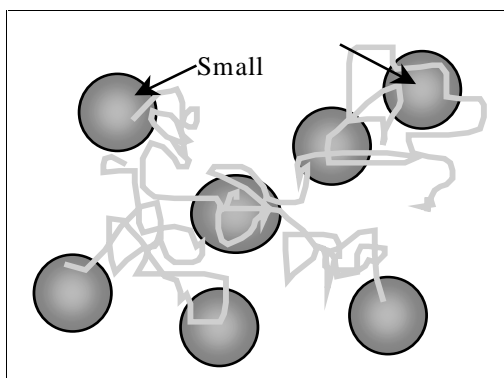


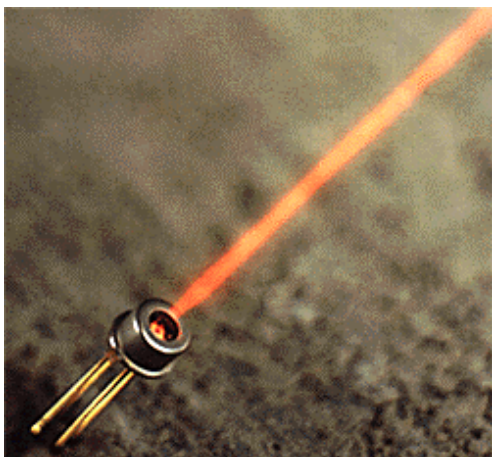
Figure 1. Schematic for nanoparticle-reinforced polymeric materials (after Schadler et al. 1998).

The ATP Ongoing Partnership has started in October 1997 for five years. The partnership includes: NIST-ATP, Dow Chemical Company, Magna International of America. Total project (est.) is \$15.9 million with \$7.8 million requested government funding.

## B10. Two Examples of Nanoelectronic Devices

The proposed National Nanotechnology Initiative would invest in the science base necessary to manufacture, characterize and utilize three dimensional nanostructured systems. While this goal is years away, technologies based on assemblies of one-dimensional nanostructures (superlattices) have already penetrated the marketplace. Two examples are High Electron Mobility Transistor (HEMT) and Vertical Cavity Selective Emitter Laser (VCSEL). These examples give an indication of the potential for nanoelectronics to completely change electronic devices in the next 10-20 years. Currently, other new concepts such as single electron devices, quantum cellular automata, and use of molecular and quantum devices are under investigation.

HEMT devices were engendered by the DoD 6.1 Ultra Small Electronics Research Program (USER, FY81-88) in which \$60M was expended to develop technology capable of creating nanometer thick semiconductor films and electronic junctions. The DARPA Microwave Amplifier Front End Transistor (MAFET) program of FY92-99 used the HEMT devices as the major building block for sophisticated microwave and millimeter wave integrated circuits for radar and communications systems in various DoD applications. Today HEMT is used as a standard for the development of any military and commercial microwave or millimeter wave system requiring low noise figure and high gain. The commercial market for HEMT high frequency receiver/transmitter devices is estimated at \$140M in 1997 with growth to \$800M by 2002.



Vertical Cavity Surface Emitting Lasers are another device that relies on superlattices with nanometer thick films. VCSELs were first demonstrated in the 1970s by the Tokyo Institute of Technology (Japan) and became a commercial reality in the 1990s following innovations at ATT and DARPA funding. Fiberoptic data communications is the first major commercial application of VCSELs, with a growing list of other applications such as optical sensors, encoder, range-finders, and extended range sensing. The present market is approximately \$100M and is anticipated to grow to over \$1B in the next 3-5 years. (A Honeywell VCSEL laser is shown in the picture

and tabulated data below). The VCSEL has superior performance as compared to other solid state photon sources as shown in the following table:

	VCSEL	CD Laser	LED
Power Dissipation (mW)	20	100	200
Modulation Bandwidth (GHz)	>10	<2	>0.1
Wallplug Efficiency (%)	10	5	1

## B11. National Security: Bio Detection

Nanotechnology promises revolutionary advances in military capability. The confluence of biology, chemistry, and physics at the nanometer scale is enabling significant advances in sensors for biological and chemical warfare agents. Civilian disaster response teams and medicine will benefit as well. We cannot afford to respond to a nerve gas attack, such as the 1995 Aum Shinrikyo incident in Japan, by carrying a canary as a sensor. Defense research and development programs are pursuing many sensor options; two related technologies are nearing fruition.

One is a colorimetric sensor (Figure 1) that can selectively detect biological agent DNA; it is in commercial development with successful tests against anthrax (and tuberculosis) (C. Mirkin, Northwestern University). DNA is attached to nanometer size gold particles; when complementary DNA strands are in solution, the gold particles are bound close to each other. The nanoparticles change the suspension color as a function of the particle clustering. Compared to present technology, the sensor is simpler, less expensive (by about a factor of 10), and more selective.

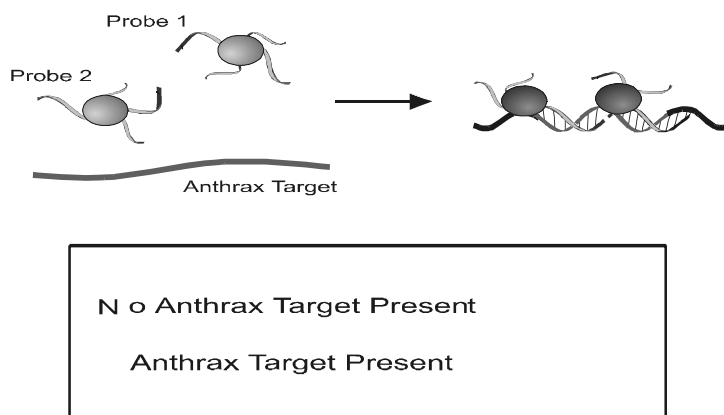


Figure 1. Anthrax detection: when the anthrax target is present, pairs of nanoparticles assemble together via the DNA filaments and change the color of the suspension.

A complementary effort is based on atomic force microscopy (AFM) in which a sandwich immunoassay attaches magnetic beads to a microfabricated cantilever (R. Colton, NRL). In the laboratory the AFM technology is already 100 to 1,000 times more sensitive than conventional immunoassays.

Both colorimetric and magnetic bead technologies might be implemented in detector arrays that provide simultaneous identification of multiple pathogens.

“Colorimetric DNA-Detection,” R. Elghanian, J.J. Storhoff, R.C. Mucic, R.L. Letsinger, and C.A. Mirkin, *Science* 277, 1078 (1997); “One-pot Colorimetric DNA Differentiation of Polynucleotides with Single Base Imperfections Using Au Nanoparticle Probes,” J.J. Storhoff,

R. Elghanian, R.C. Mucic, C.A. Mirkin and R.L. Letsinger, *J. Am. Chem. Soc.* 120, 1959 (1998).

“Sensing Molecular Recognition Events with Atomic Force Microscopy,” G.U. Lee, D.A. Kidwell and R.J. Colton, *Langmuir* 10, 354 (1994); “A High Sensitivity Micromachined Biosensor,” D.R. Baselt, G.U. Lee, K.M. Hansen, L.A. Chrisey and R.J. Colton, *Proc IEEE* 85, 672 (1997).



## **B12. Water Purification and Desalinization**

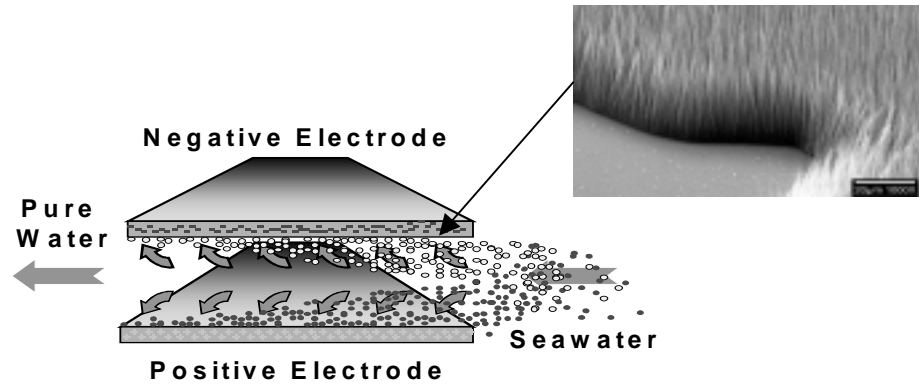
An energy-efficient Flow Through Capacitor (FTC) technology for water desalinization has been designed to desalt seawater with at least 10 times less energy than state-of-the-art reverse osmosis and at least 100 times less energy than distillation. The energy usage of the FTC is anticipated to be less than 0.5 Whr/liter and is being designed for portable use as well as for large-scale integration. The capital cost and operational costs over a 5 year period are predicted to be approximately a factor of 3 less than reverse osmosis systems. The critical experiments underpinning these estimations are underway now. This energy-efficient process is possible by fabricating of very high surface area electrodes that are electrically conductive using aligned carbon nanotubes, and by other innovations in the system design.

The DARPA-funded flow through capacitor desalinization technology being developed by Marc Andelman, its inventor at Biosource Inc, and collaborators at Sabrex of Texas, Nanopore Inc. and Boston College, is a common sense approach based on several technological advances which takes the salt out of seawater as opposed to reverse osmosis which takes the water out of the salt.

The FTC is configured as a deionizing water filter using very high surface area capacitor electrodes (1000 m<sup>2</sup>/g). Upon supplying a small dc voltage (1-2 V), the seawater is rapidly purified due to the fact that the dissolved ions become electrostatically attracted to the high surface area electrode materials. The positively charged ions (Na<sup>+</sup>, Ca<sup>++</sup>) are attracted to the negatively charged electrode, while the negatively charged ions (Cl<sup>-</sup>, SO<sub>3</sub><sup>-</sup>) in the water are electrostatically attracted to the positively charged electrode as shown in the figure below. The performance of the FTC is rooted in nanotechnology, which enable the fabrication of novel high surface area conductive electrode materials to reduce resistive losses and increase charged ion (Na, Cl, etc.) adsorption capacity. The highly conductive materials will reduce resistive losses of the electrodes and makes the desalting process energy-efficient.

Global population is increasing while fresh water supplies are decreasing. The UN predicts that by the year 2025 that 48 countries will be short of fresh water accounting for 32% of the world's population! Water purification and desalinization are some of the focus areas of preventative defense and environmental security since they can meet future water demands globally. Consumptive water use has been increasing twice as fast as the population and the resulting shortages have been worsened by contamination.

Marc Andelman, U.S. Patents: US 5,192,432, 5,196,115, 5,200,068, 5,360,540, 5,384,685, 5,415,768, 5,425,858, 5,620,598



High surface area, high-conductivity electrodes from aligned carbon nanotubes  
(after Biosource Inc., Sabres of Texas and Boston College)

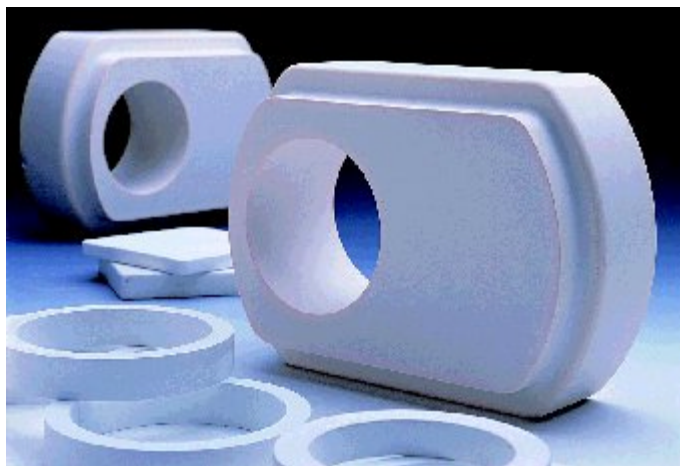
### **B13. Nanophase Technologies Corporation: A Small Business Focused on Nanotechnology**

In 1985, the Office of Basic Energy Sciences, DOE began supporting a research activity in the emerging field of nanophase materials at Argonne National Laboratories' Materials Science Division. Nanophase materials involve powders made of extremely small crystals, which are compacted to yield solid materials. Because the grain sizes are so tiny, one can obtain enhanced plasticity, chemical reactivity, optical absorption, magnetism or other properties.

Initially, the materials were too poorly understood to be developed for industrial applications, but by 1989, Argonne Researcher Dick Siegel (now at Rensselaer Polytechnic Institute) felt confident enough to start a small company commercializing nanophase products. Nanophase Technologies (NTC). Initial funding for NTC was supplied by ARCH, through their associated venture capital fund, and by the State of Illinois, through grants for new job creation. Subsequent funding was raised from a consortium of venture capital funds, and from private individuals and groups. An additional source of funding that was very important to NTC's development was an ATP grant from the Department of Commerce (in 1992), which enabled the company to develop its patented physical vapor synthesis (PVS) process for manufacturing nanocrystalline materials in commercial quantities. This process was based on the laboratory-scale technology used at ANL from 1985 onward. NTC has also developed complementary nanoparticle coating and dispersion technologies, including its proprietary discrete particle encapsulation (DPE) process, as well as capabilities for superplastic forming of ceramic parts. Together, these technologies have enabled NTC over the past decade to enter a number of viable commercial markets. The company presently employs about 40 full-time workers (about 15 of whom hold advanced degrees) in its suburban Chicago facility. NTC currently targets several markets: electronics (including advanced electronics, electromagnetic radiation protection, and advanced abrasives for chemical mechanical polishing); ceramic parts; specialty coatings and catalysts; and other technologically similar applications. In each of these market areas, NTC establishes collaborative relations with major corporate customers to develop and jointly implement nanoscale solutions for the customer's needs. In many cases, products developed to satisfy a particular market need also have significant applicability across other markets. For instance, materials used in conductive coatings also have applicability for antistatic coatings and conductive strip carriers for color toners, abrasives, cosmetics and near-net shaping of ceramic parts. The NTC Web site provides current updates: <http://www.nanophase.com>

Additional information on the government-industry partnership funded by ATP/NIST:  
“Synthesis and Processing of Nanocrystalline Ceramics on a Commercial Scale” (1992)

- ATP funding enables a 25,000-fold increase in production of materials made of nanosized particles and a 20,000-fold reduction in cost per gram (from 10 grams of material per day at \$1,000 per gram to the current capacity of 100 tons per year at 5 cents per gram).
- Sunscreens made with these materials are on the market, offering increased protection levels.
- Tests of prototype products made with these materials show that mechanical seals gain up to 10-fold increases in service life and industrial catalysts become up to four times more active.



Materials made of nanoparticles finally achieve their promise through a government-industry partnership.

The ATP funding also was used to refine and demonstrate a process for shaping nanoscale ceramics into parts quickly and economically, without machining. The company president credits the ATP with helping Nanophase attract major industry collaborators and millions of dollars in venture capital funding, leading to an agreement to distribute the materials in more than 300 countries. The materials are used in a number of commercial products, including cosmetics and skin-care sprays and powders. Independent tests show that sunscreens containing nanocrystalline titania (a non-irritating alternative to sun-blocking chemicals) provide higher SPF protection using less material by weight than do conventional products, with no skin-whitening effect. Nanophase began making commercial quantities of material in late 1996 and reported \$2.24 million in sales for the first nine months of 1997. Applications include semiconductor polishing slurries, ceramic armor, parts for medical devices, and industrial catalysts. ATP funding was \$944K, and non-ATP funding was \$2 million.

## **B.14 Molecular Electronics: UCLA-HP project sponsored by NSF and DARPA**

J. Heath (UCLA) and S. Williams (Hewlett-Packard Laboratories), in a NSF GOALI supported activity (Awards 94-57712 and 95-21392) have taken steps towards a new way to circumvent problems that will arise in the semiconductor industry when circuit feature sizes reach below the resolution of optical lithography.

If the reduction in size of electronic devices continues at its present exponential pace, the size of entire devices will approach that of molecules within two decades. However, well before this happens, both electronic devices and the manufacturing procedures used to produce them will have to change dramatically. This is because current devices are based primarily on classical mechanics, but at the scale of molecules, electrons behave as quantum mechanical objects. Also, the cost of factories for fabricating electronic devices is increasing at a rate that is much larger than the market for electronics; therefore, much less expensive manufacturing process will need to be invented.

Thus, an extremely important area of research is *molecular electronics*, in which molecules with electronics functionality are designed. synthesized using the batch processes of chemistry, and then assembled into useful circuits through the processes of self-organization and self-alignment. A major limitation of any such process is that chemically fabricated and assembled systems will necessarily contain defective components and connections. This limitation was addressed in a 1998 paper entitled “A Defect-Tolerant Computer Architecture: Opportunities for Nanotechnology” in *Science* 280:1716-1721. By describing a silicon-based computer that was designed to operate perfectly in the presence of huge numbers of manufacturing defects, researchers from Hewlett-Packard Labs and UCLA presented an architectural solution to the problem of defects in molecular electronics, as described in Figure 1, and thus demonstrated in principle that manufacture by chemical assembly is feasible.

In 1999, researchers from HP Labs and UCLA experimentally demonstrated the most crucial aspect for such a system, an electronically addressable molecular switch that operates in a totally “dry” environment (Collier et al. 1999). Logic gates were fabricated from an array of configurable molecular switches, each consisting of a monolayer of electrochemically active rotaxane molecules, as illustrated in Figure 2, sandwiched between metal electrodes.

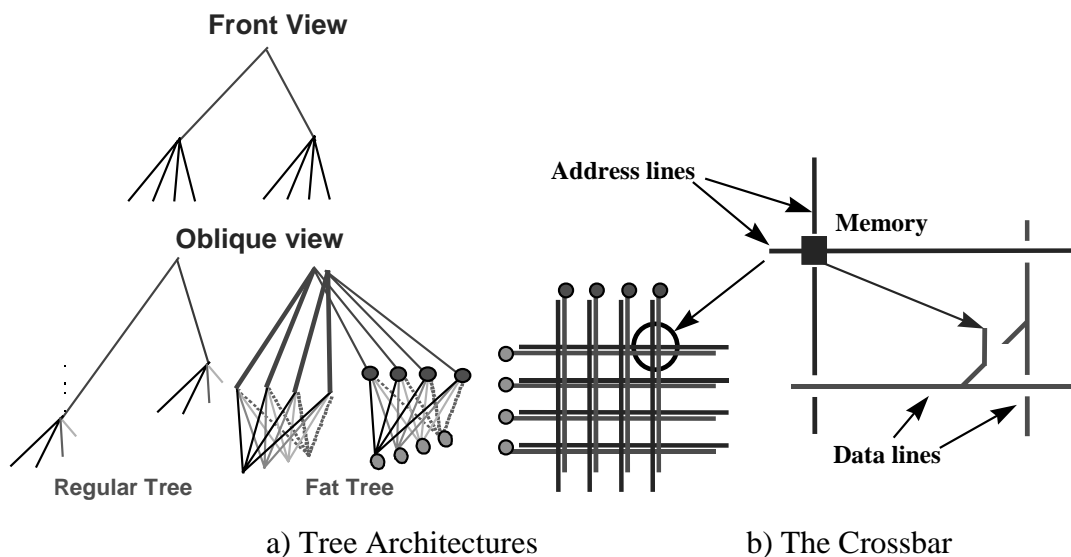


Figure 1. The logical design of a defect-tolerant circuit: (a) shows a “fat tree” architecture in which every member of a logical level of the tree hierarchy can communicate with every member at the next level. In the case of a defective component, these structures enables one to route around and avoid the defect; (b) shows how this architecture is implemented using cross bars, which are very regular structures and look like something that can be built chemically. The complexity required for a computer is programmed into the crossbars by setting the switches to connect certain elements of the tree together. Using silicon circuitry, two completely separate sets of wires (address and data lines) are required for the cross bars and seven transistors are required for each switch, since a continual application of electrical power is required to hold the sense of the switches.

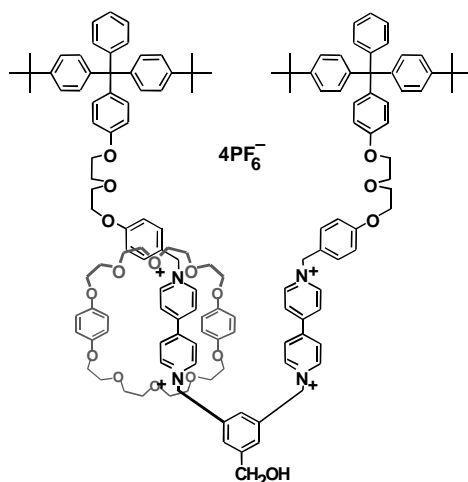


Figure 2. The atomic structure of the rotaxane molecule used in the devices described above as a molecular switch. This molecule conducts electrons via resonant tunneling through unoccupied molecular orbitals when it is in its reduced chemical state (switch closed), but it is a tunneling barrier in its oxidized state (switch open). The switch can be closed electronically in a solid-state circuit by applying the appropriate voltage across the molecule.

## B15. Academe-Industry-Government Partnerships

Federal and local governments (N.Y., N.J., Kentucky, Washington, NC, others), private profit (industry) and non-profit organizations (such as Beckman Institutes), and academic institutions have all determined that nanoscale science and engineering is an important long-term field for investment.

### Examples of universities with investments in nanotechnology in the last few years are:

- Arizona State University: Nanostructure Research Group
- California Institute of Technology: Materials and Process Simulation Center  
[<http://www.theory.caltech.edu/~quic/index.html>]
- Cornell University: Cornell Nanofabrication Facility [<http://www.nnf.cornell.edu>]; Cornell Science and Technology Center (NSF) in Nanobiotechnology
- Georgia Institute of Technology: Nanocrystal Research Laboratory; Nanostructure Optoelectronics
- Johns Hopkins University: Center for Nanostructured Materials  
<http://www.pha.jhu.edu/groups/mrsec/main.html>
- Massachusetts Institute of Technology: NanoStructures Laboratory  
[<http://www-mtl.mit.edu/MTL/NSL.html>]
- Materials Research Science and Engineering Centers (MRSECs) with interdisciplinary research groups addressing nanostructured materials. For links to their web sites see <http://www.nsf.gov/mps/dmr/mrsec.htm>
- National User Facilities (NSF sponsored) in x-ray synchrotron radiation, neutron scattering, and high magnetic fields provide access to major facilities for the benefit of researchers in a wide range of science and engineering fields including nanoscience and engineering. See <http://www.nsf.gov/mps/dmr/natfacil.htm>
- NNUN is a partnership involving NSF and five universities (Cornell University, Stanford University, UC Santa Barbara, Penn State University and Howard University). See <http://www.nnun.org/>
- Northwestern University (IL): Center for Nanofabrication and Molecular Self-assembly. See <http://www.chem.nwu.edu/NanoWeb/index.html>
- Oxford Nanotechnology (MA): Molecular nanotechnology, nanolithography
- New Jersey Institute of Technology: Nonlinear Nanostructures Laboratory (NNL)
- Pennsylvania State University: Nanotechnology
- Princeton University: Nanostructure Laboratory
- Rice University: Center for Nanoscale Science and Technology (fullerenes)
- Stanford University: Stanford National Nanofabrication Users Network (NNUN) [<http://snf.stanford.edu/NNUN>]; [<http://feynman.stanford.edu/qcomp>]
- University of California, Santa Barbara: NSF Science and Technology Center for Quantized Electronic Structures (QUEST)
- University of Illinois at Urbana-Champaign: Beckman Institute  
<http://www.beckman.uiuc.edu/themes/MENS.html>]; STM Nanofabrication and Characterization Group

- University of Notre Dame: Center for Nanoscience and Technology
- University of Washington: Center for Nanotechnology
- University of Wisconsin, Madison: Center for Nanostructured Materials and Interfaces  
<http://mrsec.wisc.edu/>
- Washington State University: Nanotechnology Think Tank
- Yale University: Optoelectronic Structures/Nanotechnology

**Examples of Federal and industry research programs collaborating with academe:**

- California Molecular Electronics Corporation (CALMEC): Molecular Electronics
- Defense Advanced Research Projects Agency (DARPA): The ULTRA Program  
[\[http://web-ext2.darpa.mil/eto/ULTRA/index.html\]](http://web-ext2.darpa.mil/eto/ULTRA/index.html)
- Hewlett Packard Lab: TERAMAK program
- IBM: Nanotech program [\[http://www.almaden.ibm.com/vis/vis\\_lab.html\]](http://www.almaden.ibm.com/vis/vis_lab.html)
- IBM's Zurich Research Laboratory: Microscopy at the atomic level
- MITRE Corporation: Covers topics on nanoelectronics and nanocomputing  
[\[http://www.mitre.org/technology/nanotech\]](http://www.mitre.org/technology/nanotech)
- Molecular Manufacturing Enterprises, Inc.(MMEI)
- Molecular Nanotechnology NanoLogic, Inc.: Integration of nanotechnology into computers
- Nanogen Co.: nanomanufacturing on a chip
- Nanophase Technologies Corporation
- NanoPowders Industries
- NanoSystems Co.: Drug delivery
- Nanotechnology Development Corporation
- NASA: Nanotechnology, Nanoelectronics [\[http://www.nas.nasa.gov\]](http://www.nas.nasa.gov)
- National Institute of Standards and Technology (NIST): Nanostructure fabrication
- Naval Research Laboratory (NRL): Nanoelectronics processing facility and Surface Nanoscience {<http://stm2.nrl.navy.mil>}
- National Science Foundation (NSF): Partnership in Nanotechnology  
[\[http://www.nsf.gov/home/crssprgm/nano/start/htm\]](http://www.nsf.gov/home/crssprgm/nano/start/htm); Nanoscale processes in biological systems [\[http://www.nsf.gov/nano\]](http://www.nsf.gov/nano)
- Office of Naval Research (ONR): Nanotechnology, nanoelectronics
- Raytheon Co.: nanoelectronics
- Texas Instruments: projects on QMOS program and TSRAM:Tunneling-based static RAM
- Xerox Palo Alto Research Center (PARC): Nanotechnology, molecular nanotechnology  
[\[http://nano.xerox.com/nano\]](http://nano.xerox.com/nano)
- Zyvex: Molecular manufacturing.

**Illustrations of partnerships:**

- Government - Industry Partnerships

Three example partnerships supported by ATP/NIST spanning about seven years in advanced materials relying on unique properties of nanosized particles. These examples show the



breadth of application (medical to cosmetics to automotive) and industrial interest (small business to large corporation) and rough time scale for commercialization (less than 10 years). These examples are purposely shown in the one narrow nanotechnology R&D field of nanoparticles. The examples further show that government-industry partnerships can play a key role in aiding U.S. industry speed nanotechnology innovations into the marketplace.

- Just started partnership – Nanoparticles for cancer therapy: NIST-ATP, NIH-NCI, CytImmune Sciences Inc., and EntreMed, Inc., “Using nanosized particles for more effective cancer therapy”
  - Ongoing partnership – Nanocomposites for the automotive industry: Industry-Government Partnership: NIST-ATP, Dow Chemical Company, Magna International of America “Nanocomposites: Materials for Automotive Parts”
  - Past Partnership, now fully commercialized – Nanoparticle synthesis: NIST-ATP and Nanophase Technologies “Synthesis and Processing of Nanocrystalline Ceramics on a Commercial Scale”
- Interdisciplinary Nanoscience Investment from University Endowment: The Harvard Center for Imaging and Mesoscale Structures (CIMS)

Harvard is making a major commitment to several areas of interdisciplinary science through the creation of several new Centers. In particular, the Faculty of Arts and Sciences has established a new Center for Imaging and Mesoscale Structures (CIMS). The emphasis of the center will be on multi-disciplinary research, bridging the disciplines of chemistry, physics, engineering, materials science, biology and medicine

The proposed initial funding for CIMS is from FAS whose main funding source is the Harvard endowment. This funding will be used for construction of new building, new major facilities and to seed new research directions. The level of funding is on the order of tens of millions of dollars and a new building. The overall aim of CIMS is to foster new interdisciplinary research on small things; the specific research areas are still under discussion but will undoubtedly include mesoscale electronics, mesoscale mechanical systems, functional nanoscale materials, and the interface between biological and physical sciences. The Center will provide space for state-of-the-art facilities (clean rooms, microscopy, synthesis - both wet and dry -, etc.), and new research space. An important point about the research space is that much of it will be assigned on a rotating basis for new interdisciplinary projects-- to provide the resources needed to pursue new directions in nanoscale research.

The length of University support of CIMS is not well defined at present. Initial plans are to provide a decreasing funding over a 10 year period with major external review after five years. This scheme is based on the desire that the researchers involved with the Center develop external funding sources (government and private) to supplement and sustain efforts. Potential partners are presently being actively pursued.

Numerous faculty members already have strong research programs in the area of nanoscience, supported in part by NIH, DoD and NSF By providing major funds to seed and support

projects and by providing world-class facilities and technical support, Harvard believes that it will create a win-win situation for academia, industry and government.

- Nanotechnology Partnership: Rice University and NASA

A collaborative effort between NASA and Rice University began in October 1998 for the development of carbon nanotechnology to be used in numerous revolutionary applications. Collaborative partners with Rice in this effort are Johnson Space Center, Ames Research Center, Jet Propulsion Laboratory, and Langley Research Center. Rice is currently working on bulk production of nanotubes in a gas-phase process, suspension of tubes in a solution, and the fabrication of membranes and arrays of nanotubes that can be grown continuously. The Johnson Space Center's primary goal for nanotubes is to produce a structural material with a strength-to-weight ratio much higher than today's best composites. This work consists of production of nanotubes using electric arc and laser ablation methods, study of growth mechanisms, purification of tubes, and insertion into polymer composites for testing. Researchers from Rice have been instrumental in pushing this work forward. Preliminary work in composites has given scientists reason for optimism for eventual widespread use. These composites show promise in revolutionizing the field of materials science. The collaboration extends to Ames Research Center for modeling of the mechanical behavior of nanotubes and nanotube composites. Ames also works directly with Rice to model the high-pressure nanotube production system being developed there. The Jet Propulsion Laboratory has been involved with the nanotube effort by looking into battery and energy storage applications and is now looking further into nanoelectronics. Although the addition of Langley Research Center is relatively new, Langley is the NASA Center of Excellence for Structures and Materials. The goal of the nanotube project is to develop breakthrough technologies such as ultralightweight composites, advanced energy storage, flat panel displays, chemical sensors, nanoelectronics, and biomedical uses. These enabling technologies will help NASA achieve its missions in the new millennium. The total planned investment of NASA in the Rice collaboration is 4 to 5 million dollars over a period of five years, and Rice's contribution will be on the same order of magnitude.

- Nanoscience university-industry-government investment: Northwestern University Center for Nanofabrication and Molecular Self-assembly.

A \$32.5 million facility for about 140 faculty, post-doctoral researchers and graduate students is in construction on campus to provide a focal place for innovative collaborative research in applying nanotechnology to improve healthcare, environment and industrial processes. Funding comes from federal Government (Department of Health and Human Services): 14 million dollars (7 million this year, 7 million next year), private donations through Northwestern (Leo Ginger, ex-VP for R & D at Baxter Diagnostics) already has donated a million dollars, and Northwestern University that will pick up the difference. The facility is scheduled to be completed by the end of 2001. The four core research areas are developing biological structures for use in human health and industry, study solar energy conversion in order to create more efficient conversion methods, designing nanostructured polymers for electronic applications and human tissues, and using theory to predict the properties and structures for accelerating the path of discovery. The Center will build on the existing support

of \$9 million per year in externally sponsored funding, including three group grants of \$0.5 million each from the National Science Foundation and a block grant over five years totaling \$5 million from Army Research Office for the study of atomic cluster-derived materials. Further information on the Center's mission, participants, and current research projects, is described on the website: <http://www.chem.nwu.edu/NanoWeb/index.html> .

## B16. International Activities in Nanotechnology

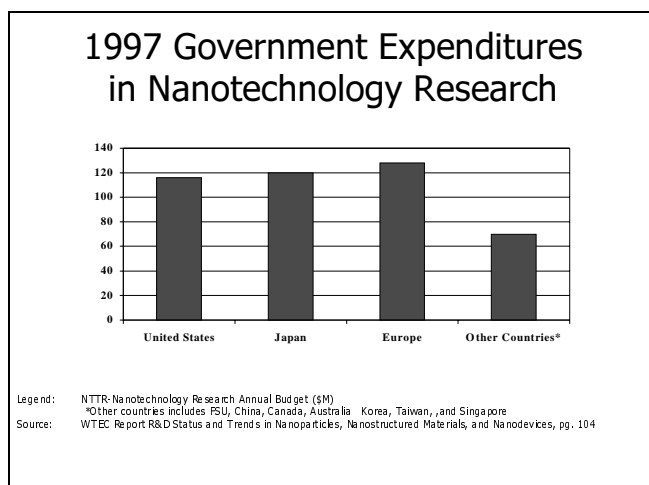
### Introduction

The United States' relative strength compared with the rest of the world has changed significantly. While the United States is still the world's undisputed economic and technological leader, the world's knowledge and wealth is found in more and more locations. In 1950, the United States contributed approximately 40 percent of the developed world's GDP and carried out two to three times the total research and development (R&D) carried out by the rest of the world. By 1997, the U.S. contribution was 27 percent of world GDP, and the United States conducted about 40 percent of the world's R&D.

Nanotechnology is a prime example of the global spread of R&D. The United States, Japan and Europe all are world leaders in this area. (for further reference see "Nanostructure Science and Technology: A Worldwide Study Study", NSTC, 1999,

(<http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.Worldwide.Study/toc.htm>).

While it is difficult to estimate the extent and quality of nanotechnology research taking place especially within industry, there is at least twice as much government-funded nanotechnology research going on outside of the United States as there is within it. Therefore, it is imperative the United States build international awareness and analysis, and investigate into collaborative opportunities into the National Nanotechnology Initiative initiative from the very beginning.



The United States can be the world's leader in commercializing nanoscale devices and materials. The United States, however, is not the only nation with this capability. Many foreign countries, companies and scientists believe that nanotechnology will be the leading technology of the 21<sup>st</sup> century. They see that it has the potential to become so broad and pervasive that it will influence all areas of science, technology, and manufacturing by changing the nature of almost every human-made object. This potential, along with the fact

that there is still a chance to get in on the ground floor in this technology's development, helps explain the phenomenal levels of R&D activity worldwide.

### **Examples of Regional Research**

The Japanese government has designed programs to establish its companies as the leaders in the development of this technology. Germany and the United Kingdom have programs comparable in scale and sophistication to Japan, but with differences in research emphasis. China also is undertaking major efforts in nanotechnology. Other major players are Australia, France, India, Taiwan, Korea, Singapore, Russia, Switzerland, and Canada. It is essential, therefore, to be able to transcend geographic location to understand and craft this technology.

#### **1. Japan**

The Japanese Government spent about \$120 million on nanotechnology research in 1997. It has significant capital infrastructure for nanotechnology in its national laboratories, universities and companies. The quality of its science in this area is high, it has ample human resources and has a large number of first-class collaborations among national laboratories, academic institutions and company researchers. Government and very large corporations are the main sources of funding for nanotechnology in Japan. Japan is attempting in the relatively new field of nanotechnology to provide an opportunity for researchers to become more proactive and less traditional. Japanese research centers around three main areas: quantum functional devices, biotechnology, and smart materials. Appendix One lists major Japanese centers of excellence and projects on nanotechnology and, if available, the approximate amount they spend per year.

#### **2. Western Europe**

In Europe, there is a combination of national programs, collaborative European Union projects and networks, and large corporations investing in nanotechnology. The United Kingdom, Germany and France all have major national programs and capabilities in nanotechnology. Researchers in other countries such as the Netherlands and Switzerland also are doing significant work. European Government Expenditures on nanotechnology were about \$128 million in 1997.

The European Union's Fifth Framework Program will run for four years and began at the end of 1998. It continues work already begun on nanotechnology in previous R&D programs, and added a new emphasis on nano-biology. The European Union's ESPRIT Advanced Research Initiative in Microelectronics and the BRITE/EURAM projects on materials science both are partially dedicated to nanotechnology. The PHANTHOM (Physics and Technology Mesoscale Systems) is a network with about 40 members created in 1992 in order to stimulate nano-electronics, nanofabrication, opto-electronics, and electronic switching. The European Science Foundation sponsors NANO to promote collaboration between the aerosol and materials science communities on nano-particles. Other major European programs that are: NEOME (Network for Excellence on Organic Materials for Electronics); the European

Society for Precision Engineering and Nanotechnology, and the Joint Research Center Nanostructured Materials Network.

The German Federal Ministry of Education and Research (BMBF) spends approximately \$50 million per year on nanotechnology. BMBF is supporting precompetitive R&D projects in nanotechnology with a plan to scale-up spending over the next few years. Areas of emphasis include: nanoanalysis, ultrathin films, lateral nanostructures, nanomaterials, and ultraprecision engineering. In 1998, it began an initiative to fund six competence centers as a platform for the accelerated development of nanotechnology. The goal of these centers is to bring together science, economics and venture capital to quickly spread information and results, coordinate an educational effort, and stimulate the formation of start-up companies.

The British Government created the LINK Nanotechnology Programme in 1988 with an annual budget of about \$2 million. The Engineering and Physical Sciences Research Council funded \$7 million worth of materials science projects related to nanotechnology from 1994-1999, and plans to continue funding this area. The National Physical Laboratory established the National Initiative on Nanotechnology to promote nanotechnology in universities, industry, and government. In addition, some British universities, such as Oxford University, conduct leading edge nanotechnology research.

### **3. Other Examples**

- Singapore has a national program initiated in 1995.
- Australia's National Research Council sponsors significant amounts of nanotechnology R&D. There are also programs in Australian universities and industry.
- Korea has included nanotechnology as a national focus area since 1995 and is in the process of establishing a special research center on nanoscale semiconductor devices.
- Taiwan is increasing nanotechnology research through the Industrial Technology research Institute and its National Science Council to ensure it can retain a leading position in information technology.
- China is just completing a ten-year nanotechnology program "Climbing Project on Nanometer Science" and plans major new activities. It also has significant relevant research on advanced materials, nanoprobes and manufacturing processes using nanotubes.
- Russia has established the Russian Society of Scanning Probe Microscopy and Nanotechnology, and has particular strengths in preparation processes of nanostructured materials and nanocrystalline structures.

#### **List of Japanese Centers of Excellence and Major Funders in 1997**

##### Ministry of International Trade and Industry (\$60 million)\*

- National Institute for Advancement of Interdisciplinary Research (\$28 million)
- Electrotechnical Laboratory (\$17 million)
- Osaka National Research Institute (\$3 million)
- National Industrial Research Institute of Nagoya (\$2.5 million)
- Quantum Functional Devices Program (\$6.4 million)

- Ultimate Manipulation of Atoms and Molecules Program (\$25 million)
- Frontier Carbon Technology Program (\$15 million)
- Smart Materials Program (\$9 million)
- Optical Disk Systems with Nano-Precision Control Program (\$12 million)
- Super Metal Technology Program (\$10 million)

\*Subtotals are higher than total MITI funding because some programs listed do not clearly delineate nanotechnology research.

#### Science and Technology Agency (\$35 million)

- Institute of Physical and Chemical Research, Frontier Materials Research
- National Research Institute for Metals
- Core Research for Evolutional Science and Technology (CREST) Projects
  - Quantum Devices
  - Single Atomic and Molecular Manipulations
- Japan Science and Technology Corporation's ERATO Projects
  - Quantum Wave Project
  - Atomcraft Project
  - Electron Wavefront Project
  - Quantum Fluctuation Project

#### Ministry of Education, Sports, Science and Culture

- Tokyo University
  - Research Center for Advanced Science and Technology
  - Institute of Industrial Engineering
  - Chemical Engineering
- Kyoto University
- Tokyo Institute of Technology, Bioelectric Devices
- Tohoku University, Institute of Materials Science
- Nagoya University
- Osaka University
- Institute of Molecular Science
- Exploratory Research on Novel Artificial Materials and Substances for Next Generation Industries

#### Industry

- Hitachi Central R&D Laboratory
- NEC Fundamental Research Labs
- Toshiba Research Center
- Nihon Shinko Gijutsu (ULVAC)
- NTT
- Fujitsu
- Sony
- Fuji Photo Film Company

## NATIONAL NANOTECHNOLOGY INITIATIVE PUBLICATIONS

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Below is a list of nanotechnology publications that have been prepared by the Interagency Working Group on Nanoscience, Engineering and Technology (IWGN) of the National Science and Technology Council's Committee on Technology.

### **Nanotechnology: Shaping the World Atom by Atom**

(<http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.Public.Brochure/welcome.htm>).

This glossy publication sets the stage for increasing the public's understanding of what nanotechnology is, how nanotechnology came to be, and its potential impact on society. "The emerging fields of nanoscience and nanoengineering are leading to unprecedented understanding and control over the fundamental building blocks of all physical things. This is likely to change the way almost everything – from vaccines to computers to automobile tires to objects not yet imagined – is designed and made."

### **National Nanotechnology Initiative – Leading to the Next Industrial Revolution**

(<http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.FY01BudSuppl/toc.htm>)

This report supplements the President's FY 2001 Budget and highlights the nanotechnology funding mechanisms developed for this new initiative as well as the funding allocations by each participating Federal agency. This report unveils the President's bold, new initiative coordinating focused areas of research and development (R&D) among the Federal government, academia and university to advancing nanotechnology.

### **Nanostructure Science and Technology: A Worldwide Study Study**

(<http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.Worldwide.Study/toc.htm>).

This report reviews the status of R&D in nanoparticles, nanostructured materials, and nanodevices, including innovative approaches to synthesis and characterization. The report highlights applications in dispersions, high-surface area materials, electronic and magnetic devices, nanostructured materials, and biological systems. It includes a comparative review of research programs around the world – the United States, Japan, Western Europe, and other countries – to help provide a global picture of the field.

### **IWGN Workshop Report: Nanotechnology Research Directions**

(<http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.Research.Directions/toc.htm>)

This publication builds upon *Nanostructure Science and Technology: A Worldwide Study* (<http://www.whitehouse.gov/WH/EOP/OSTP/NSTC/html/iwgn/IWGN.Worldwide.Study/toc.htm>), and incorporates a vision for how the nanotechnology community -- Federal agencies, industries, universities, and professional societies -- can more effectively coordinate efforts to develop a wide range of revolutionary commercial applications. *Nanotechnology Research Directions* identifies challenges and opportunities in the nanotechnology field and begins to make recommendations on how to develop a balanced R&D nanotechnology infrastructure, advance critical research areas, and nurture the scientific and technical workforce of the next century. It incorporates perspectives developed at a January 1999 IWGN-sponsored workshop by experts from universities, industry, and the Federal government.



**President's Committee of Advisors on Science and Technology Endorsement to the President**

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**EXECUTIVE OFFICE OF THE PRESIDENT  
PRESIDENT'S COMMITTEE OF ADVISORS ON SCIENCE AND TECHNOLOGY  
WASHINGTON, D.C. 20502**

December 14, 1999

The President of the United States  
The White House  
Washington, DC 20500

Dear Mr. President:

Your Committee of Advisors on Science and Technology (PCAST) strongly endorses the establishment of a National Nanotechnology Initiative (NNI), beginning in Fiscal Year 2001, as proposed by the National Science and Technology Council (NSTC). Our endorsement is based on a technical and budgetary review of a comprehensive report prepared by the NSTC Committee on Technology's Interagency Working Group on Nanoscience, Engineering and Technology (IWGN).

We believe that the Administration should make the NNI a top priority. America's continued economic leadership and national security in the 21st century will require a significant, sustained increase in nanotechnology R&D over the next 10 to 20 years. We strongly endorse the robust funding and the research strategy that has been proposed by the NSTC's IWGN.

Nanotechnology is the science and engineering of assembling materials and components atom by atom, or molecule by molecule, and integrating them into useful devices. It uses new discoveries, new eyes (high resolution microscopes) and hands (laser tweezers) to work, at the scale of a nanometer (one billionth of a meter – ten thousand times smaller than the diameter of a human hair).

Nanotechnology thrives from modern advances in chemistry, physics, biology, engineering, and materials research. We believe that nanotechnology will have a profound impact on our economy and society in the early 21st century, perhaps comparable to that of information technology or of cellular, genetic, and molecular biology. Nanotechnology also promotes the convergence of biological, chemical, materials and physical sciences and engineering disciplines.

Nanotechnology is the first economically important revolution in science and technology (S&T) since World War II that the United States has not entered with a commanding lead. Federal and industrial support of R&D in the United States for this field already is significant,

but Europe and Japan are each making greater investments than the United States is, generally in carefully focused programs. Now is the time to act.

In our view, the Federal government, together with academia and industry, plays a vital role in advancing nanotechnology. This role will require a new, bold national initiative coordinating focused R&D in the decade ahead. Today nanoscale S&T is roughly where the fundamental R&D on which transistors are based was in the late 1940s or early 1950s. Most of the work currently required is still fundamental, with a much longer time horizon than what most industries can support. The NNI is balanced well across fundamental research, grand challenges, centers and networks of excellence, research infrastructure, and education and training.

We believe that the science, technology, applications, products, and programs catalyzed by the NNI will inspire a new generation of young Americans with exciting new opportunities and draw them to careers in S&T. Potentially the NNI will help provide for a better world through advances in environmental technologies, lowering of energy consumption, and advances in medical diagnostics and therapeutics.

The NNI is an excellent multi-agency framework to ensure U.S. leadership in this emerging field that will be essential for economic and national security leadership in the first half of the next century. We recommend that progress toward NNI goals be monitored annually by an appropriate external body of experts, such as the National Research Council.

A brief summary of our review of the IWGN report, National Nanotechnology Initiative – Leading to the Next Industrial Revolution, is enclosed. We hope that our recommendations will be helpful as you consider your priorities for Federal investments.

We look forward to discussing this review with you, with members of your Administration, and with members of Congress.

Sincerely,

Neal Lane  
Co -Chair

John Young  
Co-Chair

**PRESIDENT'S COMMITTEE OF ADVISORS  
ON SCIENCE AND TECHNOLOGY  
PANEL ON NANOTECHNOLOGY  
REVIEW OF PROPOSED NATIONAL NANOTECHNOLOGY INITIATIVE  
NOVEMBER 1999**

**Summary**

PCAST believes that the benefits to the United States of the National Nanotechnology Initiative (NNI) are compelling, and we endorse the funding level, balance, and mechanism recommended by Interagency Working Group on NanoScience, Engineering and Technology (IWGN).

**Our Review**

A PCAST Nanotechnology Panel, composed of industry and university experts and chaired by Dr. Charles Vest, carefully reviewed the report entitled National Nanotechnology Initiative – Leading to the Next Industrial Revolution, written by the National Science and Technical Council (NSTC) Committee on Technology's Interagency Working Group on NanoScience, Engineering and Technology (IWGN). This report frames a new interagency R&D initiative, the NNI, starting in Fiscal Year 2001, and proposes a 5-year funding plan, appropriately distributed across both agencies and funding mechanisms. The NNI has an essential exploratory and scientific component and focuses on fundamental aspects of nanoscale science and engineering that collectively have high potential to eventually lead to important applications, processes, and products. These outcomes will strengthen both scientific disciplines and create critical interdisciplinary opportunities. Our Panel reviewed the technical merits and the funding profiles in the NNI proposal and supports the IWGN recommendation for a substantial budget increase in Fiscal Year 2001 with sustained funding in this area.

The NNI research portfolio is balanced well across fundamental research, Grand Challenges, centers and networks of excellence, research infrastructure, and education and training. The NNI also provides mechanisms for building workforce skills necessary for future industrial and academic positions, proposes cross-disciplinary networks and partnerships, includes a mechanism for disseminating information, and suggests tools for encouraging small businesses to exploit nanotechnology opportunities. If it is implemented, we recommend that the NNI be annually reviewed by a non-government advisory committee, such as the National Research Council, to monitor and assess progress toward its goals.

**Nanotechnology is the future.**

Nanotechnology is the builder's new frontier – one where properties and phenomena are very different than those utilized in traditional technologies. Nature builds things with atomic precision. Every living cell is filled with natural nanomachines of DNA, RNA, proteins, etc., which interact to produce tissues and organs. Humans are now learning to build non-biological materials and machines on the nanometer scale, imitating the elegance and economy of nature. This embryonic capability may portend a new industrial revolution. In the coming decades, nanotechnology will enable us to manufacture devices that conduct electricity efficiently, compute, move, sense their environment, and repair themselves.

Nanostructures will revolutionize materials and devices of all sorts, particularly in nanoelectronics and computer technology, medicine and health, biotechnology and agriculture, as well as national security. For example, we anticipate computers with a thousand-fold increase in power but which draw a millionth the amount of electricity, materials far stronger than steel but with ten percent the weight, and devices that can detect tumors when they are only clusters of a few cells.

It may eventually be possible to develop technologies for renewable, clean energy; to replace metals with lightweight, recyclable polymeric nanocomposites; to provide low-cost access to space; and to develop new classes of pharmaceuticals. Investments in nanotechnology have the potential to spawn the growth of future industrial productivity. When allied with the biosciences, nanotechnology will accelerate the development of early detection instruments for physicians, as well as the development of noninvasive diagnosis and medical treatment. It will also lower the cost of pure water and healthy food for the world's population.

The United States cannot afford to be in second place in this endeavor. The country that leads in discovery and implementation of nanotechnology will have great advantage in the economic and military scene for many decades to come.

**A bold, Federally funded national program is needed now.**

Nanotechnology, which is based on phenomena first observed and characterized in the 1980s, is now emerging as an important new frontier. Direct, strategic investments made now in fundamental science and engineering will position the U.S. science and technology (S&T) community to discover and apply nanoscale phenomena, and transfer them to industry. Nanoscale S&T today is roughly where the fundamental R&D on which transistors are based was in the late 1940s or early 1950s. Most foreseeable applications are still 10 or 20 years away from a commercially significant market; however, industry generally invests only in developing cost-competitive products in the 3 to 5 year timeframe. It is difficult for industry management to justify to their shareholders the large investments in long-term, fundamental research needed to make nanotechnology-based products possible. Furthermore, the highly interdisciplinary nature of some of the needed research is incompatible with many current corporate structures.

There is a clear need for Federal support at this time. Appropriately, Federal and academic investments in nanotechnology R&D to date have evolved in open competition with other research topics, resulting in some fragmentation and duplication of efforts, which is natural at this stage. Going forward, however, nanotechnology will require a somewhat more coherent, sustained investment in long-term research. The NNI would support critical segments of this research and increase the national infrastructure necessary to conduct it.

**International Activity in Nanotechnology**

The United States does not dominate nanotechnology research. Yet we strongly believe that the United States must lead in this area to ensure economic and national security leadership. Compared to our nation, other countries are investing much more in relevant areas of ongoing research. Many other countries have launched major initiatives in this area, because their scientists and national leaders have determined that nanotechnology has the potential to be a major economic factor during the next several decades. Japan and Europe are supporting scientific work of the same quality and breadth of that done in the United States. Unlike in the other post-war technological revolutions, the United States does not enjoy an early lead in nanotechnology.

We must act now to put in place an infrastructure for nanoscale research that is equal to that which exists anywhere in the world. A suitable U.S. infrastructure will enable us to collaborate appropriately, as well as compete, with other nations. Without the NNI, there is a real danger that our nation could fall behind other countries. To ensure leadership in the future, the United States must make a large and sustained investment in this area.

**Nanotechnology will inspire the public and the next generation workforce.**

Our future workforce in S&T is decreasing, in part because far too many young people perceive that action is no longer in the physical sciences and engineering, and do not see how S&T connects to the

world as they know it. Yet chemistry, physics, biology, engineering, and materials research are at the core of nanotechnology, which likely will play a dominant role in future decades. The NNI should parallel investments in R&D with a creative and entrepreneurial program that offers young people a truly interdisciplinary education, and that prepares the next generation of researchers and industrial leaders.

As nanotechnology develops, the core areas of the physical sciences, engineering and biomedicine in our nation's universities will become much more intimately coupled to each other. Future research efforts in these fields need a far better integration among each other and to industry and society as a whole. The relevance and inherent excitement of nanoscale R&D should attract young men and women to science as never before and also create exciting and important career options for them.

### **Nanotechnology and Global Challenges**

In the next century, the world population will likely grow to over ten billion. Without revolutionary advances in environmentally sustainable technologies, global society will struggle with the implications of this growth. Nanotechnology, as broadly supported by the NNI, has the potential to develop lightweight, recyclable materials and energy efficient devices that will contribute to such sustainability. Therefore, the United States should move to develop this area quickly, not only for economic benefit, but also for its potential contribution to a more sustainable future.

In closing, we note that when radically new technologies are developed, social and ethical issues can arise. Accordingly, we recommend that a modest amount be set aside for the study of such implications of nanotechnology.