# FINANCIAL ASSISTANCE
# FUNDING OPPORTUNITY ANNOUNCEMENT

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

### FY 2012 Continuation of Solicitation for the
### Office of Science Financial Assistance Program

### Funding Opportunity Number: DE-FOA-0000600
### Announcement Type: Amendment
### CFDA Number: 81.049

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| **Amendment Issued:** | **10/7/2011** |
| **Issue Date:** | **9/30/2011** |
| **Letter of Intent Due Date:** | **Not Applicable** |
| **Pre-Application Due Date:** | **Not Applicable** |
| **Application Due Date:** | **Not Applicable**<br>This Funding Opportunity Announcement (FOA) will remain open until September 30, 2012 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 point of contact listed for each program area within this Funding Opportunity Announcement. |

This Funding Opportunity Announcement (FOA) was deleted from Grants.gov and reposted on October 7, 2011. A new Application Package (Forms) was posted at that time. The new Application Package is identical to the old one except it is encoded differently behind the scenes, so the information requested on the forms remains the same. Application Packages downloaded prior to October 7 will generate errors upon submission. If you downloaded the Application Package prior to October 7, please discard it, download a new Application Package, and use the new one for submitting your application. No other changes were made to this FOA on October 7. We apologize for the inconvenience.

## 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 Central Contract Registry (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 (i.e., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the CCR, register with the credential provider, and register with Grants.gov). To register with Grants.gov go to "Get Registered" at http://grants.gov/applicants/get_registered.jsp. 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

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# 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 area 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 Funding Opportunity Announcement (FOA), DE-FOA-0000600, is our annual, broad, open solicitation that covers all of the research areas in the Office of Science and is open throughout the Fiscal Year.

This FOA will remain open until September 30, 2012, 11:59 PM Eastern Time, or until it is succeeded by another issuance, whichever occurs first. This annual FOA DE-FOA-0000600 succeeds FOA DE-FOA-0000411 and FOA DE-FOA-0000412, which were published September 30, 2010.

## 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://science.energy.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 up 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) Research and Evaluation Prototypes
(e) 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 (AMOS)
(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) Magnetic Fusion Energy Science: ITER & Advanced Tokamak Optimization
(b) Magnetic Fusion Energy Science: Theory and Simulation
(c) Magnetic Fusion Energy Science: Targeted Validation Platforms
(d) High-Energy-Density Plasma Science
(e) General Plasma Science: Experiment and Theory
(f) Materials Science and Enabling Technologies for Fusion
(g) Diagnostic Development for Fusion and Plasma Science

**5. High Energy Physics (HEP)**
(a) Experimental Research at the Energy Frontier
(b) Experimental Research at the Intensity Frontier
(c) Experimental Research at the Cosmic Frontier
(d) Theoretical High Energy Physics Research
(e) Advanced Accelerator and Detector 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
(e) Nuclear Data and Nuclear Theory Computing
(f) Isotope Development and Production for Research and Applications
(g) 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://science.energy.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 computing systems and architectures, which will require numerous significant modifications to today's tools and techniques to deliver on the promise of Exascale science.

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 and numerical algorithms 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, including those solution methods that take into consideration the possibilities brought about by future HPC architectures; (2) optimization techniques and next-generation solvers; (3) numerical methods for modeling multiscale, multi-physics or multi-component continuous or discrete systems that span a wide range of time and length scales; (4) methods of simulation and analysis of systems that account for the uncertainties of the systems, or are inherently stochastic or uncertain; and (5) innovative approaches for analyzing and extracting insight from large-scale data sets.

Subprogram Contacts: Sandy Landsberg, (301) 903-8507, Sandy.Landsberg@science.doe.gov; and Karen Pao, (301) 903-5384, Karen.Pao@science.doe.gov
Website: http://science.energy.gov/ascr/research/applied-mathematics/

**(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 are:

- Methods for increasing application-level resilience, through theories and methods of error correction in an Exascale environment.
- Methods for improving productivity of application users and developers. Scientific workflow systems that support management of highly complex, multi-scale, multi-physics scientific simulations and analysis of the resulting data;
- Knowledge representation and machine learning for analysis of extreme scale scientific data from simulations and experiments; visual analysis of uncertainty and the sources thereof; techniques for comparative analysis of data sets; and scientific databases for extreme scale data.

Applications in this open FOA must explain their relevance to current Petascale and future Exascale high performance computing platforms as well as their relevance to the mission of the Office of Science. Research aimed at developing quantum computing, networking, computer-supported collaboration, social computing, natural language processing/understanding/ generation, generalized research in human-computer interaction and research which is only applicable to hand-held, portable, desktop, cluster or cloud computing are out of scope for this program.

Subprogram Contacts: Lenore Mullin, (301) 903-3113, Lenore.Mullin@science.doe.gov; Lucy Nowell, (301) 903-3191, Lucy.Nowell@science.doe.gov; and Sonia R. Sachs, (301) 903-0060, Sonia.Sachs@science.doe.gov
Website: http://science.energy.gov/ascr/research/computer-science/

**(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 Contacts:
Randall Laviolette, (301) 903-5195, Randall.Laviolette@science.doe.gov;
Steven Lee, (301) 903-5710, Steven.Lee@science.doe.gov; and
Ceren Susut, (301) 903-0366, Ceren.Susut-Bennett@science.doe.gov
Website: http://science.energy.gov/ascr/research/scidac/

**(d) Research and Evaluation Prototypes**

This subprogram supports projects that will provide the ASCR research community with an opportunity to experiment with cutting-edge Exascale computer node architectures, specifically processor and memory technologies and associated software environments. This area will support partnerships with vendors to accelerate and influence the development of critical technologies for Exascale computing. It is a requirement that the proposed technologies have a viable product path from a research team that has a proven track record for developing research projects that transition to commercial products.

Subprogram Contact: William Harrod, (301) 903-5800, William.Harrod@science.doe.gov.
Website: http://science.energy.gov/ascr/facilities/rep/

**(e) Network Environment Research**

This program element focuses on research activities in high-performance networks and scientific collaboration to support distributed science. The current program priorities are in two major areas: a) federated end-to-end terabit networks and b) highly extensible scientific collaborations.

**End-to-End Terabit Networks**. The focus of this effort is on the research and development of high-speed network protocols, algorithms, tools and services that effectively utilize multiple 100 Gbps links in backbone networks and allow distributed high-end science applications to achieve a significant fraction of this network capacity in the end systems. Potential activities to achieve this objective include but are not limited to: a) advanced technologies built on MPLS, GMPLS, OSCARS, and OpenFlow to enable dynamic multi-layer networking capabilities such on-demand circuits, bandwidth reservation, on-demand protection, and hybrid (packet/circuit) networking across multiple domains; b) advanced data transfer toolkits and services that can be dynamically optimized and configured for a wide range of transport network technologies to deliver 100 Gbps throughput to science applications; c) advanced tools and services to perform

end-to-end performance monitoring and fault diagnosis; and d) Intelligent network management and control systems such as resources brokers/co-schedulers, end-to-end performance monitoring and fault diagnosis, and end-systems traffic shaping.

**Highly Extensible Scientific Collaborations**. This effort focuses on scientific collaboration systems for extreme-scale science. The current interest is on effective collaborative systems for distributed data-intensive science and multi-scale computing ecosystems which range from mid-range to Exascale computing. These include but are not limited to a) innovative concepts, methodologies, frameworks, tools and services that enable large multi-disciplinary teams in multi-institutions to collaborate effectively; b) innovative collaboration tools for data –intensive science frameworks and tools such as domain-science data architectures (data semantic, data placement, data discoveries, self-describing data, workflows, etc); c) Scalable and secure tools and services to support concurrent and real-time collaboration activities; and d) new techniques, frameworks, and services to enable remote/concurrent scientific visualization, remote computational steering, and tele-operation of scientific instruments.

Subprogram Contacts: Richard Carlson, (301) 903-9486, Richard.Carlson@science.doe.gov; and Thomas Ndousse-Fetter, (301) 903-9960, Thomas.Ndousse-Fetter@science.doe.gov
Website: http://science.energy.gov/ascr/research/next-generation-networking/

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

**2. Basic Energy Sciences (BES)**
Program Website: http://science.energy.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 BES divisions, program areas, 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 program areas listed below.

Website: http://science.energy.gov/bes/mse/

**(a) Materials Chemistry**

This activity supports fundamental research in the 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. Research to understand carbon capture phenomena will focus on kinetics and environments that include contaminants found in flue gases, with specific emphasis on the discovery and design of new materials tuned for optimum separation properties; understanding and controlling the atomic and molecular level interactions of the targeted species with the separation media; and tailored capture/release processes with alternative driving forces. 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: Michael Sennett, (301) 903-6051, michael.sennett@science.doe.gov
Website: http://science.energy.gov/bes/mse/research-areas/materials-chemistry/

**(b) Biomolecular Materials**

This activity supports fundamental 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://science.energy.gov/bes/mse/research-areas/biomolecular-materials/

**(c) Synthesis and Processing Science**

This activity supports fundamental 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://science.energy.gov/bes/mse/research-areas/synthesis-and-processing-science/

**(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 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 and 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://science.energy.gov/bes/mse/research-areas/experimental-condensed-matter-physics/

**(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 Davenport, (301) 903-0035 james.davenport@science.doe.gov
Website: http://science.energy.gov/bes/mse/research-areas/theoretical-condensed-matter-physics/

**(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), 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://science.energy.gov/bes/mse/research-areas/physical-behavior-of-materials/

**(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, as well as utilizing newly developed and more powerful parallel computational platforms and 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://science.energy.gov/bes/mse/research-areas/mechanical-behavior-and-radiation-effects/

**(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 tabletop laser sources.

Subprogram Contact: Lane Wilson, (301) 903-5877, lane.wilson@science.doe.gov
Website: http://science.energy.gov/bes/mse/research-areas/x-ray-scattering/

### (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.

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### (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.

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**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://science.energy.gov/bes/csgb/

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

This activity supports experimental and theoretical research aimed at understanding the structural and dynamical properties of atoms, molecules and nanostructures. The research emphasizes fundamental interactions of these systems with photons and electrons to characterize and control their behavior. The goal is to develop accurate quantum mechanical descriptions of dynamical processes such as chemical bond breaking and forming, interactions in strong fields, electron correlation, ultracold chemistry, and light-matter interactions in nanoscale structures. Topics of interest include the development and application of novel, ultrafast optical probes of matter; the interactions of atoms and molecules with intense electromagnetic fields; and studies of collisions and highly correlated interactions in atomic and molecular systems. The AMOS activity will continue to support science that advances DOE and BES mission priorities. Closely related experimental and theoretical efforts will be encouraged. AMOS will continue to have a prominent role at BES facilities in understanding the interaction of intense x-ray pulses with matter and in the control and investigation of ultrafast light-matter interactions. Key targets for greater investment include ultrafast electron diffraction, attosecond science, electron-driven processes, and quantum control of molecular systems.

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.

The program emphasizes ultrafast, ultra-intense, short-wavelength science, and correlated dynamics in atoms and molecules. Examples include the use of high-harmonic generation or its variants as soft x-ray sources, intense, ultrafast x-ray science at the Linac Coherent Light Source (LCLS), and development and characterization of femtosecond and attosecond pulses of x-rays at synchrotrons as well as accelerator-based and table-top sources. Applications of these light sources include ultrafast imaging of chemical reactions, diffraction and harmonic generation from aligned molecules, and atomic and molecular inner-shell photoionization. Control of nonlinear optical processes and tailoring of quantum mechanical wave functions with lasers will continue to be of interest, particularly in molecular systems. Theoretical advances are enabling modeling and simulation of increasingly complex systems to provide interpretation of existing

data, and predictions for new experiments. These experimental and theoretical 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. Experimental and theoretical tools also will be used in the study of low-energy electron-molecule interactions in the gas and condensed phases, and collisions of ultracold molecules.

The AMOS program does not support research in quantum information science, ultracold quantum gases, condensates, or plasmas.

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Website: http://science.energy.gov/bes/csgb/research-areas/atomic-molecular-and-optical-science/

**(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 and 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 toward 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.

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**(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 ineractions, 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.

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**(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 understanding 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 research is toward 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. Future emphasis includes the need to probe the chemical physics of energy transfer and reactivity 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 CPIMS program does not fund research in bulk fluid dynamics, such as studies of laminar or turbulent flows. In addition, the program does not support applications such as micro-scale devices, and the CPIMS program does not support research on molecules or cells that is directed toward medical applications.

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**(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 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, $CO_2$, and multifunctional molecules will continue to receive attention. Increased emphasis will be placed on the use of theory, intense-radiation-source spectroscopy, microscopy and ultrafast techniques 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.

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**(p) Separations and Analysis**

This activity supports fundamental research to advance understanding and control of the atomic and molecular interactions between target species and separations media associated with a broad spectrum of new or improved separation concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, and complexation. Also supported is work to improve the sensitivity, reliability, and productivity of analytical determinations and to the development of new approaches to analysis in complex, heterogeneous environments, including techniques that combine chemical selectivity and spatial and temporal resolution to achieve chemical imaging. The separations and analysis activity is inspired by the common, and often tightly coupled, fundamental underpinnings associated with a wide range of energy related chemical recognition, separation, and analysis problems. These problems include those arising in the development, processing and utilization of current and future fuels, including emerging carbon capture requirements, and the production of strategic energy-relevant materials. The overall goal is to obtain a predictive understanding, at molecular and nanoscale dimensions, of the basic chemical and physical principles involved in separations systems and analytical tools so that innovative approaches to these problems may be discovered and advanced.

Separations research will continue to seek innovative science involving multifunction separations media; supramolecular recognition (using designed, multi-molecule assemblies to attract specific target species); synthesis of new porous/hierarchical materials, understanding and control of interface properties at the molecular/nanoscale; ligand design and synthesis of extractant molecules; mechanisms of transport and fouling in polymer and inorganic membranes; and relevant solvation in supercritical and ionic liquids. Analytical research will pursue the elucidation of ionization, ion chemistry, 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; and laser and tip-enhanced methods for high-resolution spectroscopy and for presentation of samples for mass spectrometry. This research will also pursue the underlying science needed to achieve true chemical imaging, i.e., the ability to image selected chemical moieties at the molecular scale and to do so with temporal resolution that allows one to follow physical and chemical processes relevant to energy science.

This activity does not support engineering or scale up of particular processes or devices. Research that is directed toward medical applications is not supported.

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Website: http://science.energy.gov/bes/csgb/research-areas/separations-and-analysis/

**(q) Heavy Element Chemistry**

The mission of the Heavy Element Chemistry (HEC) program is to support basic chemical research of the heavy elements, focusing primarily on the actinides (elements with atomic numbers from 89 to 103 – actinium through lawrencium), but also including some fission products and the transactinide elements (the elements beyond lawrencium). Modern experimental techniques and relativistic quantum theory are utilized to explore the unique molecular bonding of these heavy elements, their reaction thermodynamics, and their reaction kinetics in order to understand the underlying chemical and physical principles that determine the behavior of these elements. Knowledge of the chemical characteristics of materials that incorporate actinides and fission-products, under realistic conditions, provides a basis for advanced fission fuel cycles. Fundamental understanding of the chemistry of these long-lived radioactive species is required to accurately predict and mitigate their transport and fate in environments associated with the storage of radioactive wastes.

The role of 5f electrons in bond formation remains the major fundamental topic in actinide chemistry. As most actinide species have partly-filled 5f electron subshells and all have highly charged nuclei, simple models cannot be extrapolated to the heavy elements. Resolving the role of the 5f-electrons is one of the grand challenges identified by the Department of Energy. Efforts aimed at implementing quantum-mechanical theories that allow more quantitative treatments of spin-orbit interactions and relativistic effects are necessary in order to better understand the role of the 5f-electrons. Determining the chemical behavior of the actinide and transactinide elements

assists the development and validation of computer codes at the extreme limits of the periodic table and can expand our ability to predict actinide and fission product chemical behavior under conditions relevant to all stages of fuel reprocessing and environmental remediation.

Improved modeling of actinide transport requires an understanding of the processes describing sorption on surfaces such as colloidal particles. Greater understanding of chemical bonding, reactivity, and spectroscopic properties of molecules that contain actinides in environmentally relevant species leads to a more fundamental understanding of separations processes and aids the development of ligands to sequester actinides in the environment.

This program directly addresses the training of undergraduates, graduate students, and postdoctoral researchers in radiochemistry at national laboratories and universities. This is a specific challenge the nation faces now and in the immediate future.

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Website: http://science.energy.gov/bes/csgb/research-areas/heavy-element-chemistry/

**(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.

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Website: http://science.energy.gov/bes/csgb/research-areas/geosciences/

**(s) Solar Photochemistry**

This activity supports fundamental, 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, charge separation, and charge transport within a number of chemical systems, including those with significant nanostructured composition. Although the long term mission of this Program is an understanding

of the science behind solar-driven production of fuels and electricity, it is recognized that fundamental research in the interaction of light, matter and electrons in these systems is essential to the achievement of Program goals.

Supported research areas include organic and inorganic photochemistry, catalysis and photocatalysis, and 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. An enhanced theory and modeling effort is needed for rational design of these artificial solar conversion systems.

Among the challenges for catalytic fuels production, knowledge gained in charge separation and electron transfer needs to be applied in a meaningful way to activation of small molecules including, among others, $CO_2$ in its reduction to fuels and $H_2O$ in its oxidation or reduction via transformative catalytic cycles. This spans the range from dark catalytic reactions to those driven by the energy of an absorbed photon and in both homogeneous and heterogeneous environments. The major scientific challenge for photoelectrochemical energy conversion for fuel generation is that small band gap semiconductors capable of absorbing solar photons are susceptible to oxidative degradation, whereas wide band gap semiconductors, which are resistant to oxidative degradation in aqueous media, absorb too little of the solar spectrum. Also of emphasis are new hybrid systems that feature molecular catalysis at solid surfaces and new nanoscale structures for the photochemical generation of fuels.

Research areas concerned with separation of charge that might result in electricity include multi-bandgap, multilayer cascade-type semiconductors, photosensitized nanoparticulate solids, and the study of the mechanism of multiple exciton generation within nanoparticles. There are also challenges in fundamental understanding of photoconversion processes – energy transfer and the generation, separation, and recombination of charge carriers – in organic-based molecular semiconductors, which could lead to a new type of inexpensive and flexible solar cell

Another regime of chemistry initiated through creation of high energy excited states is highly ionizing radiation, as can be produced through electron pulse radiolysis, to investigate reaction dynamics, structure, and energetics of short-lived transient intermediates in the condensed phase. Among many topics, fundamental research is of interest in areas which have a long term impact upon the understanding of radiolytic degradation of nuclear tank waste, the reactivity of solid surfaces in reactor coolant systems, and the chemistry of reagents used in separations processes in nuclear cycles.

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

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Website: http://science.energy.gov/bes/csgb/research-areas/solar-photochemistry/

**(t) Photosynthetic Systems**

This activity supports basic research on the biological capture and conversion of solar energy to chemically stored forms of energy in plants, algae, and photosynthetic microbes. 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). Also of interest are studies to increase understanding of the processes and mechanisms of biological energy transduction and storage, such as redox reactions and carbon storage in organic molecules and polymers. Research involving strong intersection between biological sciences and energy-relevant chemical sciences and physics is particularly encouraged, such as in self-assembly of photosynthetic components, efficient photon capture and charge separation, and self-regulating/repairing systems.

Such research will lead to increased understanding and control of the weak intermolecular forces governing molecular assembly in photosynthetic systems; knowledge of the biological machinery for cofactor insertion into proteins and protein subunit assemblies; adaptation and use of combinatorial, directed evolution, and other methods to enhance energy production in photosynthetic systems; characterization of the structural and mechanistic features of photosynthetic complexes; and discovery of the physical and chemical rules that underlie biological mechanisms of repair and photo-protection. The strengths of the Photosynthetic Systems program in biochemistry and molecular biology combined with advances in powerful technologies, such as imaging and computation/modeling, will allow an unprecedented biophysical understanding of photosynthesis and related processes such as carbon fixation and metabolism. Such fundamental knowledge, in turn, can provide important insights and strategies for the future development of bio-inspired, bio-hybrid, and biomimetic energy systems.

Photosynthetic Systems does not fund research: 1) in prokaryotic systems related to human/animal health or disease; 2) on development or optimization of devices/processes; or 3) on development or optimization of microbial strains or plant varieties for biofuel/biomass production. Projects should ideally be hypothesis-driven. Projects that develop or rely solely on high-throughput screening approaches will not be supported.

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?

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Website: http://science.energy.gov/bes/csgb/research-areas/photosynthetic-systems/

**(u) Physical Biosciences**

This activity supports basic research that combines the tools from the physical sciences with biochemistry and molecular biology approaches to further our understanding of the ways plants and/or non-medical microbes capture, transduce, and store energy. Research supported includes studies that investigate mechanisms by which energy transduction systems are assembled and maintained, the 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 biological systems. For instance, the application of such tools to the 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*. Another 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: 1) in prokaryotic systems related to human/animal health or disease; 2) on development or optimization of devices/processes; or 3) on development or optimization of microbial strains or plant varieties for biofuel/biomass production. Projects should ideally be hypothesis-driven. Projects that develop or rely primarily on high-throughput screening approaches will not be supported.

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?

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Website: http://science.energy.gov/bes/csgb/research-areas/physical-biosciences/

**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 announcement is listed below.

Website: http://science.energy.gov/bes/suf/

**(v) BES Accelerator and Detector Research**

Research areas include ultrashort (attosecond) free electron laser (FEL) pulses, new seeding techniques and other optical manipulations to improve performance of next generation FELs, and very high frequency laser photocathodes which can influence the design of linac-based FELs at

high repetition rates. Research includes studies on creating, manipulating, transporting, and performing diagnostics of ultrahigh brightness beams, studies of properties of cathodes materials and factors that limit cathode lifetime, and modeling of ultrashort beam dynamics.

Detector research is a crucial component in the optimal utilization of user facilities. The emphasis is on research leading to new and more effective generation of photon and neutron detectors. 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 area strongly interacts with BES research divisions that use synchrotron radiation and neutron sources.

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Website: http://science.energy.gov/bes/suf/accelerator-and-detector-research/

**3. Biological and Environmental Research (BER)**
Program Website: http://science.energy.gov/ber/

The Biological and Environmental Research (BER) program addresses diverse and critical global challenges, from the sustainable and affordable production of renewable biofuels in an environmentally conscientious manner to understanding and predicting how climate change depends on natural and anthropogenic greenhouse gas emissions. These practical arguments and challenges are driven by a foundation of scientific knowledge and inquiry in atmospheric chemistry and physics, ecology, biology, and biogeochemistry.

The BER subprograms and their objectives follow:

**(a) Biological Systems Science**

The BER science portfolio includes research programs and scientific user facilities that examine 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. BER research explores the inner workings of a wide diversity of microbes and plants to understand how biological systems function, how they interact with each other, and how they can be manipulated to harness their processes and products. By starting with an organism's DNA, BER-funded scientists seek to understand whole biological systems as the systems respond to and modify their environments. The biological systems that BER scientists investigate span organization scales ranging from individual molecular components such as proteins, multi-component molecular machines, interconnected metabolic and regulatory networks within cells, interactive communities of cells or organisms, and intact ecosystems.

The major objectives are:

1. to develop systems biology approaches leading to the predictive understanding of functional properties of microbes, plants, multispecies communities, and intact ecosystems. This provides the foundational knowledge enabling advanced bioenergy

solutions, understanding microbial processes mediating transformation of environmental contaminants, and delineating key biological mechanisms involved in carbon cycling in terrestrial ecosystems;
2. to develop radiochemistry synthetic and advanced technologies for imaging and high through-put characterization and analysis of plants and microbes;
3. to understand the integrated gene function and response of biological systems to low dose radiation exposure;
4. to provide high-throughput genome sequencing and analysis at the national user facility, the Joint Genome Institute; and
5. to facilitate biological structure-function analyses at experimental biological stations at synchrotron and neutron sources.

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**(b) Climate and Environmental Sciences**

BER plays a vital role in supporting research on atmospheric processes, climate change modeling, interactions between ecosystems and greenhouse gases (especially carbon dioxide, $CO_2$), and analysis of impacts and interdependencies of climatic change with energy production and use. Understanding the Earth's radiant energy balance associated with clouds, aerosols, and atmospheric greenhouse gases represent the largest uncertainty in determining the rate of global climate change. BER supports research on the factors determining that balance—the role of different types of clouds, atmospheric particles, and greenhouse gases. BER also supports research to understand the impacts of climatic change—warmer temperatures, changes in precipitation, increased levels of greenhouse gases, changing distributions of weather extremes—on different ecosystems such as forests, grasslands, and farmland. Finally, the Earth's subsurface is critical in understanding the role that biogeochemical processes play in controlling the cycling and mobility of materials in the subsurface and across key surface-subsurface interfaces in the environment.

The major objectives are:
1. to understand and simulate the processes and dynamics governing the atmosphere's cloud and aerosol characteristics, and radiation balance, by exploiting the unique observational capabilities of the Atmospheric Radiation Measurement (ARM) Climate Research Facility;
2. to enhance and evaluate the earth system models necessary to predict natural climatic variability and quantify the role of human- caused forcing of climate change at global and regional scales;
3. to understand and simulate the net exchange of carbon dioxide between the atmosphere and terrestrial systems, as well as quantifying the effects of climate change on the global carbon cycle;
4. to understand interactions and interdependencies between climate change on ecosystems, from regional to global scales, and improve approaches to assess effects of, and options to mitigate, climatic change;

5. to support subsurface biogeochemical research to understand and predict the fate and transport of subsurface contaminants;
6. to support research taking advantage of the national user facility, the Environmental Molecular Sciences Laboratory (EMSL), providing integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences.

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Website: http://science.energy.gov/ber/research/cesd/

**4. Fusion Energy Sciences (FES)**
Program Website: http://science.energy.gov/fes/

The Fusion Energy Sciences (FES) mission is to expand the fundamental understanding of matter at very high temperatures and density and to build the scientific foundation needed to develop a fusion energy source. This is accomplished by studying plasma and its interactions with its surroundings across wide ranges of temperature and density, developing advanced diagnostics to make detailed measurements of its properties and dynamics, and creating theoretical and computational models to resolve the essential physics principles.

To accomplish its mission, the FES program is organized into three subprograms. The Science subprogram is developing a predictive understanding of plasma properties, dynamics, and interactions with surrounding materials. It encompasses magnetic fusion energy science, high energy density laboratory plasma science, plasma-material interactions, and general plasma science. The Facility Operations subprogram includes efforts to build, operate, maintain, and upgrade the large facilities needed to carry out research on fusion energy science. It also includes funding for the U.S. share of the ITER project. The Enabling R&D subprogram supports research to optimize and control plasma states in the laboratory, increasing the scientific output of present experiments and the likelihood of success of future fusion facilities.

FES has four strategic goals:

- Advance the fundamental science of magnetically confined plasmas to develop the predictive capability needed for a sustainable fusion energy source;
- Support the development of the scientific understanding required to design and deploy the materials needed to support a burning plasma environment;
- Pursue scientific opportunities and grand challenges in high energy density plasma science to explore the feasibility of the inertial confinement approach as a fusion energy source, to better understand our universe, and to enhance national security and economic competitiveness, and;
- Increase the fundamental understanding of basic plasma science, including both burning plasma and low temperature plasma science and engineering, to enhance economic competiveness and to create opportunities for a broader range of science-based applications.

Specific information about FES program areas and their objectives follow:

**(a) Magnetic Fusion Energy Science: ITER and Advanced Tokamak Optimization**

The ITER and Advanced Tokamak (AT) Optimization program seeks to utilize unique magnetic fusion research facilities to develop the physics knowledge needed to advance the FES energy mission. The FES major experimental facilities, which are operated as national facilities and involve users from many national laboratories and universities, provide the essential tools for the U.S. research community to explore and solve fundamental issues of fusion plasma physics. A high priority for these facilities is to extend and optimize advanced tokamak operating scenarios, including providing data for the validation of theoretical models and the development of predictive understanding. A primary goal of the program is to improve and refine concepts for future fusion power plants. In addition, research at these facilities focuses on developing the predictive science needed for ITER operations and providing solutions to high-priority ITER technical issues. U.S. scientists also participate in leading experiments on fusion facilities abroad and conduct comparative studies to supplement the scientific understanding they can obtain from domestic facilities.

Subprogram Contact: Mark Foster, (858) 455-3360, Mark.Foster@science.doe.gov
Website: http://science.energy.gov/fes/research/

**(b) Magnetic Fusion Energy Science: Theory and Simulation**

The Magnetic Fusion Energy Science (MFES) Theory and Simulation program focuses on advancing the scientific understanding of the fundamental physical processes governing the behavior of magnetically confined plasmas and on using this knowledge to improve the design and performance of future fusion power reactors. Among the fundamental problems addressed by this program are the macroscopic stability and dynamics of fusion plasmas; the understanding and controlling of the multiscale, collisional, and turbulent physical mechanisms responsible for the loss of heat, momentum, and particles from the confining region; the interaction of externally launched radiofrequency waves with the background plasma and surrounding structures; the nonlinear interaction between background plasma, various instabilities, and energetic particle populations; and the effect of multiscale and multiphysics processes at the plasma edge on the plasma performance and on the interaction and interface of the hot plasma boundary with the material walls. The efforts supported by this program provide the foundations for integrated simulations of fusion systems and range from analytical work to the development and application of advanced simulation codes capable of exploiting the potential of next generation high performance computers.

Subprogram Contact: John Mandrekas, (301) 903-0552, John.Mandrekas@science.doe.gov
Website: http://science.energy.gov/fes/research/

**(c) Magnetic Fusion Energy Science: Targeted Validation Platforms**

The Targeted Validation Platforms (VP) program provides experimental data in regimes of relevance to the FES mainline magnetic confinement and materials science efforts and helps validate theoretical models and simulation codes in support of the FES goal to develop an experimentally validated predictive capability for magnetically confined fusion plasmas. The goal of the program is to generate sufficient experimental data to elucidate the underlying physics principles upon which concepts of toroidal confinement are based and, as needed, to develop computational models to a sufficient degree of scientific fidelity to allow an assessment of the relevance of those concepts to future fusion energy systems. VP experiments have intrinsic value to the plasma science and fusion energy missions of the FES program since they provide unique tests and extensions to enhance the understanding of magnetically confined plasmas. The program places emphasis on research that can best help deepen the scientific foundations of understanding and improve the tokamak concept. Recent investments have supported the operation of a range of facilities, a center that provides theory and computational support to VP experiments, and several small topic-specific investigations.

Subprogram Contact: Sam Barish, (301) 903-2917, Sam.Barish@science.doe.gov
Website: http://science.energy.gov/fes/research/

**(d) High-Energy-Density Plasma Science**

High-Energy-Density Laboratory Plasma (HEDLP) physics is the study of ionized matter at extremely high density and temperature, specifically when matter is heated and compressed to a point that the stored energy in the matter reaches approximately 100 billion Joules per cubic meter (the energy density of a hydrogen molecule). This corresponds to a pressure of approximately 1 million atmospheres or 1 Mbar. Systems in which free electrons play a significant role in the dynamics and for which the underlying assumptions and methods of traditional ideal-plasma theory and standard condensed matter theory do not apply (e.g., Warm Dense Matter at temperatures of a few eV) can have pressures as low as 0.1 Mbar and are also considered HED plasmas. Discovery-driven and use-inspired scientific explorations of high-energy-density states of matter are being supported in this program. Topical examples being emphasized include (1) high-energy-density hydrodynamics, (2) radiation-dominated dynamics and material properties, (3) magnetized high-energy-density plasmas, (4) nonlinear optics of plasmas and laser-plasma interactions, (5) relativistic HED plasmas and intense beam physics, and (6) warm dense matter.

Subprogram Contact: Sean Finnegan, (301) 903-4920, Sean.Finnegan@science.doe.gov
Website: http://science.energy.gov/fes/research/

**(e) General Plasma Science: Experiment and Theory**

The General Plasma Science program is directed toward research that addresses fundamental issues in plasma science and engineering not directly related to fusion energy. This research strengthens the fundamental underpinnings of the discipline of plasma physics that complements burning plasma science and reaches beyond into many basic and applied physics areas. The

focus of this program continues to be on fundamental issues of plasma science and engineering that can have impact in other areas or disciplines in which improved understanding of the plasma state is needed. General plasma science is a broad, multidisciplinary field that spans many science issues such as interaction of waves with plasmas, magnetic reconnection and particle acceleration, physics of non-neutral plasmas and antimatter, chaos, turbulence, and structure in plasmas. Areas of interest include but are not limited to: (1) astrophysical, solar, and space plasmas, (2) plasmas in biological and environmental science, (3) plasma modification, synthesis and processing of materials, (4) dusty, non-neutral and antimatter plasmas, (5) advanced plasma diagnostics, and (6) advanced methods for plasma modeling and simulation.

Subprogram Contact: Nirmol Podder, (301) 903-9536, Nirmol.Podder@science.doe.gov
Website: http://science.energy.gov/fes/research/

**(f) Materials Science and Enabling Technologies for Fusion**

The Enabling Technology 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.

Subprogram Contact: Peter Pappano, (301) 903-4883, Peter.Pappano@science.doe.gov
Website: http://science.energy.gov/fes/research/

**(g) Diagnostic Development for Fusion and Plasma Science**

Diagnostics provide the compass that scientists use to navigate the voyage of scientific discovery. New observations leading to scientific breakthroughs are often enabled by the development of a new diagnostic technique or methodology. Advances in diagnostic systems are needed to serve two important functions: to provide a link between theory/computation and experiments; and to provide sensory tools for active control of plasma properties to optimize device operation and plasma performance. The program also supports development of ITER-relevant diagnostic systems.

Subprogram Contact: Francis Thio, (301) 903-4678, Francis.Thio@science.doe.gov
Website: http://science.energy.gov/fes/research/

**5. High Energy Physics (HEP)**
Program Website: http://science.energy.gov/hep

The mission of the High Energy Physics (HEP) program 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.

The HEP program focuses on three scientific frontiers:

- *The Energy Frontier*, where powerful accelerators are used to create new particles, reveal their interactions, and investigate fundamental forces;
- *The Intensity Frontier*, where intense particle beams and highly sensitive detectors are used to pursue alternate pathways to investigate fundamental forces and particle interactions by studying events that occur rarely in nature; and
- *The Cosmic Frontier*, where non-accelerator-based experiments and telescopes are used to make measurements of naturally occurring phenomena that will offer new insight and information about the nature of dark matter, dark energy, and other phenomena to understand fundamental properties of matter and energy.

Together, these three interrelated and complementary discovery frontiers offer the opportunity to answer some of the most basic questions about the world around us. Also integral to the mission of HEP are two additional cross-cutting subprograms that enable new scientific opportunities by developing the necessary tools and methods for discoveries:

- *Theoretical Particle Physics*, where the foundation and mathematical framework for understanding and extending the knowledge of particles, forces, space-time, and the universe are developed; and
- *Advanced Accelerator and Detector Technology Research and Development*, where the technologies and basic science needed to design, build, and operate the accelerator and detector facilities essential for making new discoveries are developed.

The scientific objectives of the HEP program are aligned with the priorities for the field recommended by the High Energy Physics Advisory Panel, which are detailed in their recent long-range plan available at:
http://science.energy.gov/~/media/hep/pdf/files/pdfs/p5_report_06022008.pdf

To accomplish its mission, the HEP program supports basic research and technology development through the following five subprograms:

**(a) Experimental Research at the Energy Frontier**

This subprogram seeks to support studies of fundamental particles and their interactions using proton-(anti)proton collisions at the highest possible energies. This is accomplished through direct detection of new phenomena or through sensitive measurements that probe the Standard Model and new physics beyond it. In particular, applications are sought for physics research

utilizing the D0 and CDF experiments at the Tevatron and the ATLAS and CMS experiments at the LHC. This subprogram also provides graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities. Support for Heavy Ion Physics research is not provided under this subprogram.

Subprogram Contact: Saul Gonzalez, (301) 903-2359, saul.gonzalez@science.doe.gov
Website: http://science.energy.gov/hep/research

**(b) Experimental Research at the Intensity Frontier**

This subprogram seeks to support precision studies that are sensitive to new physics at very high energy scales, beyond what can be directly probed with energy frontier colliders. Often these studies involve observing rare processes that require intense particle beams. In addition, recent advances in neutrino physics have opened the first window beyond the Standard Model of particle physics, perhaps signaling significant new properties of neutrinos that will have wide ranging impact in particle physics and cosmology. This subprogram includes studies of high intensity electron-positron collisions; studies of the properties of neutrinos produced by accelerators, nuclear reactors, and certain rare nuclear decays; and studies of rare processes using high intensity beams on fixed targets. In addition, this subprogram includes searches for proton decay. This subprogram also provides graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities.

Subprogram Contact: Alan Stone, (301) 903-7998, alan.stone@science.doe.gov
Website: http://science.energy.gov/hep/research

**(c) Experimental Research at the Cosmic Frontier**

This subprogram supports studies of particle physics using naturally occurring particles and phenomena. High-energy cosmic rays, photons and neutrinos serve as some of the non-accelerator-based particle sources used in this area of research. In addition, this program seeks to support studies of dark energy; studies of primordial antimatter; and direct detection of the particles constituting dark matter. This subprogram also provides graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities. Studies of gravitational physics, classical astrophysics phenomena, or fundamental symmetries are not included in this subprogram.

Subprogram Contact: Kathy Turner, (301) 903-1759, kathy.turner@science.doe.gov
Website: http://science.energy.gov/hep/research

**(d) Theoretical High Energy Physics Research**

This program supports activities that range from detailed calculations of the predictions of the Standard Model to the extrapolation of current knowledge to a new level of understanding and the identification of the means to experimentally search for them. Topics studied in the theoretical research program include, but are not limited to: phenomenological and theoretical studies that support the experimental HEP research program, both in understanding the data and

in finding new directions for experimental exploration; development of analytical and numerical computational techniques for these studies; and exploration of theoretical frameworks for understanding fundamental particles and forces at the deepest level possible. This subprogram also provides graduate and postdoctoral research training for the next generation of scientists and computational resources needed for theoretical calculations.

Subprogram Contact: Simona Rolli, (301) 903-0504, simona.rolli@science.doe.gov
Website: http://science.energy.gov/hep/research

**(e) Advanced Accelerator and Detector Technology Research and Development**

The Advanced Technology R&D subprogram develops the next generation of particle accelerators, detectors, and computing 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 the science of particle acceleration, control, detection and instrumentation. This subprogram supports long-range, exploratory research aimed at developing new concepts. This subprogram also provides graduate and postdoctoral research training, equipment for experiments and related computational efforts.

Topics studied in the accelerator science 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; high resolution, fast-readout calorimeters and particle identification detectors; techniques for improving the radiation tolerance of particle detectors; and advanced electronics and data acquisition systems. In addition, this subprogram develops next-generation computational tools and techniques in support of the experimental and theoretical physics research programs.

Subprogram Contact: L. K. Len, (301) 903-3233, lk.len@science.doe.gov
Website: http://science.energy.gov/hep/research

**6. Nuclear Physics (NP)**
Program Website: http://science.energy.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 unknown. 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, including those that are no longer commonly found in our universe.

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 mysteries surrounding the fundamental 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 five subprograms: Medium Energy, Heavy Ion, Low Energy, Nuclear Theory, and Nuclear Data and Nuclear Theory Computing (a through e). The program is the steward of the isotopes program for the nation (f) and supports the development of the tools and capabilities that make fundamental research possible (g).

The NP subprograms and their objectives follow:

**(a) Medium Energy Nuclear Physics**

The Medium Energy subprogram primarily explores the scientific frontier of Quantum Chromodynamics (QCD) to develop a complete understanding of how quarks and gluons assemble themselves into protons and neutrons and how the resulting quark structure of protons and neutrons is modified in the interior of light and heavy nuclei. 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: Frank (Ted) Barnes, (301) 903-3212, ted.barnes@science.doe.gov
Website: http://science.energy.gov/np/research/

**(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 early universe. 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://science.energy.gov/np/research/

**(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 spanning the entire nuclear chart, to utilize rare isotope beams to reveal new nuclear phenomena and structures unlike those gleaned from studies using stable nuclei, and to measure the cross sections of nuclear reactions that power stars and spectacular stellar explosions 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://science.energy.gov/np/research/

**(d) Nuclear Theory**

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.

Subprogram Contact: G. Fai, (301) 903-8954, george.fai@science.doe.gov
Website: http://science.energy.gov/np/research/

**(e) Nuclear Data and Nuclear Theory Computing**

The mission of the Nuclear Data program is to continually validate, refine, and maintain a set of publicly accessible online databases that contain a broad spectrum of nuclear physics data. The archives supported by the Nuclear Data program are of interest for academic research, for, applied and basic research at national laboratories, and to industries involved in nuclear applications such as nuclear energy and medical isotopes. This information includes the properties of both stable and unstable nuclei, experimental results and theoretical predictions for nuclear reactions and nuclear cross sections, and an extensive set of relevant publications on nuclear physics and specialized databases.

The Nuclear Theory Computing program provides computer time and funding support to nuclear scientists whose research has major computational requirements. Thrusts supported by this program include projects jointly supported by the Nuclear Physics and Advanced Scientific Computing Research (ASCR) Offices under the Scientific Discovery through Advanced Computation (SciDAC) initiative and the National Energy Research Super Computer (NERSC) allocation program. SciDAC provides support, in partnership with other DOE Offices, for resource intensive computational science topics; NERSC provides allocations of supercomputer time and storage to NP and other researchers. The research supported through Nuclear Theory

Computing covers a wide range of computational nuclear physics topics. Recent examples include predictions based on the fundamental theory of quark and gluon interactions, "Quantum Chromodynamics" (QCD) calculated on a space-time lattice; predictions of the properties of nuclei using Density Functional Theory formalism; studies of problems in nuclear astrophysics, including simulations of core collapse supernovae and the birth of the heavy elements; computer studies of novel particle accelerators; and the development of networking software for experimental data applications.

Subprogram Contact: Frank (Ted) Barnes, (301) 903-3212, ted.barnes@science.doe.gov
Website: http://science.energy.gov/np/research/

**(f) 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 BNL and the Isotope Production Facility (IPF) at 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://science.energy.gov/np/research/

**(g) 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://science.energy.gov/np/research/

**7. Workforce Development for Teachers and Scientists (WDTS)**
Program Website: http://science.energy.gov/wdts/

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

This is accomplished through support of undergraduate internships and visiting faculty programs at the DOE laboratories; a graduate fellowship program, which also involves the DOE laboratories; the Albert Einstein Distinguished Educator Fellowship for K–12 teachers, which is administered by WDTS for DOE and for a number of other federal agencies; and Nation-wide, middle- and high-school science competitions that culminate annually in the National Science Bowl® in Washington D.C.

These investments help develop the next generation of scientists and engineers to support the DOE missions, administer its programs, and conduct the research that will realize the Nation's science and innovation agenda. Today, DOE's federal and contractor workforce includes more than 30,000 workers with STEM backgrounds; ensuring the availability and readiness of its future workforce is a key responsibility of the DOE.

The priority areas for WDTS include the following:

- Support of undergraduate internships and visiting faculty programs at the DOE laboratories;
- Support for 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;
- Support to increase the research competitiveness of faculty members and their students at institutions historically underrepresented in the research community in order to expand the workforce that addresses DOE mission areas.

Program Contact: Ping Ge, (202) 287-6490, ping.ge@science.doe.gov
Website: http://science.energy.gov/wdts/

# 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 $400 million will be available for DOE Office of Science new, renewal, continuing, and supplemental grant and cooperative agreement awards under this and other, more targeted FOAs in FY 2012, subject to the availability of FY 2012 appropriated funds. The amount of funding allocated under this specific FOA will be decided based on a number of factors, including peer review, the number of applications received, and the availability of appropriated funds.

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 2012 appropriated funds. Historically, applications that arrive in response to the open solicitation for applications have resulted in 200 to 350 new awards per year.

## E. ANTICIPATED AWARD SIZE.

N/A

## F. PERIOD OF PERFORMANCE.

N/A

## G. TYPE OF APPLICATION.

DOE will accept new, renewal, and supplemental applications under this FOA.

Applications for conference or workshop support must be submitted at least six months before the meeting date and no later than April 1, 2012 to be considered for FY 2012 funding.

### NEW APPLICATION INSTRUCTIONS.

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 new applications.

### 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 a Grant 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://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms, 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 for 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-0000600
**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.

Collaborative applications submitted from different institutions should clearly indicate they are part of a collaborative project/group. Every partner institution must submit an application through its own sponsored research office. Each application within the collaborative group, including the narrative and all required appendices and attachments, should be identical with one exception: The exception is that each application should contain unique budget and budget justification documents corresponding to the expenditures for that application's submitting institution only. Each collaborative group can have only one lead institution, which should be identified in the common narrative. The common narrative should also contain a summary table describing the budget breakdown by institution for all participants.

Each application belonging to a collaborative group should have the same title in Block 11 of the SF 424 (R&R) form.

Our intent is to create from the various applications associated with a collaborative group one document for merit review that consists of the common, identical application materials combined with a set of detailed budgets from the partner institutions. Thus, it is very important that every application in the collaborative group be exactly identical (including the title) with the exception of the budget and budget justification pages.

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 and 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 and 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 Other Attachments 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 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, 2012, 11:59 PM Eastern Time, or until it is succeeded by another issuance, whichever occurs first. This Annual FOA DE-FOA-0000600 succeeds FOA DE-FOA-0000411 and FOA DE-FOA-0000412, which were published September 30, 2010.

## 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. 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. To register with Grants.gov go to "Get Registered" at http://grants.gov/applicants/get_registered.jsp. Use the Grants.gov Organization Registration Checklist 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 Part 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://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms. 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://energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards.

**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 F4600.2, attached to the award agreement. For a sample checklist, see http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms, under Awards Forms.

# 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 confidentional 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://ecfr.gpoaccess.gov/cgi/t/text/text-idx?c=ecfr&tpl=/ecfrbrowse/Title10/10cfr784_main_02.tpl.

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.