III. Major Laboratory Initiatives

The Laboratory's second strategic objective is stated in Chapter II: "Argonne will develop important new R&D initiatives and scientific facilities that serve emerging national needs consistent with its mission and will implement them cost-effectively and expeditiously to the benefit of DOE and the nation." This chapter provides planning "snapshots" of Argonne's major Laboratory initiatives, for consideration by DOE.[1] The Laboratory's initiatives represent important opportunities to enhance U.S. research capabilities, to serve the broader scientific community, and to advance scientific understanding and engineering achievement across a wide range of disciplines.

Argonne carefully considers the implications of the National Environmental Policy Act (NEPA) for its scientific and technical initiatives, as early as it is reasonable to do so. For initiatives where NEPA implications are expected to be significant, the implications are discussed explicitly in this *Institutional Plan*.

The six major Argonne initiatives relate most closely to two DOE mission areas, Science and Energy:

- Science
  - Nanosciences and Nanotechnology — Center for Nanoscale Materials
  - Rare Isotope Accelerator
  - Functional Genomics
  - Petaflops Computing and Computational Science
- Energy
  - Advanced Nuclear Fuel Cycle
  - Hydrogen Research and Development

In addition to these six major Laboratory initiatives, we are applying our capabilities to national security. In the next chapter, Section IV.A.3 explains these efforts and presents six programmatic initiatives in the areas of (1) nuclear national security and (2) infrastructure assurance and counterterrorism. These initiatives individually are too specialized and exploratory to be included among the Laboratory's current major initiatives. However, they point toward more extensive future program development in support of DOE's core national security mission, from which flow all of the Department's missions.

A. Science

1. Nanosciences and Nanotechnology — Center for Nanoscale Materials

The National Nanotechnology Initiative is an interagency effort driven by the realization that present-day materials and processes are reaching their limits of performance. Fundamentally new approaches are needed to transcend these limits. The emerging field of nanoscience offers the requisite scientific and technological opportunities. Accordingly, DOE has taken the bold step of establishing five new Nanoscale Science Research Centers at its national laboratories. Argonne's Center for Nanoscale Materials (CNM) was approved in FY 2002 as one of the five.

Our vision is to go beyond present-day semiconductor materials and processing methods to create new functional materials on the nanoscale. Highlights of our plan include focusing on chemical methods to self-assemble nano-structures, to pattern nontraditional electronic

[1] Inclusion of initiatives in this chapter does not necessarily imply approval, or an intention to implement, by DOE. All funds received for initiatives during FY 2003 are included in the resource tables in Chapter VI of this *Institutional Plan*. However, resources required for proposed growth of initiatives in years beyond FY 2003 are generally not included in those projections. Projected resource requirements for all initiatives include costs associated with protection of the environment and the health and safety of workers and the public.

materials, and to create new probes for exploring nanoscale phenomena. Moreover, we aspire to help pioneer the new fields of molecular and magnetic electronics and to help lay the foundations for new sensor technologies in the chemical and biological arenas.

The CNM will serve simultaneously as a forefront research center and as a user facility for the regional and national research communities. Previously, DOE's stewardship of the nation's major materials science user facilities (such as the Advanced Photon Source [APS] and Intense Pulsed Neutron Source [IPNS] at Argonne) focused on the advanced *characterization* of materials. The CNM will be part of a new generation of DOE user facilities, because its primary goal is to *fabricate* advanced nanoscale materials.

The CNM will complement our existing user facilities and enhance their value by creating cutting-edge nanomaterials that require advanced characterization. To maximize this synergy, the new building for the CNM will adjoin the APS, and the CNM will construct a state-of-the-art, hard x-ray nanoprobe beamline at the APS. The new beamline will focus hard (i.e., 10 keV) x-rays down to an unprecedented spot size of 30 nanometers. This capability will enable a variety of imaging, spectroscopic, and diffraction experiments that cannot be performed similarly anywhere else in the world.

A signature new technology of the last half of the 20th century was solid-state electronics. The 21st century is expected to be marked by the creation of connections across the biointerface, and a major focus of the CNM will be creating novel interconnections between soft matter (complex organic and biological molecules) and hard matter (solid-state nanoparticles and patterned systems). Major areas of interest will include the flow of chemical energy and the propagation of light. Our initial work in these areas has been supported by Laboratory Directed R&D funding and, more recently, by funding of proposals we made to the DOE Nanoscale Science, Engineering, and Technology call.

Magnetic nanomaterials hold much promise to advance the future of electronics, despite the fact that magnetic materials are among the oldest of technological materials (starting with the use of lodestones for ships' compasses). Today, magnetic nanomaterials promise to revolutionize computer design. Computers already use magnetic nanosystems in hard disk drives to store and read data, and the data density of such magnetic recording devices is doubling every nine months. In the future, nanomagnetic devices may also be used to control the flow of current in the computer's logic elements, which could enable programmable processors that transcend the fixed architectures of today's circuitry. Such processors could be reconfigured dynamically to optimize performance for the particular task at hand. Currently under industrial development are magnetic random access memories that may ultimately provide nonvolatile electronics, including laptop computers capable of "instant bootup."

Realizing these technological opportunities requires fundamental studies of magnetic materials on the nanoscale. We are positioned to take a leadership role within the DOE system in this challenging area. Work on nanomagnetism at the CNM will create new nanostructures by using chemical methods of self-assembly, as well as lithographic patterning of novel thin-film hybrid systems. Utilizing the spin (magnetism) of the electron, in addition to its charge, is opening the new field of magnetic electronics (spintronics). The mission of the CNM will include spintronics, along with molecular electronics and nanophotonics, in the effort to develop new functionalities at the nanoscale.

The CNM will energize new collaborations and partnerships that broaden the user community throughout the nation, particularly in the Midwest. To foster this user community and stimulate feedback from users, general and specialized workshops have been held, and more are being planned. Research themes already covered include the x-ray nanoprobe, neutrons and nanoscience, and industrial microfabrication. The University of Chicago-Argonne Consortium for Nanoscience Research was launched in 2001. Investigators from both institutions are cooperating to pursue initial research themes that embrace major focal areas for the CNM. The investigators also have begun ambitious planning for intellectual cross-pollination and educational outreach.

An emerging prime interest for the CNM is the role of theory in creating computational algorithms that simulate nanoscale phenomena. Now under way are efforts to define the scope of a research theme within the CNM dubbed the "Virtual Fab Lab." The objective is to use large-scale computational strategies to transform nanofabrication from an art into a science. The concept of the Virtual Fab Lab in the context of the CNM will be the topic of a future workshop, and it creates linkages with the Petaflops Computing and Computational Science initiative described in Section III.A.4.

The excitement of planning science for the CNM is being enhanced by planning for its infrastructure. The state of Illinois has committed funds for construction of the CNM building. M.W. Zander was selected as the architectural and engineering firm to design the building, and its work has begun. Jacob Facilities, Inc., is the construction management firm.

The CNM initiative requires investments in the following three complementary areas:

1. *Personnel.* Our staff includes some of the researchers required for this initiative, and several of our core programs will naturally move in directions complementary to the CNM. Many new staff members with special expertise will be recruited in areas such as self-assembly, lithography, advanced spectroscopies, and imaging. In addition, creation of the Virtual Fab Lab will require critical new staff in the areas of theory and computational nanosciences.

2. *New Tools for Nanofabrication.* Electron lithography and focused-ion-beam lithography are essential tools for fabrication of nanostructures. Also required is equipment for etching, deposition, and other processes. Several of these tools do not exist elsewhere in the Midwest and will strongly attract outside users. Clean rooms and related infrastructure will be developed; nanostructures are much smaller than a speck of dust, and scrupulously clean conditions are needed for their fabrication.

3. *New Tools for Nanocharacterization.* Tools for visualizing nanostructures, especially microscopes (x-ray, electron, scanning probe, and near-field optical), will be further developed at Argonne. The x-ray nanoprobe will be developed to use the brilliance of the APS to probe at the nanoscale. Our Electron Microscopy Center (Section IV.A.1.b) will be enhanced by synergies with the CNM, and the IPNS will attract new users because of new materials created by the CNM.

Resources required for this initiative are summarized in Table III.1. We are working with the state of Illinois to construct the building for the CNM by January 2006. Further funding for instrumentation and research operations is being provided by DOE-Basic Energy Sciences (DOE-BES; KC-02 and KC-03) and also by the state of Illinois and other sources.

Table III.1 Nanosciences and Nanotechnology — Center for Nanoscale Materials ($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating[a]	1.5	1.5	6.0	10.0	18.0	18.0	18.0
Capital Equipment	-	10.0	12.0	14.0	-	-	-
Construction[b]	17.0	17.0	-	-	-	-	-
Total	18.5	28.5	18.0	24.0	18.0	18.0	18.0
Direct Personnel	5.0	5.0	24.0	40.0	60.0	60.0	60.0

[a] Not included here is funding for in-house nanoscience research, for which Argonne will compete separately. The magnitude of this additional funding is expected to be similar to that of the initiative's operating funding.

[b] The state of Illinois is funding construction of a building for the CNM.

2. Rare Isotope Accelerator

Present understanding does not allow reliable prediction of the properties of unexplored forms of nuclei having unusual ratios of protons to neutrons. These forms hold the keys to unlocking fundamental questions of matter and the cosmos. Beams of short-lived nuclei (rare isotopes) provide the opportunity to determine the properties and structure of these nuclei and promise answers to these scientific questions:

- How do short-lived nuclei derive their properties from the interactions of their individual constituents, and why do such complex systems exhibit such simple symmetries?

• How are the heavy elements created, and how do nuclear properties influence the characteristics of stars?

• What are the fundamental symmetries of nature, and how can the rare isotopes help us investigate them?

• What new uses of radioactive isotopes can be developed to serve society and the nation?

Exploration at these frontiers will require extension of today's technical capabilities and facilities. This need and its scientific basis have been discussed thoroughly in a number of forums in the past decade, both in the United States and abroad, including the 1999 National Research Council's Committee on Nuclear Physics. Most recently, the compelling scientific opportunities offered by research with rare isotopes led the DOE-National Science Foundation Nuclear Science Advisory Committee (NSAC) in its *2002 Long Range Plan for Nuclear Science* to recommend the Rare Isotope Accelerator (RIA) as the field's highest priority for major new construction and to conclude that RIA is required to ensure U.S. leadership in the areas of nuclear structure and nuclear astrophysics. Most recently, NSAC reaffirmed this priority in its published recommendations supporting the DOE Office of Science strategic plan for major construction projects.

We have developed a facility concept for RIA that will achieve the physics goals set forth by NSAC. The project is currently preparing to complete the initial steps of DOE's major systems acquisition process. Approval of mission need ("critical decision zero") is expected in 2003 or 2004.

Our work on RIA is a collaboration with other U.S. research institutions. Technology development related to RIA is currently under way at ten institutions, including both universities and national laboratories. We are working with the research community to organize the RIA team and prepare a preconceptual design report.

In parallel with consideration of the fundamental science to be pursued, Argonne's design for RIA has aroused significant interest in the technological applications of the rare isotopes to be created. In addition to potential applications to research in materials science, biology, and medicine, RIA has an important national security role identified in the science-based stockpile stewardship program.

Our concept for RIA is based on two accelerators. It uses a flexible approach for the primary production accelerator, which will be a high-power superconducting heavy-ion linac. The heavy-ion driver can deliver beams of any element from hydrogen to uranium, so a variety of production mechanisms can be selected to optimize rare isotope yields. One mechanism, heavy-ion fragmentation, can be used with a magnetic fragment separator and a new kind of fast gas catcher. This mechanism operates independently of the chemical properties of the exotic species being used. Our approach to RIA also capitalizes on the capabilities of Argonne's existing state-of-the-art heavy-ion accelerator — ATLAS (Argonne Tandem-Linac Accelerator System) — as the postaccelerator. ATLAS is unique in the world in its ability to provide intense, high-quality, continuous-wave (100% duty cycle), heavy-ion beams for all elements up to and including uranium. ATLAS has excellent transverse and longitudinal phase space properties, and it excels in beam transmission and timing characteristics. These capabilities are important for nuclear structure investigations and astrophysics experiments, where the beam quality requirements are especially stringent.

In the past year we have achieved significant technical advances demonstrating the feasibility of key elements of the RIA design: (1) construction of a full-scale RIA gas-stopping cell and initial tests that demonstrate the required ion extraction efficiency; (2) operation of a half-scale, windowless, flowing-liquid lithium target, to serve as the prototype for heavy-ion fragmentation targets; (3) construction and testing of three new classes of intermediate-velocity superconducting accelerating cavities; (4) construction and testing of a cold model of a new class of hybrid radio frequency quadrupole structure; and (5) detailed simulations of beam dynamics and beam loss for the entire driver accelerator.

Preliminary estimates of effort, time lines, and cost suggest that this major new facility can be constructed at Argonne within the planning window established by DOE, following approximately two years of detailed facility design. Funding (Table III.2) is being sought from the Nuclear Physics (KB-04) program. A major challenge is to increase DOE's total nuclear physics budget sufficiently to allow RIA to proceed. Argonne's plan for RIA calls for substantial completion of capital construction in 2010, with commissioning extending through 2012. This plan achieves the objectives of the RIA project while recognizing the need of DOE's Office of Science to set priorities across its full portfolio of prospective major construction projects.

3. Functional Genomics

Recent developments in genome-scale DNA sequencing, high-throughput analytical tools, and computing technology have made feasible the genome-wide analysis of biomolecular function. Construction of a complete functional map of cellular behavior now appears to be achievable. Functional analysis of the thousands of proteins and other macromolecules needed for a comprehensive analysis of even the simplest prokaryote is a significant technological challenge that will require substantial enhancement of currently available experimental and computational capabilities. The amount of data needed for functional characterization of an organism greatly exceeds the amount required to sequence the genome. Furthermore, unlike genome sequencing, functional analysis requires multiple high-throughput experimental technologies and novel computational approaches. At the deepest level, the biological sciences now stand at the threshold of developing new conceptual structures — facilitated by informatics and large-scale computation — that will transform biology from a science that is almost exclusively experimental to one in which theory plays a key role.

It is widely appreciated that the comprehensive characterization of biomolecular function has huge potential payoffs. It will provide the basis for developing entirely new strategies for modulating cellular activities and engineering novel cellular capabilities. These opportunities can provide the basis for novel solutions to problems associated with the DOE science mission, and they will be particularly important for advancing the DOE national security mission through the study of organisms used as biowarfare agents. More broadly, the resulting capabilities will enable major benefits for environmental management, human health, and general economic productivity.

To help seize these opportunities, we are continuing a major Laboratory initiative to undertake the large-scale functional characterization of genomes and thereby advance the goals of DOE's Genomes to Life program. The Functional Genomics initiative comprises three components: structural genomics, high-throughput molecular biology and biochemistry, and bioinformatics. The structural genomics component will evolve from the crystallographic resources of our Structural Biology Center (SBC) — one of the best facilities in the world for collecting high-resolution data from crystals of macromolecules and macromolecular complexes. Meeting the needs of this initiative will require greater throughput at the SBC, which can be achieved by enhancing existing detectors and upgrading optics and robotics capabilities.

Table III.2 Rare Isotope Accelerator ($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09	FY10	FY11	FY12
Costs										
Operating	3.5	14.0	13.0	9.0	4.0	3.0	25.5	40.0	68.0	96.0
Capital Equipment	-	-	-	-	-	-	-	-	-	-
Construction	-	-	24.0	76.0	150.0	183.0	149.0	120.0	78.0	-
Total	3.5	14.0	37.0	85.0	154.0	186.0	174.5	160.0	146.0	96.0
Direct Personnel	10.0	35.0	70.0	120.0	200.0	250.0	250.0	300.0	300.0	300.0

The high-throughput molecular biology and biochemistry component of this initiative will develop through the growth of facilities and capabilities originally created for the Midwest Center for Structural Genomics (MCSG), funded by the National Institutes of Health (NIH). The MCSG has robotic facilities for high-throughput cloning, expression, and purification of proteins. Significant expansion of those robotic facilities will be required for production of proteins at a rate adequate for the Functional Genomics initiative. In summary, our intention is to establish the premier protein production facility in the nation.

The initiative's informatics component will encompass computational structural biology and development of novel genome and proteome databases that support high-throughput experimentation. Integrating the massive amounts of data to be generated by the Functional Genomics initiative with the vast amounts of data accumulating in public databases throughout the world will be a significant challenge in itself.

We have sought input on the development of strategies and procedures for this initiative throughout the research community. In September 2001 we hosted a workshop on the challenges of integrating genome and proteome databases. Additional workshops addressing other aspects of the program are being planned.

Our efforts in functional genomics will take advantage of a number of important existing resources at Argonne and the University of Chicago. The SBC at the APS will be key for the production of high-resolution images of gene products. Such high-resolution images are the best way to link the sequence information generated by genome projects to the functional data that will be generated by the Functional Genomics initiative. Resources at the APS and the IPNS will be used for small-angle scattering studies of macromolecular complexes (molecular machines) that will be identified by protein-protein interaction mapping and generated in high-throughput protein production facilities. Protein chips for the study of protein-protein interactions will be developed in cooperation with our biochip program (see Section IV.A.2.f). Studies of gene expression will be carried out in partnership with biochip facilities at the University of Chicago. Finally, our computer scientists will create a computational environment for information management and for analysis and integration of functional data. Computer simulations are essential to the development of systems biology capabilities. The Functional Genomics initiative will include a major effort to advance the systems biology of prokaryotes by using simulation.

To develop comprehensive functional information on whole organisms, we will both enhance our existing capabilities and establish new capabilities. Existing resources for protein production will be enhanced. Novel resources for high-throughput mapping of protein-protein interactions will be established, as will facilities for identifying high-affinity, high-specificity ligands for all gene products and for the biochemical and biophysical characterization of protein function (e.g., enzyme assays). To house these resources, we have proposed that the state of Illinois fund construction of a new facility providing over 40,000 square feet of laboratory space, including space for high-throughput crystallization facilities. To develop state-of-the-art intermediate-voltage cryoelectron microscopy and associated image processing capabilities, we will partner with the University of Chicago. The facilities developed for this initiative will serve the entire research community. They will provide researchers from universities and industry with a broad range of capabilities needed to study molecular processes in the cell.

Our Functional Genomics initiative is designed to advance the goals of the Genomes to Life program of DOE's Office of Biological and Environmental Research (DOE-BER). The four goals of this program are to (1) identify and characterize the molecular machines of life, (2) characterize gene regulatory networks, (3) characterize the functional repertoire of complex microbial communities in their natural environments at the molecular level, and (4) develop the conceptual framework and the computational capabilities needed to advance understanding of complex biological systems and predict their behavior. Key to this program is a systems biology approach to understanding how molecular machines and other cellular components function together in a living system. Developing capabilities for comprehensive functional characterization of entire genomes is critical to the success of this program.

Elements of our Functional Genomics initiative should attract sponsorship from NIH. Table III.3 describes the overall resources required, including the efforts of computer scientists, environmental scientists, and APS staff, as well as biologists working in the areas of structural and functional genomics. The increase in resources leading up to FY 2005 reflects anticipated expansion of computational and robotics capabilities and NIH funding to support sector development and operation of an experimental station (the GM/CA-CAT) at the APS. These increases will support multiple Argonne research divisions working — in the areas of computation, engineering, and molecular biology — to determine the molecular structure and function of macromolecular complexes. DOE funding will be sought from DOE-BES (Energy Biosciences; KC-03) and from DOE-BER (KP-11), including the latter office's Genomes to Life program.

Table III.3 Functional Genomics ($ in millions BA, personnel in FTE)[a]

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating[b]	14.3	16.5	17.7	18.6	19.5	20.5	21.5
Capital Equipment	1.5	1.3	1.3	1.6	1.6	1.6	1.6
Construction[c]	-	2.0	16.0	16.0	-	-	-
Total	15.8	17.8	19.0	20.2	21.1	22.1	23.1
Direct Personnel	55.2	67.3	69.4	69.4	69.4	69.4	69.4

[a] Resource projections include funding from the National Institute of General Medical Sciences for the MCSG, plus anticipated funding from NIH, DOE-BER, and other organizations.

[b] Includes anticipated funding from NIH and the National Institute of General Medical Sciences for development of the GM/CA-CAT sector at the APS (enclosures, utilities, and undulators and other insertion devices).

[c] Funding of construction has been proposed to the state of Illinois.

4. Petaflops Computing and Computational Science

Our Petaflops Computing and Computational Science initiative builds on Argonne's existing long-term base program in mathematics and computer science, which is supported by DOE's Office of Advanced Scientific Computing. DOE and other agencies support work in the areas of mathematical software, parallel programming tools, advanced visualization systems, grid computing and distributed systems, collaboration technologies, scalable systems software, and performance analysis and modeling. Strong internal and external scientific collaborations tie this computer science research work to diverse applications in biology, high energy physics, climate modeling, computational chemistry, chemical engineering, subsurface modeling, biomedical computing, astrophysics, and other areas. We plan to continue building our base activities in fundamental computer science and mathematics while increasing our computational science efforts by applying advanced computing to leading-edge scientific investigations, both theoretical and experimental.

Our Petaflops Computing and Computational Science initiative aims to accelerate progress in these directions through three major components: (1) a Laboratory-wide computational science program, (2) a targeted R&D program, and (3) a new advanced computation building. Details are as follows:

- The *Laboratory-wide computational science program* will provide expertise and midrange computing resources to the Laboratory. The purpose is to enable all research groups at Argonne to begin to apply state-of-the-art computational methods to their work and to help them prepare to take advantage of emerging large-scale computing opportunities. Current exploratory efforts involve all of our scientific and engineering programs.

- The *targeted R&D program* will lead to deployment of a petascale system (one capable of 10^{15} operations per second) by 2006 and will include development of next-generation modeling capabilities in diverse scientific applications ranging from the life sciences and nanosciences to energy systems and the environment. The program will take advantage of the development of advanced analysis techniques for constructing predictive models of overall systems performance; recent advances in computer-aided design tools for applying an integrated software-hardware co-design approach to large-scale systems; and the expected availability by 2005 of the billion-transistor chips needed to build petascale systems.

• The *new advanced computation building* will support integrated research in mathematics, computer science, computational science and theory, collaborative research with industry, and joint programs with the University of Chicago (e.g., the Computation Institute). The building will include a large-scale computer room capable of housing a petaflops computing system and will incorporate digital collaboration technologies to support distributed meetings and collaboratories.

We have made substantial progress in several areas that support the Petaflops Computing and Computational Science initiative. A newly established collaboration with IBM's advanced architecture group has begun studying design options for specific classes of applications. A collaboration involving Argonne computer scientists and computational biologists and researchers at the University of Chicago aiming to advance large-scale computing in systems biology has begun to analyze model organisms and to design a whole-cell modeling system targeting petascale architectures. Laboratory researchers in computational nanoscience have begun development of an integrated simulation environment that combines models at multiple temporal and spatial scales; the researchers are also developing a virtual fabrication line simulation capability that will complement facilities being deployed in the Center for Nanoscale Materials (see Section III.A.1).

Resources required for the Petaflops Computing and Computational Science initiative are specified in Table III.4. Included are costs for facilities and for a concomitant increase in personnel (systems staff, postdoctoral researchers, scientific programmers, and permanent research staff). Funding will be sought from the Mathematical, Information, and Computational Sciences Division (KJ-01) and from other sponsors within DOE's Office of Science.

Table III.4 Petaflops Computing and Computational Science ($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	2.0	4.0	12.0	16.0	24.0	24.0	24.0
Capital Equipment	-	1.0	2.0	4.0	40.0	40.0	40.0
Construction[a]	-	-	-	7.7	7.7	7.7	7.7
Total	2.0	5.0	14.0	27.7	71.7	71.7	71.7
Direct Personnel	10.0	20.0	60.0	80.0	120.0	120.0	120.0

[a] Detailed planning for the advanced computation building will be done in FY03. Calculation of construction costs assumes third-party financing for FY04 and FY05, with leasing to begin in FY06. The calculated leasing cost is based on 240,000 square feet at $28 per square foot, plus overhead at approximately 1.15%.

B. Energy

1. Advanced Nuclear Fuel Cycle

The need to produce increasing amounts of energy and still reduce the burden of energy production on the environment dictates that nuclear energy will have a major role in the future. Nuclear energy on the required scale cannot be realized without addressing problems associated with spent fuel disposition and nuclear nonproliferation. The best way to address those two problems is through an advanced nuclear fuel cycle that returns fuel to the reactor and produces a more benign waste form.

The requirement for an advanced nuclear fuel cycle is recognized in the May 2001 report of the National Energy Policy Development Group: "The United States should reexamine its policies to allow for research, development, and deployment of fuel conditioning methods (such as pyroprocessing) that reduce waste streams and enhance proliferation resistance." This need was also recognized more recently in the May 2002 summit meeting between President Bush and Russian President Putin. The two presidents agreed that their governments see promise in advanced technologies for nuclear reactors and nuclear fuels that would significantly reduce the volume of waste produced by civilian reactors, would be highly proliferation resistant, and could be used to reduce excess stocks of weapons-grade plutonium and other dangerous nuclear materials.

Argonne has been collaborating with DOE-Nuclear Energy, Science and Technology, as well as with other national laboratories, industry, and international partners, to formulate an Advanced Nuclear Fuel Cycle initiative. The initiative's objective is to develop the technology base for a new globally secure, sustainable nuclear regime that will allow nuclear power to become a publicly acceptable, growing part of the energy supply mix in the United States and abroad. Such a regime would also be marked by reduced and stabilized inventories of spent nuclear fuel, secure management of problematic nuclear materials, enhanced proliferation resistance, and restoration of U.S. global leadership in nuclear technology.

Working with international partners, the Advanced Nuclear Fuel Cycle initiative would demonstrate the technologies and nuclear systems needed to establish the desired new nuclear regime. The two key technologies and systems that must be developed and demonstrated are a closed, proliferation-resistant fuel cycle and an advanced fast-neutron-spectrum facility. Argonne proposes to develop and demonstrate a fuel cycle based on pyroprocessing and a fast-spectrum nuclear reactor.

In addition to its work on the pyroprocess fuel cycle and the fast reactor, Argonne is a leader in developing advanced aqueous separation technologies that might also help to close the nuclear fuel cycle. We will assess both pyroprocessing and advanced aqueous options to determine their appropriate roles in meeting the objectives of the Advanced Nuclear Fuel Cycle initiative. Moreover, Argonne plans to continue supporting the development of transmutation system models and assessing transmutation options, including thermal reactors.

Primary support for the Advanced Nuclear Fuel Cycle initiative will be sought from DOE-Nuclear Energy, Science and Technology (AF). Required resources are summarized in Table III.5.

Our Advanced Nuclear Fuel Cycle initiative has four components: (1) oxide fuel reduction and actinide recovery, (2) the demonstration of reactor transmutation, (3) a spent fuel treatment facility, and (4) design studies for a prototype reactor.

Table III.5 Advanced Nuclear Fuel Cycle
($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	27.0	35.0	41.0	49.0	54.0	57.0	59.0
Capital Equipment	5.0	8.0	10.0	8.0	5.0	5.0	5.0
Construction	-	-	-	-	-	-	-
Total	32.0	43.0	51.0	57.0	59.0	62.0	64.0
Direct Personnel	135.0	170.0	190.0	220.0	230.0	230.0	230.0

Oxide Fuel Reduction and Actinide Recovery. Pyroprocessing is now being used on a production basis at Argonne-West to treat spent fuel from the Experimental Breeder Reactor-II (EBR-II). However, the current system cannot process oxide spent fuel, nor can it separate and recover plutonium and higher actinides. Necessary advances are the development and demonstration of (1) a front-end process for reducing oxide fuel to metal suitable as input for electrorefining and (2) a process for recovering plutonium and other actinides for recycling into fast reactor fuel. Also required is completed qualification of the metal and ceramic waste forms for disposal in a repository. Those waste forms contain metals and fission products remaining after the separation and recovery of uranium, plutonium, and other actinides.

Demonstration of Reactor Transmutation. Demonstration of transmutation of actinides in a fast reactor requires fabrication of fuel containing actinides and irradiation of the fuel in a fast reactor to about 10% burnup. Such a demonstration will show that fuel containing actinides can be fabricated successfully in a remote process, that the fuel performs reliably in the reactor, and that the fuel has the necessary inherent safety characteristics. With no fast reactor operating today in the United States, the demonstration will require international collaboration. (Argonne currently supports the fabrication of samples of various actinide-bearing fuels for irradiation in both domestic and international facilities.)

Spent Fuel Treatment Facility. As the third component of this initiative, we propose that a spent fuel treatment facility be designed, constructed, licensed, and operated to treat spent fuel from light-water reactors. This facility would be larger than that employed in demonstrations of separations technologies, nominally in the range of 100-500 metric tons of heavy metal per year. Operation of this facility would further demonstrate the technical and economic viability of fuel recycling, particularly fabrication of new fuel containing recycled actinides and production of waste forms for disposal. In addition, the facility's operation would reduce the amount of spent fuel destined for a geologic repository and would support the deployment of subsequent treatment facilities.

Design Studies for a Prototype Reactor. Finally, we propose to conduct nuclear system R&D and design studies focusing on a medium-sized fast reactor (with a power rating of 300-400 MWe) that incorporates lessons learned about fast-reactor technology from around the world, particularly lessons from Argonne's successful EBR-II program. Past experience in designing and operating fast reactors will be combined with new technologies to design a power plant having optimal capital costs. International collaboration will facilitate the incorporation of worldwide lessons learned, and Argonne will seek partnerships with countries having significant experience with fast reactors and sustained interest in the technology, particularly Japan, France, and Russia.

2. Hydrogen Research and Development

In his 2003 State of the Union address, President Bush announced a major hydrogen initiative. The goal is to reverse America's growing dependence on foreign oil by developing the technology for commercially viable fuel cells that use hydrogen to power cars, trucks, homes, and businesses without directly emitting pollution or greenhouse gases. This national initiative encompasses R&D on, and eventual deployment of, the technologies and infrastructure needed to produce, store, and distribute hydrogen for use in fuel cell vehicles, industrial production, heating, and electricity generation. Combined with the FreedomCAR Partnership, the President's new program is expected to accelerate the development of hydrogen-powered fuel cells and a hydrogen infrastructure. Achieving the President's comprehensive vision for our energy future requires an aggressive, interdisciplinary R&D effort spanning the fields of materials science, chemistry, and engineering. It is broadly appreciated that a hydrogen economy will not be economically competitive until fundamental breakthroughs occur in many areas, including more efficient hydrogen production, far more effective storage at high energy densities, more efficient hydrogen distribution, and more effective ultimate utilization.

In response to this national initiative, Argonne has mounted a coordinated effort that integrates its expertise in basic science and technology and in nearer-term technology development and deployment with its state-of-the-art user facilities. Central to our research program are two cross-cutting objectives that drive progress toward the hydrogen economy: (1) high-performance materials for hydrogen separation and fuel cell membranes and (2) new catalysts that improve hydrogen production and combustion. In pursuit of these objectives, we draw on our broad knowledge of materials science and chemistry to orchestrate comprehensive research programs that coordinate advances across the spectrum from basic science to applications. In particular, our program builds on insights and research directions identified by two recent workshops: (1) the May 2003 Workshop on Hydrogen sponsored by DOE-BES, in which Argonne played a leading role, and (2) the August 2002 Workshop on Hydrogen Storage Materials sponsored by DOE-Energy Efficiency and Renewable Energy, which the Laboratory hosted.

The unique capabilities of Argonne's IPNS, APS, and Electron Microscopy Center will be particularly valuable in our work on high-performance materials and catalysts for the hydrogen economy. To investigate the production of hydrogen from nuclear power, we will rely on Argonne's extensive expertise in nuclear reactor technology. To address hydrogen utilization issues, we will take full advantage of experience and facilities developed through our participation in the FreedomCAR Partnership and in the stationary fuel cell distributed generation program for electric utilities.

We are already one of DOE's leading resources for developing the technologies required for hydrogen production, distribution, storage, and utilization. Key elements of our current programs are funded by DOE through the Offices of Science; Energy Efficiency and Renewable Energy; Fossil Energy; and Nuclear Energy, Science and Technology. Further valuable work is sponsored by industrial collaborators. Current R&D programs are investigating the following areas:

- Hydrogen production
- Hydrogen storage
- Fuel cell development and testing
- Fuel and power systems
- Vehicle simulation and testing
- Economic and technical analysis
- Infrastructure assurance
- Environmental research
- Technology validation projects

Primary support for the Hydrogen Research and Development initiative will be sought from the DOE Offices of Science (KC); Energy Efficiency and Renewable Energy (EE); Fossil Energy (AA); and Nuclear Energy, Science and Technology (AF). Required resources are summarized in Table III.6.

Table III.6 Hydrogen Research and Development ($ in millions BA, personnel in FTEs)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09
Costs							
Operating	2.0	5.0	9.0	16.0	24.0	24.0	24.0
Capital Equipment	-	0.5	1.5	3.0	3.0	2.0	1.5
Construction	-	0.2	5.0	5.0	-	-	-
Total	2.0	5.7	15.5	24.0	27.0	26.0	25.5
Direct Personnel	10.0	25.0	45.0	80.0	120.0	120.0	120.0

The Hydrogen Research and Development initiative we now propose has six coordinated components: (1) production, (2) storage, (3) utilization, (4) infrastructure, (5) environmental research, and (6) technology validation.

Hydrogen Production. We will explore a variety of options for efficiently producing hydrogen by using domestic energy resources — fossil, nuclear, and renewable. We will continue to develop fuel processing technology as a near-term means of producing hydrogen from fossil fuels or from renewable fuels such as ethanol. The main transition strategy envisioned involves co-production of electricity and hydrogen from fossil fuels, with stringent environmental controls and carbon sequestration. Much of the required research on fossil fuels will be applicable to our longer-term emphasis on co-generating electricity and hydrogen by nuclear power and to our focus on developing novel low-temperature thermochemical cycles and advanced membranes to use the heat from a nuclear power plant to generate hydrogen from water. By developing the next generation of nuclear reactors ("Generation IV") in conjunction with efficient hydrogen generation technology, we will address the nation's two major energy needs: electricity and transportation fuels. In the meantime we are also working to facilitate the use of existing nuclear power plants to produce hydrogen.

Hydrogen Storage. A major challenge to the success of hydrogen-powered vehicles is the development of lightweight, compact, and safe onboard storage capabilities for adequate quantities of hydrogen. Building on a DOE-sponsored workshop that Argonne hosted in FY 2002, we will explore new and innovative concepts for storing hydrogen. Laboratory-directed research is already investigating two such novel concepts, and other ideas are being considered. Some of this research will benefit importantly from work at Argonne's emerging Center for Nanoscale Materials. We propose to lead a DOE-supported virtual center for research on storage of hydrogen through novel approaches such as chemical hydrides, metal-organic frameworks, and nanoclusters and nanofibers. We also propose to participate in other DOE virtual centers that are to investigate storage using carbon-based materials and advanced hydrides.

Hydrogen Utilization. Our work on hydrogen utilization will build on our extensive, wide-ranging partnerships with nonfederal organizations in areas that will be crucial to developing this aspect of the hydrogen economy. We have conducted research on the FreedomCAR with the automotive industry and its suppliers, helped fuel cell companies in product development, worked with state and local government agencies on alternative fuel demonstrations, and helped electric power companies analyze the technological requirements for load management and transmission.

Infrastructure Development. In collaboration with Canadian partners on the "2050 Study," we are examining long-range supply-and-demand scenarios for transportation fuels. For the Hydrogen Research and Development initiative we propose further technical and economic analyses focusing specifically on issues related to hydrogen distribution. Our expertise in infrastructure assurance will allow us to identify the steps needed to ensure that a national network for hydrogen transmission and distribution is safe and secure.

Environmental Research. Environmental impacts from the transition to a hydrogen economy must be considered. In particular, we will draw on our broad expertise in environmental research to investigate largely unanswered questions regarding effects on the atmosphere and on global warming from leaks and other losses of hydrogen from a national hydrogen infrastructure and vehicles.

Technology Validation. DOE is soliciting partnerships to conduct cost-shared demonstrations of hydrogen-powered vehicles and of hydrogen production and other infrastructure. We will form a regional partnership with vehicle developers, energy suppliers, and vehicle fleet operators for needed hydrogen technology demonstrations. In addition, at Argonne-West we propose to construct and operate a hydrogen technology demonstration facility utilizing nuclear power.