

**FINANCIAL ASSISTANCE
FUNDING OPPORTUNITY ANNOUNCEMENT**



**U.S. Department of Energy
Office of Science**

**FY 2011 Annual Notice
Submission of Renewal and Supplemental Applications
for Office of Science Grants and Cooperative Agreements**

**Funding Opportunity Number: DE-FOA-0000412
Announcement Type: Initial
CFDA Number: 81.049**

Issue Date: 9/30/2010
Letter of Intent Due Date: Not Applicable
Pre-Application Due Date: Not Applicable
Application Due Date: Not Applicable

This Funding Opportunity Announcement (FOA) will remain open until September 30, 2011 or until replaced by a successor FOA. Applications may be submitted any time during this period.

Program Manager Contact: Questions regarding the program technical requirements must be directed to the DOE Program Manager for your Award.

Where to Submit:

NOTE: REQUIREMENTS FOR GRANTS.GOV

Where to Submit: Applications must be submitted through Grants.gov to be considered for award. You cannot submit an application through Grants.gov unless you are registered. Please read the registration requirements carefully and start the process immediately. Remember you have to update your CCR registration annually. If you have any questions about your registration, you should contact the Grants.gov Helpdesk at 1-800-518-4726 to verify that you are still registered in Grants.gov.

Registration Requirements: There are several one-time actions you must complete in order to submit an application through Grants.gov (e.g., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the Central Contract Registry (CCR), register with the credential provider, and register with Grants.gov). See <http://www.grants.gov/GetStarted>. Use the Grants.gov Organization Registration Checklist at <http://www.grants.gov/assets/OrganizationRegCheck.pdf> to guide you through the process. Designating an E-Business Point of Contact (EBiz POC) and obtaining a special password called an MPIN are important steps in the CCR registration process. Applicants, who are not registered with CCR and Grants.gov, should allow at least 21 days to complete these requirements. It is suggested that the process be started as soon as possible.

IMPORTANT NOTICE TO POTENTIAL APPLICANTS: When you have completed the process, you should call the Grants.gov Helpdesk at 1-800-518-4726 to verify that you have completed the final step (i.e. Grants.gov registration).

Questions: Questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@grants.gov. Part VII of this FOA explains how to submit other questions to the Department of Energy (DOE).

Application Receipt Notices

After an application is submitted, the Authorized Organization Representative (AOR) will receive a series of four e-mails. It is extremely important that the AOR watch for and save each of the emails. It may take up to two (2) business days from application submission to receipt of email Number 2. The titles of the four e-mails are:

- Number 1 - Grants.gov Submission Receipt Number
- Number 2 - Grants.gov Submission Validation Receipt for Application Number
- Number 3 - Grants.gov Grantor Agency Retrieval Receipt for Application Number
- Number 4 - Grants.gov Agency Tracking Number Assignment for Application Number

TABLE OF CONTENTS

PART I – FUNDING OPPORTUNITY DESCRIPTION

PART II – AWARD INFORMATION

- A. Type of Award Instrument**
- B. Estimated Funding**
- C. Maximum and Minimum Award Size**
- D. Expected Number of Awards**
- E. Anticipated Award Size**
- F. Period of Performance**
- G. Type of Application**

PART III – ELIGIBILITY INFORMATION

- A. Eligible Applicants**
- B. Cost Sharing or Matching**
- C. Other Eligibility Requirements**

PART IV – APPLICATION AND SUBMISSION INFORMATION

- A. Address to Request Application Package**
- B. Letter of Intent and Pre-Application**
- C. Content and Form of Application**
- D. Submissions from Successful Applicants**
- E. Submission Dates and Times**
- F. Intergovernmental Review**
- G. Funding Restrictions**
- H. Other Submission and Registration Requirements**

PART V – APPLICATION REVIEW INFORMATION

- A. Criteria**
- B. Review and Selection Process**
- C. Anticipated Notice of Selection and Award Dates**

PART VI – AWARD ADMINISTRATION INFORMATION

- A. Award Notices**
- B. Administrative and National Policy Requirements**
- C. Reporting**

PART VII – QUESTIONS/AGENCY CONTACTS

- A. Questions**
- B. Agency Contacts**

PART VIII – OTHER INFORMATION

- A. Modifications**
- B. Government Right to Reject or Negotiate**
- C. Commitment of Public Funds**

- D. Proprietary Application Information**
- E. Evaluation and Administration by Non-Federal Personnel**
- F. Intellectual Property Developed under this Program**
- G. Notice of Right to Request Patent Waiver**
- H. Notice Regarding Eligible/Ineligible Activities**
- I. Availability of Funds**

PART I – FUNDING OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) SHOULD BE DIRECTED TO:

Program Manager Contact: Questions regarding the specific program areas/technical requirements should be directed to the points of contact listed for each program office within the FOA and not to the FOA Administrative Contact.

STATUTORY AUTHORITY

Public Law 95-91, US Department of Energy Organization Act
Public Law 109-58, Energy Policy Act of 2005

APPLICABLE REGULATIONS

U.S. Department of Energy Financial Assistance Rules, codified at 10 CFR Part 600
U.S. Department of Energy, Office of Science Financial Assistance Program Rule, codified at 10 CFR Part 605

SUMMARY: The Office of Science of the Department of Energy hereby announces its continuing interest in receiving grant applications for support of work in the following program areas: Advanced Scientific Computing Research, Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, High Energy Physics, Nuclear Physics, and Workforce Development for Teachers and Scientists. On September 3, 1992, DOE published in the Federal Register the Office of Energy Research Financial Assistance Program (now called the Office of Science Financial Assistance Program), 10 CFR Part 605, Final Rule, which contained a solicitation for this program. Information about submission of applications, eligibility, limitations, evaluation and selection processes and other policies and procedures are specified in 10 CFR Part 605.

This FOA will remain open until September 30, 2011, 8:00 PM Eastern Time, or until it is succeeded by another issuance, whichever occurs first. This annual FOA DE-FOA-0000412 succeeds FOA DE-FOA-0000179, which was published December 4, 2009.

SUPPLEMENTARY INFORMATION

The following program descriptions are offered to provide more in-depth information on scientific and technical areas of interest to the Office of Science.

OFFICE OF SCIENCE OVERVIEW

Website: <http://www.science.doe.gov>

The mission of the Office of Science is the delivery of scientific discoveries and major scientific tools to transform our understanding of nature and to advance the energy, economic, and national security of the United States.

The Office of Science accomplishes its mission by supporting:

- ***Science for Discovery***, focused on unraveling nature’s mysteries—from the study of subatomic particles, atoms, and molecules that make of the materials of our everyday world to DNA, proteins, cells, and entire biological systems;
- ***Science for National Need***, focused on advancing a clean energy agenda through basic research on energy production, storage, transmission, and use; and advancing our understanding of the Earth’s climate through basic research in atmospheric and environmental sciences and climate change; and
- ***National Scientific User Facilities***, the 21st century tools of science, engineering, and technology—providing the Nation’s researchers with the most advanced tools of modern science including accelerators, colliders, supercomputers, light sources and neutron sources, and facilities for studying the nanoworld.

The Office of Science manages its research portfolio through six scientific program offices and a workforce development program. The following program descriptions are offered to provide more in-depth information on scientific and technical areas of interest to the Office of Science:

Research opportunities exist in the following Office of Science research programs and subprograms. Additional details, websites, and technical points of contact are provided in the materials that follow.

1. Advanced Scientific Computing Research (ASCR)

- (a) Applied Mathematics
- (b) Computer Science
- (c) Computational Partnerships
- (d) Network Environment Research

2. Basic Energy Sciences (BES)

- (a) Materials Chemistry
- (b) Biomolecular Materials
- (c) Synthesis and Processing Science
- (d) Experimental Condensed Matter Physics
- (e) Theoretical Condensed Matter Physics
- (f) Physical Behavior of Materials
- (g) Mechanical Behavior and Radiation Effects
- (h) X-ray Scattering
- (i) Neutron Scattering
- (j) Electron and Scanning Probe Microscopies
- (k) Atomic, Molecular, and Optical Sciences
- (l) Gas Phase Chemical Physics
- (m) Computation and Theoretical Chemistry
- (n) Condensed Phase and Interfacial Molecular Science (CPIMS)
- (o) Catalysis Science
- (p) Separations and Analysis

- (q) Heavy Element Chemistry
- (r) Geosciences Research
- (s) Solar Photochemistry
- (t) Photosynthetic Systems
- (u) Physical Biosciences
- (v) BES Accelerator and Detector Research

3. Biological and Environmental Research (BER)

- (a) Biological Systems Science
- (b) Climate and Environmental Sciences

4. Fusion Energy Sciences (FES)

- (a) FES Science and Facility Operations
- (b) FES Enabling Research and Development

5. High Energy Physics (HEP)

- (a) Experimental High Energy Physics Research
- (b) Theoretical High Energy Physics Research
- (c) HEP Advanced Technology Research and Development

6. Nuclear Physics (NP)

- (a) Medium Energy Nuclear Physics
- (b) Heavy Ion Nuclear Physics
- (c) Low Energy Nuclear Physics
- (d) Nuclear Theory (including the Nuclear Data subprogram)
- (e) Isotope Development and Production for Research and Applications
- (f) Accelerator Research and Development for Current and Future Nuclear Physics Facilities

7. Workforce Development for Teachers and Scientists (WDTS)

1. Advanced Scientific Computing Research (ASCR)

Program Website: <http://www.sc.doe.gov/ascr/>

The mission of the Advanced Scientific Computing Research (ASCR) program is to discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to the Department of Energy (DOE). A particular challenge of this program is fulfilling the science potential of emerging multi-core computing systems and other novel “extremescale” computing architectures, which will require significant modifications to today’s tools and techniques.

The priority areas for ASCR include the following:

- Develop mathematical models, methods and algorithms to accurately describe and predict the behavior of complex systems involving processes that span vastly different time and/or length scales.

- Advance key areas of computer science that:
 - Enable the design and development of extreme scale computing systems and their effective use in the path to scientific discoveries; and
 - Transform extreme scale data from experiments and simulations into scientific insight.
- Advance key areas of computational science and discovery that support the missions of the Office of Science through mutually beneficial partnerships.
- Develop and deliver forefront computational, networking and collaboration tools and facilities that enable scientists worldwide to work together to extend the frontiers of science.

The computing resources and high-speed networks required to meet Office of Science needs exceed the state-of-the-art by a significant margin. Furthermore, the system software, algorithms, software tools and libraries, programming models and the distributed software environments needed to accelerate scientific discovery through modeling and simulation are beyond the realm of commercial interest. To establish and maintain DOE's modeling and simulation leadership in scientific areas that are important to its mission, ASCR operates Leadership Computing facilities, a high-performance production computing center, and a high-speed network, implementing a broad base research portfolio in applied mathematics, computer science, computational science and network research to solve complex problems on computational resources that are on a trajectory to reach well beyond the petascale within a few years.

The ASCR subprograms and their objectives follow:

(a) Applied Mathematics

This subprogram supports basic research leading to fundamental mathematical advances and computational breakthroughs across DOE and Office of Science missions. Applied Mathematics research includes and supports efforts to develop robust mathematical models, algorithms and numerical software for enabling predictive scientific simulations of DOE-relevant complex systems. Important areas of supported research include: (1) novel numerical methods for the scalable solution of large-scale, linear and nonlinear systems of equations; (2) innovative approaches for analyzing and extracting insight from large-scale data sets; (3) efficient techniques for characterizing, propagating, and/or quantifying uncertainties and errors in next-generation solver, optimization, simulation, analysis, and other codes; and (4) multiscale methods for continuous and/or discrete systems that efficiently account for physics and subcomponent interactions across vastly different time and length scales.

Subprogram Contacts: Karen Pao, (301) 903-5384, Karen.Pao@science.doe.gov, and Sandy Landsberg, (301) 903-8507, Sandy.Landsberg@science.doe.gov
 Website: <http://www.sc.doe.gov/ascr/Research/AppliedMath.html>

(b) Computer Science

This subprogram supports basic research to advance extreme scale scientific computing and data management and analysis. It also supports research in computer science that enables scientific applications and data-driven computational science through advances in petascale and exascale computing systems.

In the context of ASCR-supported high performance computing environments, research topics of interest include: computing systems architecture; hardware and software approaches to power/energy management; scalable and fault tolerant operating and runtime systems; programming and execution models; programming environments, programming languages, and compilers; auto-tuning and performance modeling; methods for interoperability and for improving software resilience; formal verification and validation metrics and methods; and large scale data management, data analytics and visual techniques for understanding and representing complex physical or biological phenomena across multiple spatial and temporal scales.

The development of new computer and computational science techniques will allow scientists to use the most advanced computers without being overwhelmed by the complexity of rewriting their codes with each new generation of high performance architectures.

Subprogram Contacts: Lucy Nowell, (301) 903-3191, Lucy.Nowell@science.doe.gov, and Sonia R. Sachs, (301) 903-0060, Sonia.Sachs@science.doe.gov
Website: <http://www.sc.doe.gov/ascr/Research/ComSci.html>

(c) Computational Partnerships

This subprogram supports research in pioneering science applications for the next generation of high-performance computing. It also supports research that incorporates and integrates applied mathematics, computer science, and computational sciences, and enables scientists to effectively exploit petascale-and-beyond machines in their pursuit of transformational scientific discovery through simulation and modeling. In order to advance science relevant to the DOE mission, it is expected that the research will utilize or lead to partnerships with SC, NNSA, or other DOE programs. For examples of computational partnerships, refer to the website <http://www.scidac.gov>.

Subprogram Contact: Randall Laviolette, (301) 903-5195, Randall.Laviolette@science.doe.gov
Website: <http://www.sc.doe.gov/ascr/Research/SciDAC.html>

(d) Network Environment Research

This subprogram supports research and development in next-generation network and scientific collaboration technologies that support distributed high-end science applications and enhance large-scale scientific collaborations. DOE's national science facilities are typically accessed by distributed collaborative teams of scientists in academia, industry, and national laboratories. The subprogram supports research activities to develop technologies that enable DOE scientists and collaborators to effectively communicate and access science facilities securely and seamlessly.

The current priority of the program is to develop network and middleware technologies that will deliver end-to-end throughput a thousand times (1000x) faster than currently available.

Research topics of interest include, but are not limited to: radically new architectures and protocols for hybrid terabit/s networking, multi-layer and multi-domain network provisioning and security, virtual optical network services, composable transport protocols and data transfer services that work effectively at 100 Gbps and beyond, multi-level end-to-end performance analysis tools and services, scientific workflows, and distributed data management toolkits. Respondents are encouraged to use component-based approaches to facilitate the adoption of their proposed algorithms/software into DOE science infrastructures.

Subprogram Contacts: Thomas Ndousse-Fetter, (301) 903-9960, Thomas.Ndousse-Fetter@science.doe.gov, and Richard Carlson, (301) 903-9486, Richard.Carlson@science.doe.gov
Website: <http://www.sc.doe.gov/ascr/Research/NextGen.html>

Proposed research may include one or more of the areas listed above.

2. Basic Energy Sciences (BES)

Program Website: <http://www.sc.doe.gov/bes>

The mission of the Basic Energy Sciences (BES) program is to support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security. The portfolio supports work in the natural sciences by emphasizing fundamental research in materials sciences, chemistry, geosciences, and biosciences. BES-supported scientific facilities provide specialized instrumentation and expertise that enable scientists to carry out experiments not possible at individual laboratories.

The four long-term goals in scientific advancement that the BES program is committed to and against which progress can be measured are:

- Understand, design, model, synthesize, characterize, analyze, assemble, and use a variety of new materials and structures, emphasizing nanoscale materials, including metals, alloys, ceramics, polymers, bioinspired and biomimetic materials, and hybrid materials for energy-related applications.
- Understand, model, and control chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic and biological systems.
- Develop new concepts and improve existing methods to assure a secure energy future, e.g., for solar energy conversion, energy storage, and other energy sources.
- Conceive, design, fabricate, and use new scientific instruments to characterize and ultimately control materials, especially instruments for x-ray, neutron, and electron beam scattering and for use with high magnetic and electric fields.

The BES divisions and subprograms and their objectives follow:

Materials Sciences and Engineering

The Materials Sciences and Engineering (MSE) Division supports fundamental experimental and theoretical research to provide the knowledge base for the discovery and design of new materials with novel structures, functions, and properties. This knowledge serves as a basis for the development of new materials for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use. The MSE research portfolio consists of the research focus areas listed below.

Website: <http://www.sc.doe.gov/bes/mse/index.html>

(a) Materials Chemistry

This activity supports basic research in chemical synthesis and discovery of new materials. The major programmatic focus is on the discovery, design and synthesis of novel materials with an emphasis on the chemistry and chemical control of structure and collective properties. Major thrust areas include: nanoscale chemical synthesis and assembly; solid state chemistry for exploratory synthesis and tailored reactivities; novel polymeric materials and complex fluids; surface and interfacial chemistry including electrochemistry; and the development of new, science-driven laboratory-based analytical tools and techniques.

With the completion of the recent cycle of BES Basic Research Needs (and other) workshops and reports, the scientific community has articulated very clearly those areas of science and materials which are most relevant to energy. All of the reports variously identify the overarching goal of materials chemistry research as providing the knowledge needed to design and produce new materials with tailored properties from first principles. This program will make progress towards that goal by increasing activity in the following areas: development of new chemical means to direct and control the non-covalent assembly of materials, such as strategies to organize electron donors and acceptors; creation of ways to tailor the symmetry and dimensionality of crystalline lattices; and utilization of chemistry to control and design interfaces between dissimilar materials. Research will be conducted on materials that have potential for use in the next generation energy technologies, including research that underpins new approaches and chemistries related to carbon capture. The program will seek to increase the proportion of research in classes that demonstrate promise in providing the properties required for energy solutions. Some examples of these classes include complex inorganic oxides, metamaterials, and liquid crystals with novel electronic, magnetic, photonic and thermal properties.

Subprogram Contact: Mary Galvin, (301) 903-8334, mary.galvin@science.doe.gov

Website: http://www.sc.doe.gov/bes/mse/materials_chemistry.html

(b) Biomolecular Materials

This activity supports basic research in the discovery, design and synthesis of biomimetic and bioinspired functional materials and complex structures, and materials aspects of energy conversion processes based on principles and concepts of biology. The major program emphasis

is the creation of robust, scalable, energy-relevant materials and systems with emergent behavior that work with the extraordinary effectiveness of molecules and processes of the biological world. Major thrust areas include: understanding, controlling, and building complex hierarchical structures by mimicking nature's self- and directed-assembly approaches; design and synthesis of environmentally adaptive, self-healing multi-component materials and systems that demonstrate energy conversion and storage capabilities found in nature; biomimetic and/or bioinspired routes for the synthesis of energy relevant materials, e.g., semiconductor and magnetic materials under mild conditions; functional systems with collective properties not achievable by simply summing the individual components; and development of science-driven tools and techniques for the characterization of energy-relevant biomolecular and soft materials.

Enhanced integration of theory, computation, and experiment is sought to develop a more comprehensive understanding of bioinspired and biomimetic synthesis of inorganic materials, nanoscale structure, and non-equilibrium behavior of bioinspired/bioderivative materials and systems, leading to new design ideas and opportunities for discovery of transformational materials and processes for future energy technologies. In addition, research will be enhanced in areas for the discovery, design, and synthesis of materials for energy: dynamically adaptive and self-repairing materials; low temperature synthesis; effective and unique strategies for interfacing biological and non-biological materials and systems in search of emergent behavior; artificial enzymes; material architectures for efficiently integrating light-harvesting, photo-redox, and catalytic functions; and functional structures that take inspiration from biological gates, pores, channels, and motors.

Subprogram Contact: Michael Markowitz, (301) 903-6779, mike.markowitz@science.doe.gov
Website: <http://www.sc.doe.gov/bes/mse/biomolecular.html>

(c) Synthesis and Processing Science

This activity supports basic research to understand the physical phenomena that underpin materials synthesis including diffusion, nucleation, and phase transitions; and for developing new techniques such as *in situ* diagnostics. The emphasis is on the synthesis of complex thin films and nanoscale materials with atomic layer-by-layer control; preparation techniques for high-quality single crystal and bulk materials with novel physical properties; understanding the contributions of the liquid and other precursor states to the processing of bulk nanoscale materials; and low energy processing techniques for large-scale nanostructured materials. The program includes research that couples experiments and theory for discovery and design of materials. The focus of this activity on materials discovery and design by physical means is complementary to the BES Materials Chemistry and Biomolecular Materials research activities, which emphasize chemical and biomimetic routes to new materials.

Over the past few years, the activity has evolved an increasing interest in controlling defects in deposition processes, novel synthesis methods for bulk and nanocrystalline growth, understanding nanoscale morphology through nucleation and growth kinetics and mechanisms, and complex chemical and structural materials growth. Over the next several years, these directions are expected to strengthen research in bulk materials growth, deposition, and sintering and added emphasis in the fundamental understanding of the mechanisms for interfacing soft-

hard hybrid materials and the organization of these structures. Expansion is planned in research for discovery of novel synthesis methods, especially using extreme environments of field and flux, and research to push the limits of our basic understanding in synthesis and processing related to use-inspired technologies including solid-state lighting, solar energy conversion, hydrogen storage, and electrical energy storage. This activity will continue to support hypothesis-driven fundamental science in synthesis and processing with a particular interest in high-risk, high-impact, innovative, and imaginative projects. The activity continues to support and encourages natural collaboration between theorists and experimentalists to address the opportunities described in the scientific challenges described above.

Subprogram Contact: Bonnie Gersten, (301) 903-0002, bonnie.gersten@science.doe.gov

Website: <http://www.sc.doe.gov/bes/mse/synthesis.html>

(d) Experimental Condensed Matter Physics

This activity supports experimental condensed matter physics research with an emphasis on understanding the relationships between electronic structure and properties of complex materials. The focus is largely on systems whose behavior derives from strong electron correlation effects, anisotropy, or reduced dimensionality. Scientific themes include superconductivity, magnetism and spin physics, low dimensional electron systems, nanoscale systems, and quantum-size effects. The program also supports the development of new techniques and instruments for characterizing the electronic states and properties of materials under extreme conditions, such as ultra-low temperatures (milli-Kelvin) and ultra-high magnetic fields (100 Tesla).

This program will foster research at to support the search for new materials systems with which to explore the central scientific themes of the program. The portfolio will continue support research on electronic structure, surfaces/interfaces, and development of experimental techniques. Efforts will continue to strengthen research in unconventional superconductivity, including the high-temperature cuprate superconductors, heavy fermion superconductors, and the recently discovered iron-arsenide superconductors. Continued growth in support for spin physics and nanomagnetism is expected. Most recently the program has begun to explore the potential of cold atom research to provide insights into open questions about correlated electron behavior in condensed matter systems.

Subprogram Contact: Andrew Schwartz, (301) 903-3535, andrew.schwartz@science.doe.gov

Website: <http://www.sc.doe.gov/bes/mse/experimental.html>

(e) Theoretical Condensed Matter Physics

This activity supports theoretical condensed matter physics with emphasis on the theory, modeling, and simulation of electronic correlations. Major research areas include nanoscale science, quantum transport, superconductivity, magnetism, and optics. Development of theory targeted at materials discovery and aiding the design and interpretation of experimental research supported by BES is also emphasized.

The program will continue to emphasize the development of our understanding of matter on the atomic scale, expanding to address properties of materials at nanometer length scales. A rich future exists in basic science and applications surrounding highly correlated materials as well as novel superconductors. This research is motivated by the newest science of materials, as well as by the potential for impact on longstanding problems for energy technologies and for fundamental physics, including understanding of the physics of microstructure.

Subprogram Contact: James Horwitz, (301) 903-4894, james.horwitz@science.doe.gov
Website: <http://www.sc.doe.gov/bes/mse/theoretical.html>

(f) Physical Behavior of Materials

This activity supports basic research on the behavior of materials in response to external stimuli, such as temperature, electromagnetic fields, chemical environments, and the proximity effects of surfaces and interfaces. Emphasis is on the relationships between performance (electrical, magnetic, optical, electrochemical, and thermal) and the crystal structure and defects in the material. Included within the activity is research to establish the relationship of crystal and defect structures to diffusion and transport phenomena, phase equilibria, and kinetics of reactions. Basic research is also supported to develop new instrumentation, including *in situ* experimental tools, to probe the physical behavior in real environments encountered in energy applications.

The long term goals of this program are to understand the relationships between material properties and response to external stimuli. This can be achieved by determining structure over multiple length scales, with emphasis at the atomic level, and by understanding the response of nanometer and larger features to those external stimuli. Studies of the physical response of a single nanometer-scale feature needs to be related to the macroscopic behavior of the material. This can often be done with modeling, but further advances are necessary to fully couple the length scales from atomic to macroscopic scale. Developing and applying novel experimental, theoretical, and modeling techniques to address these problems will be emphasized. Increased investment in plasmonics, metamaterials and organic electronic materials will be considered. This program also seeks to foster theory, modeling, and simulation activities that address charge and energy transfer; electronic structure calculation; exciton dynamics and transport; and spin dynamics in energy relevant materials.

Subprogram Contact: Refik Kortan, (301) 903-3308, refik.kortan@science.doe.gov
Website: http://www.sc.doe.gov/bes/mse/physical_behavior.html

(g) Mechanical Behavior and Radiation Effects

This activity supports basic research to understand defects in materials and their effects on the properties of strength, structure, deformation, and failure. Defect formation, growth, migration, and propagation are examined by coordinated experimental and modeling efforts over a wide range of spatial and temporal scales. Topics include deformation of ultra-fine scale materials, radiation-resistant material fundamentals, and microstructural design for increased strength,

formability, and fracture resistance in energy relevant materials. The goals are to understand the fundamentals of defect behavior that will allow the development of predictive models for the design of materials having superior mechanical properties and radiation resistance.

Due to the importance of defects from radiation damage and mechanical strain in self-assembly, physical behavior and chemical reactions, it is imperative to understand these interactions and synergies at a fundamental level. With the emerging importance of nanoscale structures with high surface-to-volume ratios, it is appropriate to take advantage of the new, unprecedented capabilities to fabricate and test tailored structures down to the nanoscale, taking advantage of more powerful parallel computational platforms and new experimental tools.

Radiation is increasingly being used as a tool and a probe to gain a greater understanding of fundamental atomistic behavior of materials. Incoming fluxes can be uniquely tuned to generate a material's response that can be detected *in situ* over moderate length and time scales. Materials also sustain damage after long times in high-radiation environments typical of current and projected nuclear energy reactors and in geological waste storage. As nuclear energy is projected to play a larger role in US energy production, fundamentals of the unit processes that lead to long-term damage need to be addressed.

Subprogram Contact: John Vetrano, (301) 903-5976, john.vetrano@science.doe.gov
Website: http://www.sc.doe.gov/bes/mse/mechanical_behavior.html

(h) X-Ray Scattering

This activity supports basic research on the fundamental interactions of photons with matter to achieve an understanding of atomic, electronic, and magnetic structures and excitations and their relationships to materials properties. The main emphasis is on x-ray scattering, spectroscopy, and imaging research, primarily at major BES-supported user facilities. Instrumentation development and experimental research in ultrafast materials science, including research aimed at manipulating and detecting ultrashort and ultrahigh-peak-power electron, x-ray, and laser pulses to study ultrafast physical phenomena in materials, is an integral part of the portfolio.

Advances in x-ray scattering and ultrafast sciences will continue to be driven by scientific opportunities presented by improved source performance and optimized instrumentation. The x-ray scattering activity will continue to fully develop the capabilities at the DOE facilities by providing support for instrumentation, technique development and research. A continuing theme in the scattering program will be the integration and support of materials preparation, especially when coupled to *in situ* investigation of materials processing. New investments in ultrafast science will focus on research that uses radiation sources associated with BES facilities and beam lines but also includes research with ultra short pulse x-ray, electron beam and THz radiation probes created by conventional tabletop laser sources.

Subprogram Contact: Lane Wilson, (301) 903-5877, lane.wilson@science.doe.gov
Website: <http://www.sc.doe.gov/bes/mse/xray.html>

(i) Neutron Scattering

This activity supports basic research on the fundamental interactions of neutrons with matter to achieve an understanding of the atomic, electronic, and magnetic structures and excitations of materials and their relationship to materials properties. Major emphasis is on the application of neutron scattering, spectroscopy, and imaging for materials research, primarily at BES-supported user facilities. Development of next-generation instrumentation concepts, innovative optics, novel detectors, advanced sample environments, and polarized neutrons are distinct aspects of this activity.

The neutron scattering activity will continue its stewardship role to foster growth of the US neutron scattering community in the development of innovative, time-of-flight neutron scattering and imaging instrumentation concepts and their effective utilization for transformational research. A continuing theme in the neutron scattering program will be the integration and support of materials preparation such as single crystals required to enable important experiments on correlated and complex materials. New investments will be made in the development and application of neutron scattering techniques to understand the effects of interfaces on the collective behavior of multi-component systems consisting of hard and soft matter, enabling transformational research for energy.

Subprogram Contact: P. Thiyagarajan (Thiyaga), (301) 903-9706,

p.thiyagarajan@science.doe.gov

Website: <http://www.sc.doe.gov/bes/mse/neutron.html>

(j) Electron and Scanning Probe Microscopies

This activity supports basic research in materials sciences using advanced electron and scanning probe microscopy and spectroscopy techniques to understand the atomic, electronic, and magnetic structures and properties of materials. The emphasis is to advance the instrumentation and techniques, including ultrafast diffraction and imaging techniques, to address forefront challenges in basic research.

Significant improvements in resolution and sensitivity will provide an array of opportunities for groundbreaking science. These include imaging functionality and understanding the electronic structure, spin dynamics, magnetism, and transport properties at the atomic or nanometer scale; correlation of structure and properties of nanostructured materials for energy applications; atomic-scale tomography; combining multiple probes in a single experiment; high resolution analyses of energy-relevant soft matter; and *in situ* analysis capabilities under perturbing parameters such as temperature, stress, magnetic field, and chemical environment. To address these challenges, new state-of-the-art microscopy and spectroscopy, as well as the associated theoretical tools to maximize understanding of the experiments, are needed.

Subprogram Contact: Jane Zhu, (301) 903-3811, jane.zhu@science.doe.gov

Website: <http://www.sc.doe.gov/bes/mse/electron.html>

Chemical Sciences, Geosciences, and Biosciences

The Chemical Sciences, Geosciences, and Biosciences (CSGB) Division supports experimental, theoretical, and computational research to provide fundamental understanding of chemical transformations and energy flow in systems relevant to DOE missions. This knowledge serves as a basis for the development of new processes for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use. The CSGB research portfolio consists of the research focus areas listed below.

Website: <http://www.sc.doe.gov/bes/csgb/index.html>

(k) Atomic, Molecular, and Optical Sciences (AMOS)

This activity supports theory and experiments to understand structural and dynamical properties of atoms, molecules, and nanostructures. The research emphasizes the fundamental interactions of these systems with photons and electrons to characterize and control their behavior. These efforts aim to develop accurate quantum mechanical descriptions of properties and dynamical processes of atoms, molecules, and nanoscale matter. For example, the study of energy transfer within isolated molecules provides the foundation for understanding chemical reactivity. Topics include the development and application of novel, ultrafast optical probes of matter with particular interest in x-ray sources; the interactions of atoms and molecules with intense electromagnetic fields; and studies of collisions and many-body cooperative interactions of atomic and molecular systems. The knowledge and techniques produced by this activity form a science base that underpins several aspects of the DOE mission. The AMOS activity provides new ways to control and probe interactions in the gas and condensed phases, and enhances our ability to understand materials. New methods for using photons, electrons, and ions to probe matter enable more effective use of BES light source, nanoscience, and microcharacterization facilities. This enabling aspect will continue to be emphasized, particularly with respect to research involving the generation and application of ultrafast, intense x-ray pulses. Similarly, the study of formation and evolution of energized states in atoms, molecules, and nanostructures provides a fundamental basis for understanding elementary processes in solar energy conversion and radiation-induced chemistry.

Research in AMO science is fundamental to meeting the grand challenges for basic energy sciences, as identified in the report from the Basic Energy Sciences Advisory Committee: *Directing Matter and Energy: Five Challenges for Science and the Imagination*. In recent years, AMO science has transformed from a field in which the fundamental interactions of atoms, molecules, photons, and electrons are probed to one in which they are controlled. Systems studied are increasingly complex, and exhibit highly correlated, non-perturbative interactions. AMOS scientists can shape the quantum mechanical wave functions of atoms and small molecules using controllable laser fields, trap and cool atoms and molecules to ultracold temperatures, create nanoscale structures that manifest novel light-matter interactions and properties, and coherently drive electrons to generate ultrafast x-ray pulses. Theoretical advances are enabling modeling and simulation of increasingly complex systems to provide interpretation

of existing data, and predictions for new experiments. These capabilities create opportunities to investigate chemical processes under conditions that are far from equilibrium, where complex phenomena are predominant and controllable, and on ultrafast timescales commensurate with the motions of atoms and electrons.

Subprogram Contact: Jeffrey Krause, (301) 903-5827, jeff.krause@science.doe.gov
Website: <http://www.sc.doe.gov/bes/csgb/atomic.html>

(l) Gas Phase Chemical Physics

The Gas Phase Chemical Physics (GPCP) Program supports research that improves our understanding of the dynamics and rates of chemical reactions at energies characteristic of combustion and the chemical and physical properties of key combustion intermediates. The overall aim is the development of a fundamental understanding of chemical reactivity enabling validated theories, models and computational tools for predicting rates, products, and dynamics of chemical processes involved in energy utilization by combustion devices. Important to this aim is the development of experimental tools for discovery of fundamental dynamics and processes affecting chemical reactivity. Combustion models using this input are developed that incorporate complex chemistry with the turbulent flow and energy transport characteristics of real combustion processes.

Major thrust areas supported by the GPCP program include: quantum chemistry, reactive molecule dynamics, chemical kinetics, spectroscopy, predictive combustion models, combustion diagnostics, and soot formation & growth. The GPCP program does *not* support research in the following areas: non-reacting fluid dynamics and spray dynamics, data-sharing software development, end-use combustion device development, and characterization or optimization of end-use combustion devices.

The focus of the GPCP program is the development of a molecular-level understanding of gas-phase chemical reactivity of importance to combustion. The desired evolution is to multi-phase predictive capabilities that span the microscopic to macroscopic domains enabling the computation of individual molecular interactions as well as their role in complex, collective behavior in real-world devices. Currently, increased emphasis in gas-phase chemical physics is on validated theories and computational approaches for the structure, dynamics, and kinetics of open shell systems, experimental measurements of combustion reactions at high pressures, better insight into soot particle growth and an improved understanding of the interaction of chemistry with fluid dynamics.

Subprogram Contact: Wade Sisk, (301) 903-5692, wade.sisk@science.doe.gov
Website: <http://www.sc.doe.gov/bes/csgb/gas-phase.html>

(m) Computation and Theoretical Chemistry

Computation and Theoretical Chemistry emphasizes sustained development and integration of new and existing theoretical and massively parallel computational approaches for the accurate and efficient prediction of processes and mechanisms relevant to the BES mission and for laying

the groundwork for computational design of matter for energy technologies. Part of the focus is on next-generation simulation of processes that are so complex that efficient computational implementation must be accomplished in concert with development of theories and algorithms. Efforts should be tightly integrated with the research and goals of BES, especially the chemical physics programs, and should provide fundamental solutions that enhance or enable conversion to clean, sustainable, renewable, novel or highly efficient energy use. Efforts should include application to real molecular- and nano- scale systems. This may include the development or improvement of reusable computational tools that enhance analysis of measurements at the DOE facilities or efforts aimed at enhancing accuracy, precision, and applicability or scalability of all variants of quantum-mechanical simulation methods. This includes the development of spatial and temporal multi-scale/multistage methodologies that allow for time-dependent simulations of resonant, non-resonant and dissipative processes as well as rare events. Development of capabilities for simulation of light-matter interactions, conversion of light to chemical energy or electricity, and the ability to model and control externally driven electronic and spin-dependent processes in real environments are encouraged. These phenomena may be modeled using a variety of time-independent and time-dependent simulation approaches. Examples include:

- Practical predictive methods for excited-state phenomena in complex molecular systems.
- Nontraditional or novel basis sets, meshes and approaches for quantum simulation.
- Simulation and coupling of all interactions/scales in a system including: electronic, vibrational and atomistic structure, dissipative interactions, interactions between matter, radiation, fields and environment, spin-dependent and magnetic effects and the role of polarization, solvation and weak interactions.

Current interest includes applications to (i) energy storage, (ii) solar light harvesting including sunlight-to-fuel, (iii) interfacial phenomena, (iv) selective carbon-dioxide/gas separation, storage and capture, (v) next-generation combustion modeling, (vi) reactivity and catalysis, (vii) molecular and nano-scale electronic and energy transport, (viii) quantum simulation of biologically inspired mechanisms for energy management, and (ix) alternative fuel.

Subprogram Contact: Mark Pederson, (301) 903-9956, mark.pederson@science.doe.gov
Website: <http://www.sc.doe.gov/bes/csgb/computational-theoretical.html>

(n) Condensed Phase and Interfacial Molecular Science (CPIMS)

This activity emphasizes molecular understanding of chemical, physical, and electron- and photon-driven processes in aqueous media and at interfaces. Studies of reaction dynamics at well-characterized metal and metal-oxide surfaces and clusters lead to the development of theories on the molecular origins of surface-mediated catalysis and heterogeneous chemistry. Studies of model condensed-phase systems target first-principles understandings of molecular reactivity and dynamical processes in solution and at interfaces. The approach confronts the transition from molecular-scale chemistry to collective phenomena in complex systems, such as the effects of solvation on chemical structure and reactivity. Fundamental studies of reactive processes driven by radiolysis in condensed phases and at interfaces provide improved understanding of radiolysis effects and radiation-driven chemistry in nuclear fuel and waste environments.

Research in CPIMS is fundamental to meeting the grand challenges for basic energy sciences, as identified in the report from the Basic Energy Sciences Advisory Committee: *Directing Matter and Energy: Five Challenges for Science and the Imagination*. This activity supports experimental and theoretical investigations in the gas phase, condensed phase, and at interfaces aimed at elucidating the molecular-scale chemical and physical properties and interactions that govern chemical reactivity, solute/solvent structure, and transport. The impact of this cross-cutting program on DOE missions is far reaching, including energy utilization, catalytic and separation processes, energy storage, and environmental chemical and transport processes.

The desired evolution for CPIMS is to predictive capabilities that span the microscopic to macroscopic domains enabling the computation of individual molecular interactions as well as their role in complex, collective behavior in real-world devices. In surface chemistry, continued emphasis is on the development of a structural basis for gas/surface interactions, encouraging site-specific studies that measure local behavior at defined sites. At interfaces, emphasis is on aqueous systems and the role of solvents in mediating solute reactivity. Expanding into the future, plans are to probe the chemical physics of energy transfer in large molecules, to explore the molecular origins of condensed phase behavior and the nature and effects of non-covalent interactions including hydrogen bonding, and to investigate temporally resolved interfacial chemical dynamics and charge transfer using advances in chemical imaging. Renewed emphasis is anticipated in areas such as emergent behavior in condensed phase systems and for interfacial science relevant to electrical energy storage, including studies for electrode-electrolyte interfaces.

The emphasis of research support toward the molecular level means that the CPIMS program does not fund research in bulk fluid dynamics, such as studies in laminar or turbulent flows or microfluidics. The relevance of research to the energy mission means that the CPIMS program does not support research on molecules or cells directed toward medical applications.

Subprogram Contact: Gregory Fiechtner, (301) 903-5809, gregory.fiechtner@science.doe.gov
Website: <http://www.sc.doe.gov/bes/csgb/condensed-phase.html>

(o) Catalysis Science

This activity develops the fundamental scientific principles enabling rational catalyst design and chemical transformation control. Research includes the identification of the elementary steps of catalytic reaction mechanisms and their kinetics; construction of catalytic sites at the atomic level; synthesis of ligands, metal clusters, and bio-inspired reaction centers designed to tune molecular-level catalytic activity and selectivity; the study of structure-reactivity relationships of inorganic, organic, or hybrid catalytic materials in solution or supported on solids; the dynamics of catalyst structure relevant to catalyst stability; the experimental determination of potential energy landscapes for catalytic reactions; the development of novel spectroscopic techniques and structural probes for *in situ* characterization of catalytic processes; and the development of theory, modeling, and simulation of catalytic pathways. A wealth of experimental information has been accumulated relating catalytic structure, activity, selectivity, and reaction mechanisms. However, for phenomenological catalysis to evolve into predictive catalysis, the principles

connecting those kinetic phenomena must be more clearly and thoroughly identified. Better understanding of catalysis will result from synthesis of catalyst structures that are stable and reproducible under working conditions; fast and ultrafast characterization of intermediate and transition states; and microkinetics analysis of complex reactions.

The convergence of heterogeneous, homogeneous, and biocatalysis is emerging and being used to derive new biomimetic catalysts. Designed secondary and tertiary structures add structural flexibility and chemical specificity that affect catalytic properties of inorganic catalysts. In terms of applications, the research will focus on understanding and controlling the synthesis and chemistry of novel inorganic, organic, and hybrid catalysts. New strategies for design of selective catalysts for fuel and chemical production from both fossil and renewable biomass feedstocks will be explored. Selective and low-temperature activation of alkanes, CO₂, and multifunctional molecules will continue to receive attention. Increased emphasis will be placed on the use of theory, spectroscopy and microscopy to probe and understand catalytic systems under realistic working conditions. Emphasis will also be placed on the investigation of catalytic mechanisms and pathways bond rearrangements under electrochemical and photoelectrochemical conversion of small as well as complex molecules into chemicals and fuels.

Subprogram Contact: Raul Miranda, (301) 903-8014, raul.miranda@science.doe.gov
Website: <http://www.sc.doe.gov/bes/csgb/catalysis.html>

(p) Separations and Analysis

This activity supports fundamental research covering a broad spectrum of separation concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, photodissociation, and complexation. Also supported is work to improve the sensitivity, reliability, and productivity of analytical determinations and to develop new approaches to analysis in complex, heterogeneous environments, including techniques that combine chemical selectivity and spatial resolution to achieve chemical imaging. This activity is the nation's most significant long-term investment in the fundamental science underpinning actinide separations and mass spectrometry. The overall goal is to obtain a thorough understanding, at molecular and nanoscale dimensions, of the basic chemical and physical principles involved in separations systems and analytical tools so that their full utility can be realized.

Separations research will continue to advance the understanding of multifunction separations media; supramolecular recognition (using designed, multi-molecule assemblies to attract specific target species); synthesis of new porous materials and control of interface properties at the nanoscale; ligand design and synthesis of extractant molecules; mechanisms of transport and fouling in polymer and inorganic membranes; solvation in supercritical fluids; field-enhanced mixing; and drop formation. Analytical research will pursue the elucidation of ionization and excitation mechanisms for optical and mass spectrometry; single molecule detection, characterization, and observation; nano- and molecular-scale analytical methods including biomolecules relevant to DOE's bioenergy interests; laser-based methods for high-resolution spectroscopy and for presentation of samples for mass spectrometry; characterization of interfacial phenomena, with emphasis on chromatography; surface-enhanced Raman

spectroscopy; and use of quadrupole ion traps to study gas-phase ion chemistry. This research will also pursue the underlying science needed to achieve true chemical imaging, i.e., the ability to selectively image selected chemical moieties at the molecular scale and to do so with temporal resolution that allows one to follow physical and chemical processes.

Subprogram Contact: William Millman, (301) 903-5805, william.millman@science.doe.gov
Website: <http://www.sc.doe.gov/bes/csgb/separations.html>

(q) Heavy Element Chemistry

This activity supports basic research in the chemistry of the heavy elements, including actinides and some fission products. The unique molecular bonding of the heavy elements is explored using theory and experiment to elucidate electronic and molecular structures, bond strengths, and chemical reaction rates. Additional emphasis is placed on the chemical and physical properties of actinides to determine solution, interfacial, and solid-state bonding and reactivity; on determining chemical properties of the heaviest actinide and transactinide elements; and on bonding relationships among the actinides, lanthanides, and transition metals.

Theoretical chemists predict the properties of actinides and transactinides in gaseous molecules, clusters in liquids, and solid species, using modern calculation tools such as density functional theory and sophisticated quantum mechanical calculations that include both spin-orbit and relativistic effects. Support of research to understand the chemical bonding of elements that have 5f electrons leads to fundamental understanding of separations processes and to the design and synthesis of preorganized chelating agents for the separations of particular actinide ions. Research in bonding, reactivity, and spectroscopic properties of molecules that contain heavy elements and of actinides in environmentally relevant species aids the development of ligands to sequester actinides in the environment and to remove toxic metals from the human body. Better characterization and modeling of the interactions of actinides at liquid-solid and liquid-liquid interfaces, including mineral surfaces under environmentally relevant conditions, improve separations processes that are essential for advanced nuclear fuel cycles.

Subprogram Contact: Larry Rahn, (301) 903-2508, larry.rahn@science.doe.gov
Website: http://www.sc.doe.gov/bes/csgb/heavy_element.html

(r) Geosciences Research

The Geosciences research activity supports basic experimental, theoretical and computational research in geochemistry and geophysics. Geochemical research emphasizes fundamental understanding of geochemical processes and reaction rates, focusing on aqueous solution chemistry, nanoscale geochemical processes, mineral-fluid interactions, and isotopic distributions and migration in natural systems. Geophysical research focuses on new approaches to understand the subsurface physical properties of fluids, rocks, and minerals and develops techniques for determining such properties at a distance. The activity includes improved small-scale imaging of chemical processes and properties using x-ray sources, neutron sources, and scanning microscopy, and improved large-scale imaging of physical processes and properties using seismic, electromagnetic and other sensing technology. Geosciences activities will link

physical and chemical investigations with improved analytical capabilities and with computational capabilities at the nano-, micro- and macro-scales to provide understanding of geoscience processes occurring at natural time and length scales. Because targeted topical research in Geosciences is funded by a number of applied programs across the Department priority in Basic Energy Sciences funding is placed on research that has multiple potential applications areas.

Subprogram Contact: Nicholas Woodward, (301) 903-4061, nick.woodward@science.doe.gov
Website: <http://www.sc.doe.gov/bes/csgb/geosciences.html>

(s) Solar Photochemistry

This activity supports molecular-level research on solar energy capture and conversion in the condensed phase and at interfaces. These investigations of solar photochemical energy conversion focus on the elementary steps of light absorption, electrical charge generation, and charge transport within a number of chemical systems, including those with significant nanostructured composition. Supported research areas include organic and inorganic photochemistry and photocatalysis, photoinduced electron and energy transfer in the condensed phase and across interfaces, photoelectrochemistry, and artificial assemblies for charge separation and transport that mimic natural photosynthetic systems.

In solar photochemistry, an increased emphasis on solar water splitting will explore new semiconductor and molecular systems for photoconversion. Also of emphasis are new hybrid systems that feature molecular catalysis at surfaces and new nanoscale structures for the photochemical generation of fuels. Modern combinatorial techniques will broaden and accelerate the search for new semiconductor and molecular structures. Novel quantum size structures, such as multiexciton generating quantum dots, hybrid semiconductor/carbon nanotube assemblies, fullerene-based linear and branched molecular arrays, and semiconductor/metal nanocomposites, will be examined that will allow for more complete and efficient use of the solar energy spectrum. Unresolved basic science issues in photocatalysis will be explored in coupling photoinduced charge separation to multielectron, energetically uphill redox reactions. Photoconversion systems will be investigated that are based on organic semiconductors and conducting polymers, which are inexpensive and easy to manufacture. An enhanced theory and modeling effort is needed for rational design of artificial solar conversion systems. Of particular interest is the calculation of factors controlling photoinduced long-range electron transfer, charge injection at the semiconductor/electrolyte interface, and photoconversion in biomimetic assemblies for solar photocatalytic water splitting.

Electron pulse radiolysis methods will investigate reaction dynamics, structure, and energetics of short-lived transient intermediates in the condensed phase. Fundamental studies on reactivity of nitrogen oxides in aqueous solution are pertinent to understanding radiolytic degradation of nuclear tank waste. Studies of solvent effects on free radical reaction rates in supercritical fluids are relevant to next-generation supercritical water-cooled nuclear power plants.

Solar Photochemistry does not fund research on device development or optimization.

Subprogram Contact: Mark Spitler, (301) 903-4568, mark.spitler@science.doe.gov

Website: <http://www.sc.doe.gov/bes/csgb/solar.html>

(t) Photosynthetic Systems

This activity supports basic research on the biological capture and conversion of solar energy to chemically stored forms of energy in living systems. Topics of study include light harvesting, exciton transfer, charge separation, transfer of reductant to carbon dioxide, as well as the biochemistry of carbon fixation, metabolism, and storage (e.g. Calvin-Benson cycle and RuBisCO) in plants and photosynthetic microbes. Additional areas of research include those involving strong intersection between biological sciences and energy-relevant chemical sciences and physics, such as in self-assembly of photosynthetic components, efficient photon capture and charge separation, predictive design of catalysts, and self-regulating/repairing systems. A greater understanding is also sought of the processes and mechanisms of biological energy transduction, including redox reactions and carbon storage in organic molecules and polymers.

Advances in “omics-based” technologies along with increased availability of plant genome sequences provide new opportunities to leverage the strengths of the Photosynthetic Systems program in molecular biology and biochemistry with powerful capabilities in imaging and computation. This will allow an unprecedented biophysical understanding of photosynthesis and related processes such as carbon fixation and metabolism and enable use of such knowledge for the development of bio-inspired, bio-hybrid, and biomimetic energy systems. Research will continue to examine the weak intermolecular forces governing molecular assembly in photosynthetic systems; characterize cofactor insertion into proteins and protein subunit assemblies in biological machinery; adapt combinatorial, directed evolution, and other screening methods to enhance fuel production in photosynthetic systems; investigate the structural and mechanistic features of photosynthetic complexes; and determine the physical and chemical rules that underlie biological mechanisms of repair and photo-protection.

Photosynthetic Systems does not fund research in: animal systems, prokaryotic systems related to human/animal health or disease, and device/process development or optimization.

All submitted applications must clearly state the energy relevance of the proposed research: How will the knowledge gained from the proposed work better our understanding of the ways plants, algae, and/or non-medical microbes capture, transduce, and store energy?

Subprogram Contact: Gail McLean, (301) 903-7807, gail.mclean@science.doe.gov

Website: <http://www.sc.doe.gov/bes/csgb/photosynthetic.html>

(u) Physical Biosciences

This activity supports basic research that combines experimental and computational tools from the physical sciences with biochemistry and molecular biology to increase understanding of the complex processes of energy transduction and storage in living systems. Areas of research include mechanisms by which energy transduction systems are assembled and maintained,

processes that regulate energy-relevant chemical reactions within the cell, the underlying biochemical and biophysical principles determining the architecture of biopolymers and the plant cell wall, and active site protein chemistries that provides a basis for highly selective and efficient bioinspired catalysts.

Future impact is, in general, envisioned through increased use of physical science and computational tools (ultrafast laser spectroscopy, current and future x-ray light sources, and quantum chemistry) to probe spatial and temporal properties of energy-relevant biological systems. Combined with efforts in molecular biology and biochemistry, this will give us an unprecedented architectural and mechanistic understanding of such systems and facilitate the use of such identified principles into the design of bio-inspired synthetic or semi-synthetic energy systems. The application of such tools to the detailed study of individual enzymes (and multi-enzyme complexes) will enable the design of improved industrial catalysts and processes (e.g. more cost-effective, highly-efficient, etc) through a more complete understanding of structure and mechanistic principles. One such priority area for the program is achieving a greater understanding of the active site chemistries of multi-electron redox reactions; of particular interest is carbon dioxide assimilation and reduction in the *Archaea*. A unique aspect of biological systems is their ability to self-assemble and self-repair. These capabilities occur via complex processes that are not well-understood, and enhanced efforts will be devoted to the identification of the underlying chemical/physical principles that govern such behaviors. Still another area of emphasis for the program lies in the application of these same tools to achieve a more detailed understanding of the structure – and dynamics – of complex plant and non-medical microbial systems such as cell walls, biological motors, and cytoskeletal and other assemblies involved in energy capture, transduction, and storage.

Physical Biosciences does not fund research in: animal systems, prokaryotic systems related to human/animal health or disease, and device/process development or optimization.

All submitted applications must clearly state the energy relevance of the proposed research: How will the knowledge gained from the proposed work better our understanding of the ways plants, algae and/or non-medical microbes capture, transduce, and store energy?

Subprogram Contact: Robert Stack, (301) 903-5652, robert.stack@science.doe.gov
Website: http://www.sc.doe.gov/bes/csgb/physical_biosciences.html

Scientific User Facilities

The Scientific User Facilities (SUF) Division supports the research and development, planning, construction, and operation of scientific user facilities for the development of novel nanomaterials and for materials characterization through x-ray, neutron, and electron beam scattering. These facilities provide unique capabilities to the scientific community and are a critical component of maintaining U.S. leadership in the physical sciences. The SUF Division

also supports research activities leading to the improvement of today's facilities, paving the foundation for the development of next generation facilities. The SUF research focus area for this funding opportunity announcement is listed below.

Website: <http://www.sc.doe.gov/bes/suf/index.html>

(v) BES Accelerator and Detector Research

The objective of these research activities is to improve the output and capabilities of synchrotron radiation light sources and neutron scattering facilities that are the most advanced of their kind in the world. This program supports basic research in accelerator physics and x-ray and neutron detectors. Research is supported that seeks to achieve a fundamental understanding beyond the traditional accelerator science and technology in order to develop new concepts to be used in the design of new accelerator facilities for synchrotron radiation and spallation neutron sources. Research on creating, manipulating, transporting, and diagnosing ultra-high brightness beams from their origin at a photocathode to propagation through undulators and studies on advanced seeding techniques are also supported. To exploit fully the fluxes delivered by synchrotron radiation facilities and spallation neutron sources, new detectors capable of acquiring data several orders of magnitude faster are required. Improved detectors are especially important in the study of multi-length scale systems such as protein- membrane interactions as well as nucleation and crystallization in nanophase materials. This program strongly interacts with BES programmatic research that uses synchrotron radiation and neutron sources.

Subprogram Contact: Eliane Lessner, (301) 903-9365, eliane.lessner@science.doe.gov

Website: <http://www.sc.doe.gov/bes/suf/index.html>

3. Biological and Environmental Research (BER)

Program Website: <http://www.sc.doe.gov/ober>

The Biological and Environment Research (BER) program mission is to understand complex biological, climatic, and environmental systems across spatial and temporal scales ranging from sub-micron to global, from individual molecules to ecosystems, and from nanoseconds to millennia. This is accomplished by exploring the frontiers of genome-enabled biology; discovering the physical, chemical, and biological drivers of climate change; and seeking the geochemical, hydrological, and biological determinants of environmental sustainability and stewardship.

The priority areas for BER include the following:

- Use systems biology approaches to understand enzymatic, microbial, and plant interactions for the conversion of biomass into liquid transportation fuels.
- Use advanced atmospheric measurements together with high-end computation and modeling to predict the impact of greenhouse gases on climate change.
- Model and measure the fate and transport of contaminants in the subsurface environment at DOE sites to predict contaminant flows.
- Develop new tools to explore the interface of biological and physical sciences.

The BER subprograms and their objectives follow:

(a) Biological Systems Science

Research is focused on using DOE's unique resources and facilities to develop fundamental knowledge of biological systems that can be used to address DOE needs in clean energy, carbon sequestration, and environmental cleanup and that will underpin biotechnology-based solutions to energy challenges. The major objectives are: (1) to develop the experimental and computational resources, tools, and technologies needed to understand and predict complex behavior of complete biological systems, principally plants, microbes and microbial communities or plant-microbe associations; (2) to take advantage of the remarkable high throughput and cost-effective DNA sequencing capacity at the national user facility, the Joint Genome Institute, to meet the DNA sequencing needs of the scientific community through competitive, peer-reviewed nominations for DNA sequencing; (3) to understand and characterize the risks to human health from exposures to low levels of ionizing radiation; (4) to operate experimental biological stations at synchrotron and neutron sources; and (5) to develop radiochemistry and advanced technologies for imaging and high through-put characterization and analysis for BER missions in bioenergy, subsurface, and climate change.

Subprogram Contact: Sharlene Weatherwax, (301) 903-3213,

sharlene.weatherwax@science.doe.gov

Website: http://www.science.doe.gov/ober/lmsd_top.html

(b) Climate and Environmental Sciences

The research seeks to understand the basic physical, chemical, and biological processes of the Earth's System and how these processes may be affected by energy production and use. The climate sciences research is designed to provide data to enable an objective, scientifically based assessment of the potential for, and the consequences of, human-induced climate change at global and regional scales. The activity also provides data and models to enable assessments of mitigation options to prevent such change. The research is comprehensive with emphasis on: (1) understanding and simulating the radiation balance from the surface of the Earth to the top of the atmosphere, including the effect of clouds, water vapor, trace gases, and aerosols. (The national user facility, the Atmospheric Radiation Measurement Climate Research Facility, provides key observational data to the climate research community on the radiative properties of the atmosphere, especially clouds and aerosols. This national user facility includes highly instrumented ground stations, a mobile facility, and an aerial vehicles program.); (2) enhancing and evaluating the quantitative models necessary to predict natural climatic variability and possible human- caused climate change at global and regional scales; (3) understanding and simulating the net exchange of carbon dioxide between the atmosphere, and terrestrial systems, as well as the effects of climate change on the global carbon cycle; (4) understanding impacts of climate change on ecosystems; (5) improving approaches to integrated assessments of effects of, and options to mitigate, climatic change; (6) environmental systems science research to understand the impact on and role of diverse terrestrial ecosystems on climate change, including the global carbon cycle; (7) subsurface biogeochemical research to understand and predict

subsurface contaminant fate and transport; and (8) research taking advantage of the national user facility, the Environmental Molecular Sciences Laboratory (EMSL) that houses an unparalleled collection of state-of-the-art capabilities, including a supercomputer and over 60 major instruments, providing integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences. EMSL also contributes to systems biology by providing leading edge capabilities in proteomics.

Subprogram Contact: Gary Geernaert, (301) 903-3281, Gerald.Geernaert@science.doe.gov
Website: http://www.science.doe.gov/ober/CCRD_top.html

4. Fusion Energy Sciences (FES)

Program Website: <http://www.science.doe.gov/ofes/>

The FES mission is to expand the fundamental understanding of matter at very high temperatures and densities and to develop the scientific foundations needed to develop a fusion energy source. This is accomplished by studying plasmas and their interactions with their surroundings under a wide range of temperature and density, developing advanced diagnostics to make detailed measurements of their properties, and creating theoretical and computational models to resolve the essential physics.

The priority areas for FES include the following:

- Advance the fundamental science related to magnetically confined burning plasmas and develop the predictive capability needed for a sustainable fusion energy source.
- Pursue fundamental research and scientific grand challenges in high energy density plasma science to explore the feasibility of inertial confinement for fusion energy systems and to discover the physical principles pertinent to matter at ultra-high pressures and temperatures more generally.
- Support development of the scientific understanding required to design and deploy the materials needed to support a burning plasma environment.
- Increase the fundamental understanding of basic plasma science, including low temperature plasma science and engineering, to inform the broader field and to create opportunities for innovative science-based applications.

An essential element of the FES program is the invention of advanced measurement techniques to ascertain the properties of plasma and its surroundings at a level required to test, challenge, and advance theoretical models. This validation forms the foundation of computational tools used to understand and predict the behavior of natural and man-made plasma systems, including burning plasmas for fusion energy.

The overarching FES goal is to develop the science needed to create a fusion energy source. This includes exploring basic issues in plasma science; developing the scientific basis and computational tools to predict the behavior, dynamics, and control of magnetically confined and inertially confined plasmas; using advances in tokamak research to begin investigating burning plasma physics; support the development of the scientific understanding required to design and deploy the materials needed to support a burning plasma environment; and developing the

cutting edge technologies that enable fusion facilities to achieve their scientific goals. These research areas allow us to better understand the nature of plasmas and their interactions with their environment wherever they exist, including naturally-occurring plasmas in space and on Earth, as well as man-made plasmas created in research facilities.

These activities require operation of a set of unique and diversified experimental facilities, including smaller-scale devices at universities involving individual principal investigators, larger national facilities that enable extensive domestic and international collaboration and even larger-scale experiments that require formal international partnerships to share the costs and integrate diverse scientific and engineering expertise. These facilities provide scientists with the means to test and extend theoretical understanding and computer models—leading ultimately to an improved predictive capability for fusion science. In addition, the FES program has developed a strong partnership with the Department of Energy’s National Nuclear Security Administration (NNSA) in High Energy Density Physics to take advantage of strong U.S. capabilities in inertial confinement fusion (ICF). The National Ignition Facility (NIF) is NNSA’s world-leading inertial confinement facility, which is expected to significantly advance the understanding of ICF for use as a potential energy source.

The FES long-term goal is to create an economical, abundant, and environmentally benign energy source by bringing the power of the sun and stars to Earth. Fusion energy holds the potential to provide virtually unlimited energy for mankind. FES is the U.S. participant in the construction and operation of the international ITER project. ITER, which will demonstrate a self-sustaining burning plasma for the first time, will provide an unparalleled scientific research opportunity and will test the scientific and technical feasibility of fusion power. ITER is the most significant step taken in over 25 years to advance the understanding of fusion plasmas and advance the global effort towards a feasible fusion energy source.

The specific long-term (10-year) goals for scientific advancement to which FES is committed and against which progress can be measured are:

- *Predictive Capability for Burning Plasmas*: Progress toward developing a predictive capability for key aspects of burning plasmas using advances in theory and simulation benchmarked against a comprehensive experimental database of stability, transport, wave-particle interaction, and edge effects.
- *Materials Science for Fusion Energy*: Progress toward developing plasma facing components, structural and special purpose materials, breeding blankets, and high-neutron-flux tolerant walls.
- *High Energy Density Plasma Physics*: Progress toward developing the fundamental understanding and predictability of high energy density laboratory plasmas.

To accomplish its mission and address the strategic goals described above, the FES program is organized into three subprograms—Science, Facility Operations, and Enabling R&D.

The FES subprograms and their objectives follow:

(a) FES Science and Facility Operations

The Science subprogram is developing a predictive understanding of plasma properties, dynamics, and interactions with surrounding materials. The emphasis is presently weighted towards understanding the plasma state relevant to stable magnetically confined fusion systems, but increasing emphasis is expected in the areas of plasma-material interaction physics and the materials science associated with the high heat and neutron fluxes that will be encountered in a burning plasma environment. Here is also addressed fundamental scientific questions on high-energy-density laboratory plasmas (HEDLP), nonneutral and single-component plasmas, ultracold plasmas, dusty plasmas, low-temperature plasmas, space and astrophysical plasma physics, plasma control and dynamics, plasma-related atomic and molecular physics, plasma diagnostic techniques, plasma sources, magnetic-field-line reconnection and self-organization, and plasma waves, turbulence, structures, and flows. Since these efforts are typically carried out in university environments, they also serve a critical function in educating and training scientific and technical personnel. Research is conducted on small to large-scale confinement devices to study physics issues relevant to fusion and plasma physics and to the production of fusion energy. The Facilities Operations subprogram includes efforts to build, operate, maintain, and upgrade the larger-scale facilities needed to carry out research on fusion energy science.

Subprogram Contact: Mark Koepke, (301) 903-4095, mark.koepke@science.doe.gov

Website: <http://www.science.doe.gov/ofes/>

(b) FES Enabling Research and Development

The Enabling Technology Research and Development (R&D) program supports the advancement of fusion science for both the near and long-term by carrying out research on technological topics that: (1) enable domestic experiments to achieve their full performance potential and scientific research goals; (2) permit scientific exploitation of the performance gains being sought from physics concept improvements; (3) allow the U.S. to enter into international collaborations, thus gaining access to experimental conditions not available domestically; (4) develop the technology and materials required for future fusion facilities; and (5) explore the science underlying these technological advances. Due to the harshness of the fusion environment and the significant challenge to overcome it, one of the four major goals of the FES program is to support the development of the scientific understanding required to design and deploy the materials needed to support a burning plasma environment. The Enabling Technology R&D program includes, but is not limited to, the following research topics: development of tungsten as a plasma facing material, plasma material interactions, fabrication, joining and cooling of plasma facing materials, development of both solid and liquid blanket concepts that can breed tritium and provide necessary heat transfer capabilities, and development of ferritic steels and oxide-dispersion strengthened steels as first wall structural materials.

Subprogram Contact: Gene Nardella, (301) 903-4095, gene.nardella@science.doe.gov

Website: <http://www.science.doe.gov/ofes/>

5. High Energy Physics (HEP)

Program Website: <http://www.science.doe.gov/hep>

The High Energy Physics (HEP) program's mission is to understand how the universe works at its most fundamental level, which is done by discovering the elementary constituents of matter and energy, probing the interactions between them, and exploring the basic nature of space and time.

HEP research extends the boundaries of our knowledge along three frontiers:

- The Energy Frontier: Use the highest-energy particle accelerators, discover as yet undetected elementary particles, elucidate their properties, and thereby advance our knowledge of the most fundamental forces of nature.
- The Intensity Frontier: Use high intensity particle beams and/or high precision, ultra-sensitive detectors, observe very rare events that help uncover the fundamental symmetries that govern the interactions of elementary particles or elucidate new phenomena.
- The Cosmic Frontier: Use the cosmos, not accelerators, to provide us with a wide variety of particles, from cold dark matter to ultra-high energy cosmic rays, and give us unique pathways to discover new particles, interactions, and impact on the evolution of the Universe. Additionally, HEP is responsible for stewarding a national accelerator science program with a strategy that is inclusive and cross-disciplinary.

Taken together, these interrelated and complementary discovery frontiers and the program of enabling technology research and development (R&D) offer the opportunity to answer some of the most basic questions about the world around us. All grant proposals should address specific research goals in one or more of these frontiers, or else explain how the proposed research or technology development supports the broad scientific objectives of the HEP program.

There are three broad areas within the Office of High Energy Physics that support research and technology development aimed at these objectives. New proposals should generally focus on one of these areas.

The HEP subprograms and their objectives follow:

(a) Experimental High Energy Physics Research

The experimental HEP research effort supports experiments utilizing man-made and naturally occurring particle sources to study fundamental particles and their interactions. This subprogram also provides graduate and postdoctoral research training for the next generation of scientists, equipment for experiments, and related computational support.

Topics studied in the experimental research program include, but are not limited to: proton-(anti)proton collisions at the highest possible energies; studies of neutrino properties using accelerator-produced neutrino beams as well as neutrinos from nuclear reactors; electron-

positron collisions at high intensities to make sensitive measurements of rarely occurring phenomena that can indicate new physics beyond the Standard Model; measurements of dark energy; and detection of the particles that make up cosmic dark matter.

Subprogram Contact: Glen Crawford, (301) 903-4829, glen.crawford@science.doe.gov
Website: http://www.science.doe.gov/hep/physics_research.shtm

(b) Theoretical High Energy Physics Research

The theoretical HEP research subprogram provides the vision and mathematical framework for understanding and extending the knowledge of particles, forces, space-time, and the universe. This subprogram also provides graduate and postdoctoral research training for the next generation of scientists and computational resources needed for theoretical calculations. Topics studied in the theoretical research program include, but are not limited to: phenomenological and theoretical studies that support the experimental research program, both in understanding the data and in finding new directions for experimental exploration; developing analytical and numerical computational techniques for these studies; and finding theoretical frameworks for understanding fundamental particles and forces at the deepest level possible.

Subprogram Contact: Glen Crawford, Phone (301) 903-4829, glen.crawford@science.doe.gov
Website: http://www.science.doe.gov/hep/physics_research.shtm

(c) HEP Advanced Technology Research and Development

The advanced technology R&D subprogram develops the next generation of particle accelerator and detector technologies for the future advancement of high-energy physics and other sciences, supporting world-leading research in the physics of particle beams and fundamental advances in particle detection. This subprogram also makes targeted investments in specialized or custom-built software and computing technologies in order to meet HEP research goals; and provides graduate and postdoctoral research training and equipment to support experiments and R&D activities.

This subprogram supports long-range, exploratory research aimed at developing new accelerator and detector concepts, as well as efforts which can significantly improve the cost, efficiency or efficacy of existing technologies. Topics studied in the accelerator R&D program include, but are not limited to: analytic and computational techniques for modeling particle beams; novel acceleration concepts; muon colliders and neutrino factories; the science of high gradients in room-temperature accelerating cavities; high-brightness beam sources; and cutting-edge beam diagnostic techniques. Topics studied in the detector R&D program include, but are not limited to: low-mass, high channel density charged particle tracking detectors; low-level photon detectors; high resolution, fast-readout calorimeters and particle identification detectors; improving the radiation tolerance of particle detectors; and advanced electronics and data acquisition systems.

Subprogram Contact: Michael Procaro, (301) 903-5228, michael.procaro@science.doe.gov
Website: http://www.science.doe.gov/hep/advanced_technology.shtm

6. Nuclear Physics (NP)

Program Website: <http://www.sc.doe.gov/np/>

The mission of the Nuclear Physics (NP) program is to discover, explore, and understand all forms of nuclear matter. The fundamental particles that compose nuclear matter—quarks and gluons—are relatively well understood, but exactly how they fit together and interact to create different types of matter in the universe is still largely not understood. To solve this mystery, NP supports experimental and theoretical research—along with the development and operation of particle accelerators and advanced technologies—to create, detect, and describe the different forms and complexities of nuclear matter that can exist in the universe, including those that are no longer found naturally.

The priority areas for NP include the following:

- Understand how nucleons—protons and neutrons—combine to form atomic nuclei and how these nuclei have emerged since the origin of the cosmos.
- Using particle accelerators, illuminate the structure of the nucleon—the core building block of matter; understand how quarks and gluons assemble to form matter’s core; and search for undiscovered forms of matter.
- Penetrate the respective mysteries surrounding the properties of the neutron and the neutrino.
- Conceive, construct, and operate national scientific user facilities.
- Steward isotope development, production, and technologies for research and applications.

To carry out its mission and address these priorities, the NP program focuses on three frontiers, Quantum Chromodynamics; Nuclei and Nuclear Astrophysics; and Fundamental Symmetries and Neutrinos. NP supports basic research in four subprograms: medium energy, heavy ion, and low energy nuclear physics, and nuclear theory (a through d). The program is the steward of the isotopes program for the nation (e) and supports the development of the tools and capabilities that make fundamental research possible (f).

The NP subprograms and their objectives follow:

(a) Medium Energy Nuclear Physics

The Medium Energy subprogram focuses primarily on questions having to do with Quantum Chromodynamics (QCD) and the behavior of quarks inside protons and neutrons. Specific questions that are being addressed include: *What is the internal landscape of the nucleons? What does QCD predict for the properties of strongly interacting matter? What governs the transition of quarks and gluons into pions and nucleons? What is the role of gluons and gluon self-interactions in nucleons and nuclei?* One major goal, for example, is to achieve an experimental description of the substructure of the proton and the neutron. The subprogram supports investigations into a few aspects of the second frontier, Nuclei and Nuclear Astrophysics, such as the question: *What is the nature of the nuclear force that binds protons and neutrons into stable nuclei?* The subprogram also examines aspects of the third area, Fundamental Symmetries and

Nuclei, including the questions: *Why is there now more visible matter than antimatter in the universe? What are the unseen forces that were present at the dawn of the universe, but disappeared from view as it evolved?* In pursuing these goals the Medium Energy subprogram supports different experimental approaches primarily at the Thomas Jefferson National Accelerator Facility and the Relativistic Heavy Ion Collider.

Subprogram Contact: W. B. Tippens, (301) 903-3904, brad.tippens@science.doe.gov
Website: <http://www.sc.doe.gov/np/>

(b) Heavy Ion Nuclear Physics

The Heavy Ion subprogram supports experimental research that investigates the frontier of Quantum Chromodynamics (QCD) by attempting to recreate and characterize new and predicted forms of matter and other new phenomena that might occur in extremely hot, dense nuclear matter and which have not existed since the Big Bang. This subprogram addresses what happens when nucleons "melt." QCD predicts that nuclear matter can change its state in somewhat the same way that ordinary matter can change from solid to liquid to gas. The fundamental questions addressed include: *What are the phases of strongly interacting matter, and what roles do they play in the cosmos? What governs the transition of quarks and gluons into pions and nucleons? What determines the key features of QCD, and what is their relation to the nature of gravity and spacetime?* Experimental research is carried out primarily using the U.S. Relativistic Heavy Ion Collider (RHIC) facility and the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN).

Subprogram Contact: G. Rai, (301) 903-4702, gulshan.rai@science.doe.gov
Website: <http://www.sc.doe.gov/np/>

(c) Low Energy Nuclear Physics

The Low Energy subprogram aims primarily at answering the overarching questions associated with the second frontier identified by NSAC- Nuclei and Nuclear Astrophysics. These questions include: *What is the nature of the nucleonic matter? What is the origin of simple patterns in complex nuclei? What is the nature of neutron stars and dense nuclear matter? What is the origin of the elements in the cosmos? What are the nuclear reactions that drive stars and stellar explosions?* Major goals of this subprogram are to develop a comprehensive description of nuclei across the entire nuclear chart, to utilize rare isotope beams to reveal new nuclear phenomena and structures unlike those that are derived from studies using stable nuclei, and to measure the cross sections of nuclear reactions that power stars and spectacular stellar explosions and are responsible for the synthesis of the elements. The subprogram also investigates aspects of the third frontier of Fundamental Symmetries and Neutrinos. Questions addressed in this frontier include: *What is the nature of the neutrinos, what are their masses, and how have they shaped the evolution of the universe? Why is there now more visible matter than antimatter in the universe? What are the unseen forces that were present at the dawn of the universe but disappeared from view as the universe evolved?* The subprogram seeks to measure, or set a limit

on, the neutrino mass and to determine if the neutrino is its own antiparticle. Experiments with cold neutrons also investigate the dominance of matter over antimatter in the universe, as well as other aspects of Fundamental Symmetries and Interactions.

Subprogram Contact: C. Baktash, (301) 903-0258, cyrus.baktash@science.doe.gov
Website: <http://www.sc.doe.gov/np/>

(d) Nuclear Theory (including the Nuclear Data subprogram)

The Nuclear Theory subprogram supports theoretical research at universities and DOE national laboratories with the goal of improving our fundamental understanding of nuclear physics, interpreting the results of experiments, and identifying and exploring important new areas of research. This subprogram addresses all three of the field's scientific frontiers described in NSAC's long range plan, which are Quantum Chromodynamics (QCD), Nuclei and Nuclear Astrophysics, and Fundamental Symmetries and Neutrinos, and the associated specific questions listed for the experimental subprograms above.

Theoretical research on QCD (the fundamental theory of quarks and gluons) addresses how the properties of the nuclei, hadrons, and nuclear matter observed experimentally arise from this theory, how the phenomena of quark confinement arises, and what phases of nuclear matter occur at high densities and temperatures. In Nuclei and Nuclear Astrophysics, theorists investigate a broad range of topics, including calculations of the properties of stable and unstable nuclear species, the limits of nuclear stability, the various types of nuclear transitions and decays, how nuclei arise from the forces between nucleons, and how nuclei are formed in cataclysmic astronomical events such as supernovae. In Fundamental Symmetries and Neutrinos, nucleons and nuclei are used to test the Standard Model, which describes the interactions of elementary particles at the most fundamental level. Theoretical research in this area is concerned with determining how various aspects of the Standard Model can be explored through nuclear physics experiments, including the interactions of neutrinos, unusual nuclear transitions, rare decays, and high-precision studies of cold neutrons.

Nuclear Theory activities at DOE also include the Nuclear Data subprogram, which compiles, maintains and distributes a database of information on nuclear properties and reactions that is of critical interest both to researchers and to developers of industrial applications of nuclear technology.

Subprogram Contact: G. Fai, (301) 903-8954, george.fai@science.doe.gov
Website: <http://www.sc.doe.gov/np/>

(e) Isotope Development and Production for Research and Applications

The Isotope Development and Production for Research and Applications subprogram supports the production and development of production techniques of radioactive and stable isotopes that are in short supply. The program provides facilities and capabilities for the production of research and commercial stable and radioactive isotopes, scientific and technical staff associated with general isotope research and production, and a supply of critical isotopes to address the

needs of the Nation. Isotopes are made available by using the Department's unique facilities, the Brookhaven Linear Isotope Producer (BLIP) at Brookhaven National Laboratory (BNL) and the Isotope Production Facility (IPF) at Los Alamos National Laboratory (LANL), of which the subprogram has stewardship responsibilities. The Program also coordinates and supports isotope production at a suite of university, national laboratory, and commercial accelerator and reactor facilities throughout the Nation to promote a reliable supply of domestic isotopes. Topics of interest include research that is focused on the development of advanced, cost-effective and efficient technologies for producing, processing, recycling and distributing isotopes in short supply. This includes innovative approaches to model and predict behavior and yields of targets undergoing irradiation in order to minimize target failures during routine isotope production. Integration of novel approaches to undergraduate and graduate training in radiochemistry and nuclear chemistry into proposed isotope R&D efforts is of interest.

Subprogram Contact: D. Phillips, (301) 903-7866, dennis.phillips@science.doe.gov
Website: <http://www.sc.doe.gov/np/>

(f) Accelerator Research and Development for Current and Future Nuclear Physics Facilities

The Nuclear Physics program supports a broad range of activities aimed at research and development related to the science, engineering, and technology of heavy-ion, electron, and proton accelerators and associated systems. Areas of interest include the R&D technologies of the Brookhaven National Laboratory's Relativistic Heavy Ion Collider (RHIC), with heavy ion and polarized proton beam; the development of an electron-ion collider (EIC); linear accelerators such as the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF); and development of devices and/or methods that would be useful in the generation of intense rare isotope beams for the next generation rare isotope beam accelerator facility (FRIB).

Subprogram Contact: M. Farkhondeh, (301) 903-4398,
manouchehr.farkhondeh@science.doe.gov
Website: <http://www.sc.doe.gov/np/>

7. Workforce Development for Teachers and Scientists

Program Website: <http://www.scied.science.doe.gov>

The mission of the Workforce Development for Teachers and Scientists (WDTS) program is to contribute to the national effort that will ensure that DOE and the Nation have a sustained pipeline of highly skilled and diverse science, technology, engineering, and mathematics (STEM) workers.

The priority areas for WDTS include the following:

- Increase participation of under-represented students and faculty in STEM education and careers, using opportunities afforded by the DOE national laboratories.

- Contribute to the development of STEM middle school through undergraduate educators through experiential-based programs at the DOE national laboratories.
- Provide mentored research experiences to undergraduate students and faculty through participation in the DOE research enterprise at the DOE national laboratories.
- Provide graduate fellowships for the pursuit of advanced degrees in scientific disciplines that prepare U.S. students for careers important to the Office of Science mission.

This program provides a continuum of opportunities to the Nation's STEM students and teachers/faculty in science, technology, engineering and mathematics (STEM) areas, including sponsorship of the National Science Bowl. WDTS funds undergraduate student internships, faculty and teacher fellowships and professional development programs at the DOE national laboratories. It also provides graduate fellowships for the pursuit of advanced degrees in scientific disciplines that prepare U.S. students for careers important to the Office of Science Mission. The goal of this program is to prepare a diverse workforce of scientists, engineers, and educators to keep America at the forefront of innovation, by utilizing its unique intellectual and physical resources to enhance the ability of educators and our Nation's educational systems to teach science and mathematics.

Program Contact: Ping Ge, (202) 287-6490, ping.ge@science.doe.gov
Website: <http://www.scied.science.doe.gov>

PART II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT.

DOE anticipates awarding both grants and cooperative agreements under this Funding Opportunity Announcement (FOA). If it is determined that a cooperative agreement is the appropriate award instrument, the nature of the Federal involvement will be included in a special award condition.

B. ESTIMATED FUNDING.

It is anticipated that approximately \$800 million will be available for all DOE Office of Science new, renewal, and supplemental grant and cooperative agreement awards in FY 2011, subject to the availability of FY 2011 funds. This FOA, DE-FOA-0000412, is for renewal and supplemental applications; a companion FOA, DE-FOA-0000411, exists for new applications.

The DOE is under no obligation to pay for any costs associated with the preparation or submission of an application. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this FOA.

C. MAXIMUM AND MINIMUM AWARD SIZE.

Ceiling (i.e., the maximum amount for an individual award made under this FOA):
None

Floor (i.e., the minimum amount for an individual award made under this FOA):
None

D. EXPECTED NUMBER OF AWARDS.

The number of awards is subject to availability of FY 2011 funds.

E. ANTICIPATED AWARD SIZE.

N/A

F. PERIOD OF PERFORMANCE.

N/A

G. TYPE OF APPLICATION.

DOE will accept only renewal and supplemental applications under this FOA.

RENEWAL APPLICATION INSTRUCTIONS.

Renewal applications are requests for additional funding for a period subsequent to that provided by a current award. Renewal applications compete with all other applications and must be submitted through Grants.gov at least **six months before** the scheduled expiration of the current award's project period. Earlier submission is **strongly encouraged** to allow for timely processing.

In preparing a renewal application, applicants should assume that reviewers will not have access to previous applications. The application should be developed as fully as though the applicant were applying for the first time. The application must include all the information required for a new project; additionally, the project narrative section should discuss the results from prior work.

Renewal applications must include the same forms and information categories as a new application, except for the following changes:

1. Include under the project description section information on any changes that affect the overall direction of the research being pursued.
2. Include an estimate of anticipated unexpended funds that will remain at the end of the current project period.
3. Include a progress report as a separate section that describes the results of work accomplished through the date of the renewal application and how such results relate to the activities proposed to be undertaken in the renewal period.

A renewal application generally will be subjected to the Office of Science merit review requirements. Should an application be approved and funded, the extended period of support is treated as an extension of the original project period.

Applicants should contact the appropriate DOE Program Manager or see the SC Program Website to determine if additional, program-specific guidance and/or limitations exist for the submission of renewal applications.

SUPPLEMENTAL APPLICATION INSTRUCTIONS.

Two types of supplemental applications may be submitted:

1. If the grantee is requesting support for a new task or activity to be added to the approved project, a supplemental application shall contain the same information categories as a new application. These applications will undergo merit review and will compete for funding with other new applications.

2. If the awardee needs additional funds:

- a. for increased costs that could not have been predicted when the application was originally approved; or
- b. to increase the "level of effort" or accelerate the project with no change to the project description as contained in the approved application.

A supplemental application, completed and submitted by the appropriate official, shall contain the following:

Forms as instructed in Grants.gov and an explanation of the need for the additional funding.

Applicants should contact the appropriate DOE Program Manager or see the SC Program Website to determine if additional, program-specific guidance and/or limitations exist for the submission of supplemental applications.

PART III - ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS.

All types of applicants are eligible to apply except other Federal agencies, Federally Funded Research and Development Center (FFRDC) Contractors, and non-profit organizations described in section 501(c)(4) of the Internal Revenue Code of 1986 that engaged in lobbying activities after December 31, 1995.

B. COST SHARING

Cost sharing is not required.

C. OTHER ELIGIBILITY REQUIREMENTS

N/A

PART IV – APPLICATION AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST APPLICATION PACKAGE.

Application forms and instructions are available at Grants.gov. To access these materials, go to <http://www.grants.gov>, select “Apply for Grants,” and then select “Download Application Package.” Enter the CFDA and/or the Funding Opportunity Announcement number located on the cover of this FOA and then follow the prompts to download the application package.

B. LETTER OF INTENT AND PRE-APPLICATION.

1. Letter of Intent.

Letters of Intent are not required.

2. Pre-Application.

Pre-Applications are not required.

C. CONTENT AND FORM OF APPLICATION – SF 424 (R&R).

You must complete the mandatory forms and any applicable optional forms (e.g., SF-LLL-Disclosure of Lobbying Activities) in accordance with the instructions on the forms and the additional instructions below. **Files that are attached to the forms must be in Adobe Portable Document Format (PDF) unless otherwise specified in this FOA.**

1. SF 424 (R&R).

Complete this form first to populate data in other forms. Complete all the required fields in accordance with the pop-up instructions on the form. The list of certifications and assurances referenced in Field 17 can be found on the DOE Financial Assistance Forms page at http://management.energy.gov/business_doe/business_forms.htm, under Certifications and Assurances.

2. RESEARCH AND RELATED Other Project Information.

Complete questions 1 through 6 and attach files. The files must comply with the following instructions:

Project Summary/Abstract (Field 7 on the Form)

The project summary/abstract must contain a summary of the proposed activity suitable for dissemination to publication. It should be a single page that identifies the name of the applicant, the project director/principal investigator(s), the project title, the objectives of the project, a description of the project, including methods to be employed, the potential impact of the project (i.e., benefits, outcomes), and major participants (for collaborative projects). This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must not exceed one page when printed single-

spaced with font not smaller than 11 point using standard 8.5” by 11” paper with one-inch margins (top, bottom, left and right). To attach a Project Summary/Abstract, click “Add Attachment.”

Project Narrative (Field 8 on the form)

There is no page limit to the project narrative. When printed with font not smaller than 11 point using standard 8.5” by 11” paper with one-inch margins (top, bottom, left and right). Do not include any Internet addresses (URLs) that provide information necessary to review the application because the information contained in these sites will not be reviewed. To attach a Project Narrative, click “Add Attachment.”

The application narrative should begin with a cover page that includes the project title along with the lead Principal Investigator’s name and complete contact information.

The first page of your narrative must also include the following information:

Applicant/Institution:

Street Address/City/State/Zip:

Principal Investigator (PI):

PI Postal Address:

PI Telephone Number:

PI Email:

Funding Opportunity Announcement Number: DE-FOA-0000412

DOE/Office of Science Program Office:

DOE/Office of Science Program Manager Contact:

DOE Grant Number (if Renewal or Supplemental Application):

Is this a Collaboration? If yes, please list ALL Collaborating Institutions/Pis and indicate which ones will also be submitting applications. Also indicate the PI who will be the point of contact and coordinator for the combined research activity.

Note that collaborating applications must be submitted separately.

The Project Narrative comprises the research plan for the project. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should indicate which project personnel will be responsible for which activities.

The project narrative must include:

Project Objectives

This section should provide a clear, concise statement of the specific objectives/aims of the proposed project.

Appendix 1: Biographical Sketch Appendix.

Provide a biographical sketch for the project director/principal investigator (PD/PI) and each senior/key person listed in Section A on the R&R Budget form. **Provide the biographical sketch information as an appendix to your project narrative. Do not attach a separate file.** The biographical information for each person must not exceed two pages when printed on 8.5” by 11” paper with one-inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include:

Education and Training. Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.

Research and Professional Experience: Beginning with the current position list, in chronological order, professional/academic positions with a brief description.

Publications. Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically.

Patents, copyrights and software systems developed may be provided in addition to or substituted for publications.

Synergistic Activities. List no more than five professional and scholarly activities related to the effort proposed.

Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers. Provide the following information in this section:

Collaborators and Co-editors: List in alphabetical order all persons, including their current organizational affiliation, who are, or who have been, collaborators or co-authors with you on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of this application. Also, list any individuals who are currently, or have been, co-editors with you on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of this application. If there are no collaborators or co-editors to report, state “None.”

Graduate and Postdoctoral Advisors and Advisees: List the names and current organizational affiliations of your graduate advisor(s) and principal postdoctoral sponsor(s) during the last five years. Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates during the past five years.

Appendix 2: Current and Pending Support.

Provide a list of all current and pending support (both Federal and non-Federal) for the Project Director/Principal Investigator(s) (PD/PI) and senior/key persons, including subawardees, for ongoing projects and pending applications. For each organization providing support, show the total award amount for the entire award period (including indirect costs) and the number of person-months per year to be devoted to the project by the senior/key person. **Provide the Current and Pending Support as an appendix to your project narrative. Do not attach a separate file.** Concurrent submission of an application to other organizations for simultaneous consideration will not prejudice its review.

Appendix 3: Bibliography & References Cited.

Provide a bibliography of any references cited in the Project Narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the application. **Provide the Bibliography and References Cited information as an appendix to your project narrative. Do not attach a separate file.**

Appendix 4. Facilities & Other Resources.

This information is used to assess the capability of the organizational resources, including subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. **Provide the Facility and Other Resource information as an appendix to your project narrative. Do not attach a separate file.**

Appendix 5: Equipment.

List major items of equipment already available for this project and, if appropriate identify location and pertinent capabilities. **Provide the Equipment information as an appendix to your project narrative. Do not attach a separate file.**

Appendix 6: Other Attachments.

If you need to elaborate on your responses to questions 1-5 on the “Other Project Information” document, **provide the information as an appendix to your project narrative. Do not attach a separate file.**

Do not attach any of the requested appendices described above as files for fields 9, 10, 11 and 12; instead follow the above instructions to include the information as appendices to the project narrative file.

3. RESEARCH AND RELATED BUDGET.

Complete the Research and Related Budget form in accordance with the instructions on the form (Activate Help Mode to see instructions) and the following instructions. You must complete a separate budget for each year of support requested. The form will generate a cumulative budget for the total project period. You must complete all the mandatory information on the form before the NEXT PERIOD button is activated. You may request funds under any of the categories listed as long as the item and amount are necessary to perform the proposed work, meet all the criteria for allowability under the applicable Federal cost principles, and are not prohibited by the funding restrictions in this FOA (See PART IV, G).

Budget Justification (Field K on the form).

Provide the required supporting information for the following costs (See R&R Budget instructions): equipment; domestic and foreign travel; participant/trainees; material and supplies; publication; consultant services; ADP/computer services; subaward/consortium/contractual; equipment or facility rental/user fees; alterations and renovations; and indirect cost type. Provide any other information you wish to submit to justify your budget request. **Attach a single budget justification file for the entire project period in Field K.** The file automatically carries over to each budget year.

4. R&R SUBAWARD BUDGET ATTACHMENT(S) FORM.

Budgets for Subrecipients, other than DOE FFRDC Contractors. You must provide a separate cumulative R&R budget for each subrecipient that is expected to perform work estimated to be more than \$100,000 or 50 percent of the total work effort (whichever is less). If you are selected for award, you must submit a multi-year budget for each of these subrecipients (See Section IV.D for submission of Subrecipients' multi-year budgets). Download the R&R Budget Attachment from the R&R SUBAWARD BUDGET ATTACHMENT(S) FORM and e-mail it to each subrecipient that is required to submit a separate budget. After the subrecipient has emailed its completed budget back to you, attach it to one of the blocks provided on the form. Use up to ten letters of the subrecipient's name (plus.xfd) as the file name (e.g., ucla.xfd or energyres.xfd).

5. PROJECT/PERFORMANCE SITE LOCATION(s).

Indicate the primary site where the work will be performed. If a portion of the project will be performed at any other site(s), identify the site location(s) in the blocks provided.

Note that the Project/Performance Site Congressional District is entered in the format of the two-digit state code followed by a dash and a three-digit Congressional district code, for example VA-001. Hover over this field for additional instructions.

Use the Next Site button to expand the form to add additional Project/Performance Site Locations.

6. SF-LLL DISCLOSURE OF LOBBYING ACTIVITIES.

If applicable, complete SF- LLL. Applicability: If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the grant/cooperative agreement, you must complete and submit Standard Form - LLL, "Disclosure Form to Report Lobbying."

Summary of Required Forms/Files

Your application must include the following documents:

Name of Document	Format	Attach to
SF 424 (R&R)	Form	N/A
RESEARCH AND RELATED Other Project Information	Form	N/A
Project Summary/Abstract	PDF	Field 7
Project Narrative, including required appendices	PDF	Field 8
RESEARCH & RELATED BUDGET	Form	N/A
Budget Justification	PDF	Field K
PROJECT/PERFORMANCE SITE LOCATION(S)	Form	N/A
SF-LLL Disclosure of Lobbying Activities, if applicable	Form	N/A

D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS.

If selected for award, DOE reserves the right to request additional or clarifying information for any reason deemed necessary, including, but not limited to:

- Indirect cost information
- Other budget information
- Name and phone number of the Designated Responsible Employee for complying with national policies prohibiting discrimination (See 10 CFR 1040.5)
- Representation of Limited Rights Data and Restricted Software, if applicable
- Commitment Letter from Third Parties Contributing to Cost Sharing, if applicable

E. SUBMISSION DATES AND TIMES.

1. Letter of Intent Due Date.

Letters of Intent are not required.

2. Pre-application Due Date.

Pre-applications are not required.

3. Application Due Date.

This FOA will remain open until September 30, 2011, 8:00 PM Eastern Time, or until it is succeeded by another issuance, whichever occurs first. This annual FOA DE-FOA-0000412 succeeds FOA DE-FOA-0000179, which was published December 4, 2009.

F. INTERGOVERNMENTAL REVIEW.

This program is not subject to Executive Order 12372, Intergovernmental Review of Federal Programs.

G. FUNDING RESTRICTIONS.

Cost Principles. Costs must be allowable in accordance with the applicable Federal cost principles referenced in 10 CFR part 600.

Pre-award Costs. Recipients may charge to an award resulting from this FOA pre-award costs that were incurred within the ninety (90) calendar day period immediately preceding the effective date of the award, if the costs are allowable in accordance with the applicable Federal cost principles referenced in 10 CFR part 600. Recipients must obtain the prior approval of the contracting officer for any pre-award costs that are for periods greater than this 90 day calendar period.

Pre-award costs are incurred at the applicant's risk. DOE is under no obligation to reimburse such costs if for any reason the applicant does not receive an award or if the award is made for a lesser amount than the applicant expected.

H. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS.

1. Where to Submit.

APPLICATIONS MUST BE SUBMITTED THROUGH GRANTS.GOV TO BE CONSIDERED FOR AWARD.

Submit electronic applications through the "Apply for Grants" function at www.Grants.gov. If you have problems completing the registration process or submitting your application, call Grants.gov at 1-800-518-4726 or send an email to support@grants.gov.

2. Registration Process.

You must COMPLETE the one-time registration process (all steps) before you can submit your first application through Grants.gov (See www.grants.gov/GetStarted). We recommend

that you start this process at least three weeks before the application due date. It may take 21 days or more to complete the entire process. Use the Grants.gov Organizational Registration Checklists at <http://www.grants.gov/assets/OrganizationRegCheck.pdf> to guide you through the process. **IMPORTANT:** During the CCR registration process, you will be asked to designate an E-Business Point of Contact (EBIZ POC). The EBIZ POC must obtain a special password called "Marketing Partner Identification Number" (MPIN). When you have completed the process, you should call the Grants.gov Helpdesk at 1-800-518-4726 to verify that you have completed the final step (i.e., Grants.gov registration).

You cannot submit an application through Grants.gov unless you are registered. Please read the registration requirements carefully and start the process immediately. Remember you have to update your CCR registration annually.

3. Application Receipt Notices

After an application is submitted, the Authorized Organization Representative (AOR) will receive a series of four e-mails. It is extremely important that the AOR watch for and save each of the emails. It may take up to two (2) business days from application submission to receipt of email Number 2. The titles of the four e-mails are:

Number 1 - Grants.gov Submission Receipt Number

Number 2 - Grants.gov Submission Validation Receipt for Application Number

Number 3 - Grants.gov Grantor Agency Retrieval Receipt for Application Number

Number 4 - Grants.gov Agency Tracking Number Assignment for Application Number

PART V - APPLICATION REVIEW INFORMATION

A. CRITERIA

1. Initial Review Criteria.

Prior to a comprehensive merit evaluation, DOE will perform an initial review in accordance with 10 CFR 605.10(b) to determine that (1) the applicant is eligible for the award; (2) the information required by the FOA has been submitted; (3) all mandatory requirements are satisfied; and (4) the proposed project is responsive to the objectives of the funding opportunity announcement. Applications that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

2. Merit Review Criteria

Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following evaluation criteria which are listed in descending order of importance codified at 10 CFR 605.10(d):

1. Scientific and/or Technical Merit of the Project;
2. Appropriateness of the Proposed Method or Approach;
3. Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
4. Reasonableness and Appropriateness of the Proposed Budget.

The evaluation process will include program policy factors such as the relevance of the proposed research to the terms of the FOA and the agencies' programmatic needs. Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

B. REVIEW AND SELECTION PROCESS.

1. Merit Review.

Applications that pass the initial review will be subjected to a formal merit review and will be evaluated based on the criteria codified at 10 CFR Part 605.10(d) in accordance with the guidance provided in the "Office of Science Merit Review System for Financial Assistance." This Merit Review System is available at: <http://www.sc.doe.gov/grants/merit.asp>.

2. Selection.

Selection Official Consideration: The Selection Official will consider the merit review recommendation, program policy factors, and the amount of funds available.

3. Discussions and Award.

Government Discussions with Applicant: The Government may enter into discussions with a selected applicant for any reason deemed necessary, including but not limited to: (1) the budget is not appropriate or reasonable for the requirement; (2) only a portion of the application is selected for award; (3) the Government needs additional information to determine that the recipient is capable of complying with the requirements in 10 CFR part 600 and 605; and/or (4) special terms and conditions are required. Failure to resolve satisfactorily the issues identified by the Government will preclude award to the applicant.

C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES.

DOE is striving to make **awards within six months**. The time interval begins on the date applications are due or the date the application is received, if there is no specified due date/deadline.

PART VI - AWARD ADMINISTRATION INFORMATION

A. AWARD NOTICES.

1. Notice of Selection.

Selected Applicants Notification: DOE will notify applicants selected for award. This notice of selection is not an authorization to begin performance. (See Part IV.G with respect to the allowability of pre-award costs.)

Non-selected Applicants Notification: Organizations whose applications have not been selected will be advised as promptly as possible. This notice will explain why the application was not selected.

2. Notice of Award.

An Assistance Agreement issued by the contracting officer is the authorizing award document. It normally includes, either as an attachment or by reference: 1. Special Terms and Conditions; 2. Applicable program regulations, if any; 3. Application as approved by DOE/NNSA; 4. DOE assistance regulations at 10 CFR Part 600; 5. National Policy Assurances to Be Incorporated As Award Terms; 6. Budget Summary; and 7. Federal Assistance Reporting Checklist, which identifies the reporting requirements.

For grants and cooperative agreements made to universities, non-profits, and other entities subject to OMB Circular 2 CFR, the Award also includes the Research Terms and Conditions located at <http://www.nsf.gov/bfa/dias/policy/rtc/index.jsp>

B. ADMINISTRATIVE AND NATIONAL POLICY REQUIREMENTS.

1. Administrative Requirements.

The administrative requirements for DOE grants and cooperative agreements are contained in 10 CFR 600 and 10 CFR Part 605 (See: <http://ecfr.gpoaccess.gov>). Grants and cooperative agreements made to universities, non-profits and other entities subject to Title 2 CFR are subject to the Research Terms and Conditions located on the National Science Foundation web site at <http://www.nsf.gov/bfa/dias/policy/rtc/index.jsp>.

DUNS and CCR Requirements

Additional administrative requirements for DOE grants and cooperative agreements are contained in 2 CFR, Part 25 (See: <http://ecfr.gpoaccess.gov>). Prime awardees must keep their data at CCR current. Subawardees at all tiers must obtain DUNS numbers and provide the DUNS to the prime awardee before the subaward can be issued.

Subaward and Executive Reporting

Additional administrative requirements necessary for DOE grants and cooperative agreements to comply with the Federal Funding and Transparency Act of 2006 (FFATA) are contained in 2 CFR, Part 170. (See: <http://ecfr.gpoaccess.gov>). Prime awardees must register with the new FSRS database and report the required data on their first tier subawardees. Prime awardees must report the executive compensation for their own executives as part of their registration profile in the CCR.

2. Special Terms and Conditions and National Policy Requirements.

Special Terms and Conditions and National Policy Requirements.

The DOE Special Terms and Conditions for Use in Most Grants and Cooperative Agreements are located at http://management.energy.gov/business_doe/business_forms.htm.

The National Policy Assurances to Be Incorporated As Award Terms are located at <http://www.nsf.gov/bfa/dias/policy rtc/appc.pdf>.

Intellectual Property Provisions.

The standard DOE financial assistance intellectual property provisions applicable to the various types of recipients are located at

http://www.gc.energy.gov/financial_assistance_awards.htm.

Statement of Substantial Involvement

Either a grant or cooperative agreement may be awarded under this FOA. If the award is a cooperative agreement, the DOE Contract Specialist and DOE Project Officer will negotiate a Statement of Substantial Involvement prior to award.

C. REPORTING.

Reporting requirements are identified on the Federal Assistance Reporting Checklist, DOE F 4600.2, attached to the award agreement.

PART VII - QUESTIONS/AGENCY CONTACTS

A. QUESTIONS

Questions regarding the content of the FOA must be submitted through the FedConnect portal. You must register with FedConnect to respond as an interested party to submit questions, and to view responses to questions. It is recommended that you register as soon after release of the FOA as possible to have the benefit of all responses. More information is available at https://www.fedconnect.net/FedConnect/PublicPages/FedConnect_Ready_Set_Go.pdf. DOE/NNSA will try to respond to a question within 3 business days, unless a similar question and answer have already been posted on the website. **Applications submitted through FedConnect will not be accepted.**

Questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@grants.gov. DOE cannot answer these questions.

B. AGENCY CONTACTS

Questions regarding the specific program areas/technical requirements should be directed to the point of contact listed for each program office within the FOA and not to the FOA Administrative Contact.

PART VIII - OTHER INFORMATION

A. MODIFICATIONS.

Notices of any modifications to this FOA will be posted on Grants.gov and the FedConnect portal. You can receive an email when a modification or an announcement message is posted by registering with FedConnect as an interested party for this FOA. It is recommended that you register as soon after release of the FOA as possible to ensure you receive timely notice of any modifications or other announcements. More information is available at <http://www.fedconnect.net>.

B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE.

DOE reserves the right, without qualification, to reject any or all applications received in response to this FOA and to select any application, in whole or in part, as a basis for negotiation and/or award.

C. COMMITMENT OF PUBLIC FUNDS.

The Contracting Officer is the only individual who can make awards or commit the Government to the expenditure of public funds. A commitment by other than the Contracting Officer, either explicit or implied, is invalid.

D. PROPRIETARY APPLICATION INFORMATION.

Patentable ideas, trade secrets, proprietary or confidential commercial or financial information, disclosure of which may harm the applicant, should be included in an application only when such information is necessary to convey an understanding of the proposed project. The use and disclosure of such data may be restricted, provided the applicant includes the following legend on the first page of the project narrative and specifies the pages of the application which are to be restricted:

“The data contained in pages _____ of this application have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes, provided that if this applicant receives an award as a result of or in connection with the submission of this application, DOE shall have the right to use or disclose the data herein to the extent provided in the award. This restriction does not limit the government’s right to use or disclose data obtained without restriction from any source, including the applicant.”

To protect such data, each line or paragraph on the pages containing such data must be specifically identified and marked with a legend similar to the following:

“The following contains proprietary information that (name of applicant) requests not be released to persons outside the Government, except for purposes of review and evaluation.”

E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL.

In conducting the merit review evaluation, the Government may seek the advice of qualified non-Federal personnel as reviewers. The Government may also use non-Federal personnel to conduct routine, nondiscretionary administrative activities. The applicant, by submitting its application, consents to the use of non-Federal reviewers/administrators. Non-Federal reviewers must sign conflict of interest and non-disclosure agreements prior to reviewing an application. Non-Federal personnel conducting administrative activities must sign a non-disclosure agreement.

F. INTELLECTUAL PROPERTY DEVELOPED UNDER THIS PROGRAM.

Patent Rights. The government will have certain statutory rights in an invention that is conceived or first actually reduced to practice under a DOE award. 42 U.S.C. 5908 provides that title to such inventions vests in the United States, except where 35 U.S.C. 202 provides otherwise for nonprofit organizations or small business firms. However, the Secretary of Energy may waive all or any part of the rights of the United States subject to certain conditions. (See “Notice of Right to Request Patent Waiver” in paragraph G below.)

Rights in Technical Data. Normally, the government has unlimited rights in technical data created under a DOE agreement. Delivery or third party licensing of proprietary software or data developed solely at private expense will not normally be required except as specifically negotiated in a particular agreement to satisfy DOE’s own needs or to insure the commercialization of technology developed under a DOE agreement.

G. NOTICE OF RIGHT TO REQUEST PATENT WAIVER.

Applicants may request a waiver of all or any part of the rights of the United States in inventions conceived or first actually reduced to practice in performance of an agreement as a result of this FOA, in advance of or within 30 days after the effective date of the award. Even if such advance waiver is not requested or the request is denied, the recipient will have a continuing right under the award to request a waiver of the rights of the United States in identified inventions, i.e., individual inventions conceived or first actually reduced to practice in performance of the award. Any patent waiver that may be granted is subject to certain terms and conditions in 10 CFR 784, <http://www.gc.doe.gov/documents/patwaiyclau.pdf>.

Domestic small businesses and domestic nonprofit organizations will receive the patent rights clause at 37 CFR 401.14, i.e., the implementation of the Bayh-Dole Act. This clause permits domestic small business and domestic nonprofit organizations to retain title to subject inventions. Therefore, small businesses and nonprofit organizations do not need to request a waiver.

H. NOTICE REGARDING ELIGIBLE/INELIGIBLE ACTIVITIES

Eligible activities under this program include those which describe and promote the understanding of science and technology but not those which encourage or support political activities such as the collection and dissemination of information related to potential, planned or pending legislation.

I. AVAILABILITY OF FUNDS.

Funds are not presently available for this award. The Government's obligation under this award is contingent upon the availability of appropriated funds from which payment for award purposes can be made. No legal liability on the part of the Government for any payment may arise until funds are made available to the Contracting Officer for this award and until the awardee receives notice of such availability, to be confirmed in writing by the Contracting Officer.