# FINANCIAL ASSISTANCE FUNDING OPPORTUNITY ANNOUNCEMENT



# U. S. Department of Energy Office of Science

# FY 2014 Continuation of Solicitation for the Office of Science Financial Assistance Program

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<b>Pre-Application Due Date:</b>	Not Applicable
Application Due Date:	<b>Not Applicable</b> This Funding Opportunity Announcement (FOA) will remain open until September 30, 2014 or until replaced by a successor FOA. Applications may be submitted any time during this period.

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# **REGISTRATIONS**

## A. Systems to Register In

There are several one-time actions you must complete in order to submit an application in response to this Announcement. Applicants not currently registered with SAM and Grants.gov should allow **at least 44 days** to complete these requirements. You should start the process as soon as possible.

Applicants must obtain a DUNS number at http://fedgov.dnb.com/webform.

Applicants must register with the System for Award Management (SAM) at <u>http://www.sam.gov/</u>. If you had an active registration in the Central Contractor Registry (CCR), you should have an active registration in SAM. More information about SAM registration for applicants is found at <u>https://www.sam.gov/sam/transcript/Quick\_Guide\_for\_Grants\_Registrations\_v1.7.pdf</u>.

<u>intps://www.sum.gov/sum\_dumbeript\_Quick\_Ourde\_for\_Stants\_Registrations\_v1.v.pur</u>.

Applicants must register with FedConnect at <u>www.fedconnect.net</u>. The full, binding version of assistance agreements will be posted to FedConnect.

Recipients must register with the Federal Funding Accountability and Transparency Act Subaward Reporting System at <u>https://www.fsrs.gov</u>. This registration must be completed before an award may be made: you are advised to register while preparing your application.

# **B.** Registering in Grants.gov

Applicants must register with Grants.gov.

For organizations, please follow the procedures detailed below, making use of the checklist provided below:

http://www.grants.gov/web/grants/applicants/organization-registration.html http://www.grants.gov/documents/19/18243/OrganizationRegChecklist.pdf

For individuals, please follow the procedures detailed below: <u>http://www.grants.gov/web/grants/applicants/individual-registration.html</u>

Organizations and individuals must have an E-Business (E-Biz) Point of Contact (POC). You may find the checklist at <u>http://www.grants.gov/documents/19/18243/E-Biz\_POC\_Checklist.pdf</u> useful.

Grants.gov maintains a User Guide at

http://www.grants.gov/documents/19/18243/GrantsGovApplicantUserGuide.pdf and a list of Frequently Asked Questions at http://www.grants.gov/web/grants/applicants/applicant-faqs.html. Questions relating to the registration process, **system requirements, or how an application form works** must be directed to Grants.gov at 1-800-518-4726 or <u>support@grants.gov</u>. **IMPORTANT NOTICE:** When you have completed the grants.gov registration 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).

Applicants must download the application package, application forms and instructions, from Grants.gov at <u>http://www.grants.gov/</u> (Additional instructions are provided in Section IV A of this FOA.)

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 SAM 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.

# C. DOE Office of Science Portfolio Analysis and Management System (PAMS)

After you submit your application through Grants.gov, the application will automatically transfer into the Portfolio Analysis and Management System (PAMS) for processing by the DOE Office of Science. Many functions for grants and cooperative agreements can be done in PAMS, which is available at <u>https://pamspublic.science.energy.gov</u>.

You will want to "register to" your application: a process of linking yourself to the application after it has been submitted through grants.gov and processed by DOE.

You may use the Internet Explorer, Firefox, Google Chrome, or Safari browsers to access PAMS.

Notifications sent from the PAMS system will come from the PAMS email address <<u>PAMS.Autoreply@science.doe.gov</u>>. Please make sure your email server/software allows delivery of emails from the PAMS email address to yours.

Registering to PAMS is a two-step process; once you create an individual account, you must associate yourself with ("register to") your institution. Detailed steps are listed below.

# 1. CREATE PAMS ACCOUNT:

To register, click the "Create New PAMS Account" link on the website <u>https://pamspublic.science.energy.gov/</u>.

- Click the "No, I have never had an account" link and then the "Create Account" button.
- You will be prompted to enter your name and email address, create a username and password, and select a security question and answer. Once you have done this, click the "Save and Continue" button.
- On the next page, enter the required information (at least one phone number and your mailing address) and any optional information you wish to provide (e.g., FAX number, website, mailstop code, additional email addresses or phone numbers, Division/Department). Click the "Create Account" button.

- Read the user agreement and click the "Accept" button to indicate that you understand your responsibilities and agree to comply with the rules of behavior for PAMS.
- PAMS will take you the "Having Trouble Logging In?" page. (If you have been an Office of Science merit reviewer or if you have previously submitted an application, you may already be linked to an institution in PAMS. If this happens, you will be taken to the PAMS home page.)

2. REGISTER TO YOUR INSTITUTION:

- Click the link labeled "Option 2: I know my institution and I am here to register to the institution." (Note: If you previously created a PAMS account but did not register to an institution at that time, you must click the Institutions tab and click the "Register to Institution" link.)
- PAMS will take you to the "Register to Institution" page.
- Type a word or phrase from your institution name in the field labeled, "Institution Name like," choose the radio button next to the item that best describes your role in the system, and click the "Search" button. A "like" search in PAMS returns results that contain the word or phrase you enter; you do not need to enter the exact name of the institution, but you should enter a word or phrase contained within the institution name. (If your institution has a frequently used acronym, such as ANL for Argonne National Laboratory or UCLA for the Regents of the University of California, Los Angeles, you may find it easiest to search for the acronym under "Institution Name like." Many institutions with acronyms are listed in PAMS with their acronyms in parentheses after their names.)
- Find your institution in the list that is returned by the search and click the "Actions" link in the Options column next to the institution name to obtain a dropdown list. Select "Add me to this institution" from the dropdown. PAMS will take you to the "Institutions List" page.
- If you do not see your institution in the initial search results, you can search again by clicking the "Cancel" button, clicking the Option 2 link, and repeating the search.
- If, after searching, you think your institution is not currently in the database, click the "Cannot Find My Institution" button and enter the requested institution information into PAMS. Click the "Create Institution" button. PAMS will add the institution to the system, associate your profile with the new institution, and return you to the "Institutions List" page when you are finished.

For help with PAMS, click the "External User Guide" link on the PAMS website, <u>https://pamspublic.science.energy.gov/</u>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: <u>sc.pams-helpdesk@science.doe.gov</u>. All submission and inquiries about this Funding Opportunity Announcement should reference **DE-FOA-0000995**.

# RECOMMENDATION

The Office of Science encourages you to register in all systems as soon as possible.

# Section I – FUNDING OPPORTUNITY DESCRIPTION

# GENERAL INQUIRIES ABOUT THIS FOA SHOULD BE DIRECTED TO:

**Technical/Scientific Program 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.

# 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 600 U.S. Department of Energy, Office of Science Financial Assistance Program Rule, codified at 10 CFR 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, and Nuclear Physics. 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 605, as a 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 605.

This Funding Opportunity Announcement (FOA), DE-FOA-0000995, 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, 2014, 11:59 PM Eastern Time, or until it is succeeded by another issuance, whichever occurs first. This annual FOA DE-FOA-0000995 succeeds FOA DE-FOA-0000768, which was published September 30, 2012.

# SUPPLEMENTARY INFORMATION

# **OFFICE OF SCIENCE OVERVIEW**

Website: <u>http://science.energy.gov/</u>

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

The Office of Science accomplishes its mission and advances national goals by supporting:

- *The Frontiers of Science*, discovering nature's mysteries from the study of subatomic particles, atoms, and molecules that are the building blocks of the materials of our everyday world to the DNA, proteins, and cells that are the building blocks of entire biological systems;
- *The 21<sup>st</sup> Century Tools of Science*, providing to the Nation's researchers more than 30 national scientific user facilities, the most advanced tools of modern science including accelerators, colliders, supercomputers, light sources, neutron sources, and facilities for studying the nanoworld; and
- *Energy and Environmental Science*, advancing a clean energy agenda through fundamental research on energy production, conversion, storage, transmission, and use and advancing our understanding of the earth and its climate through basic research in atmospheric and environmental sciences and climate change.

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

# 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)
- (1) 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 in High Energy Physics
- (b) Experimental Research at the Intensity Frontier in High Energy Physics
- (c) Experimental Research at the Cosmic Frontier in High Energy Physics
- (d) Theoretical Research in High Energy Physics
- (e) Computational Research in High Energy Physics
- (f) Accelerator Science and Technology Research & Development in High Energy Physics
- (g) Particle Detector Research and Development in High Energy Physics

# 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

# 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 advance applied mathematics and computer science; deliver, in partnership with disciplinary science, the most advanced computational scientific applications; advance computing and networking capabilities; and develop, in partnership with the research community, including U.S. industry, future generations of computing hardware and tools for 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 research and development of applied mathematical models, methods, and algorithms for understanding complex natural and engineered systems related to DOE's mission. 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, <u>Sandy.Landsberg@science.doe.gov</u>; Steven Lee, (301) 903-5710, <u>Steven.Lee@science.doe.gov</u>; and Karen Pao, (301) 903-5384, <u>Karen.Pao@science.doe.gov</u> Website: http://science.energy.gov/ascr/research/applied-mathematics/

## (b) Computer Science

This subprogram supports basic research to utilize computing at extreme scales and to understand extreme scale data from both simulations and experiments. 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:

- Theory and techniques that support the asynchronous data delivery to/from a very large number of lightweight threads. Operating system, messaging layers, and lightweight threads mechanisms to efficiently support dynamic and adaptive programming models. Mechanisms to dynamically manage resources across the entire system.
- 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 solicitation 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, natural language processing/understanding/generation, social computing, 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: Lucy Nowell, (301) 903-3191, <u>Lucy.Nowell@science.doe.gov</u>; and Sonia R. Sachs, (301) 903-0060, <u>Sonia.Sachs@science.doe.gov</u> Website: <u>http://science.energy.gov/ascr/research/computer-science/</u>

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

## (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, <u>William.Harrod@science.doe.gov</u> Website: <u>http://science.energy.gov/ascr</u>

## (e) Network Environment Research

This subprogram supports basic research to enable scientists, individually or in teams, to easily find and access the unique scientific facilities and data, and interact with any peers or facilities staff involved in a scientific discovery process. Research topics of interest include: (1) Software Defined Network control plan algorithms and mechanisms needed to build and operate end-to-end terabit rate networks; (2) Data management algorithms, tools, and services needed to support distributed science activities; (3) Federated Identity Management theories, tools, and services to simplify access to facilities and distributed resources; (4) The theories, algorithms, tools, and services needed to create diverse computing environments where multiple resources can be combined in unique ways to suit the needs of the science community; (5) Mechanisms and theories to enable scientists to interact with their peers and technical staff that operate a scientific facility; (7) The analytical models and simulation environments needed to understand how distributed applications behave in network infrastructures; and (8) Tools and services needed to support physical experiments in testbeds and production networks.

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

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.

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

## (a) Materials Chemistry

This program supports research on materials with a focus on the *chemical synthesis*, *chemical control, and chemical dynamics* of material composition and structure across the range of length scales from atomic to mesoscopic, with a view to elucidating fundamental aspects of materials' structure-property relationships. Major scientific areas of interest include: fundamental aspects of the chemical assembly of material structures and control of multi-scale material morphology; synthesis and characterization of novel organic, inorganic, polymeric and composite materials; synthesis and characterization of complex fluids including ionic liquids; study and control of surface and interfacial chemistry and morphology; fundamental electrochemistry of solid state materials; the study of the chemical dynamics and transformations of functional materials in operational environments; and the development of new, science-driven laboratory-based analytical tools and techniques for the elucidation of chemical processes in materials, particularly in-situ or in-operando in energy-relevant applications.

The overarching goal of materials chemistry research is to provide the *knowledge* needed to design and produce materials with tailored properties from first principles. This program will make progress towards that goal by emphasizing hypothesis-driven research on the chemistry-based synthesis of materials and/or morphologies that have the potential to enable next-generation energy-relevant technologies, and research on the chemical transformations occurring in functional materials in the operating environment. It will include the study of chemical

processes that direct and control the covalent and non-covalent assembly of materials, discovery of synthetic methods to tailor the symmetry and dimensionality of crystalline and non-crystalline lattices; and the utilization of chemistry to control interfacial properties and interactions of materials. New approaches to the integration of theory and experiment leading to new materials design ideas and opportunities for predictive materials discovery will also be supported.

Research primarily aimed at the *optimization* of synthetic methods or properties of materials for applications and research with a primary goal of device fabrication and testing will be discouraged.

Subprogram Contacts: Michael Sennett, (301) 903-6051, <u>michael.sennett@science.doe.gov</u>; and Craig Henderson, (301) 903-0805, <u>craig.henderson@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/mse/research-areas/materials-chemistry/</u>

#### (b) Biomolecular Materials

This activity supports fundamental research in the discovery, design and synthesis of functional materials and complex structures, and materials aspects of energy conversion processes based on principles and concepts of biology. Since biology provides a blueprint for translating atomic and nanoscale phenomena into mesoscale materials that display complex yet well-coordinated collective behavior, the major programmatic focus is on the hypothesis-driven creation of energy-relevant materials optimized for harsher, non-biological environments. Major thrust areas include: harnessing or mimicking the energy-efficient synthesis approaches of biology to generate new, optimized materials for a broad range of non-biological conditions; bioinspired self-, directed-, and active assembly approaches with control of assembly pathway mechanisms and kinetics to form materials that are far from equilibrium and display novel and unexpected properties; adaptive, resilient materials with self-repairing capabilities; and development of science-driven tools and techniques to achieve a fundamental understanding of how these new materials and systems are formed and how they function in real time.

Recent BES Basic Research Needs (and other) workshops and reports have clearly identified mastering the capabilities of living systems as a Grand Challenge that could provide the knowledge base to discover, design, and synthesize new materials with the precise control of complexity needed to yield totally new properties for next-generation energy technologies. Biomolecular Materials research activity will seek to advance the ability for materials to selfrepair, regulate, sequester impurities, tolerate abuse, and produce, convert and store energy, with an emphasis on achieving mechanistic understanding of these new materials and systems. New approaches that will lead to predictable and scalable synthesis of novel, hierarchically structured polymeric, inorganic, and hybrid functional materials in vitro with controllable morphology, content, behavior and performance are sought. The activity will expand research on creating materials optimized for non-biological conditions (i) in which the components work in concert to initiate, maintain, cease functions, and communicate to coordinate collective behavior in response to external signals; (ii) that are capable of spontaneous formation and deformation; (iii) that undergo self-repair without external input; and (iv) that are capable of self-replication. This activity also will expand research to design and create next generation membrane materials with programmable selectivity and transport based on biological gating and pumping functions.

Enhanced integration of theory and experiment to understand how materials complexity leads to new functionalities and the development of new design ideas and opportunities for accelerated discovery will also be emphasized.

Research aimed at optimization of materials properties for applications, device fabrication, sensor development, tissue engineering, and biomedical research will be discouraged.

Subprogram Contact: Michael Markowitz, (301) 903-6779, <u>mike.markowitz@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/mse/research-areas/biomolecular-materials/</u>

## (c) Synthesis and Processing Science

This program supports research on materials to understand the physical phenomena and unifying principles that underpin materials synthesis including diffusion, nucleation, and phase transitions, often using *in situ* diagnostics, and developing new techniques to synthesize materials with tailored structure and properties. An important element of this activity is the development of real-time monitoring tools that probe the dynamic environment and the progression of structure and properties as a material is formed. This information is essential to understand the underlying physical mechanisms and to gain atomic level control of material synthesis and processing. The emphasis is on the synthesis of complex thin films with atomic control; preparation techniques for high-quality single crystal and bulk materials with novel physical properties; understanding the contributions of the precursor states to the processing of bulk materials; and mild processing techniques for the assembly of nanostructured materials into larger scale structures. 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 approaches.

Recent BES Basic Research Needs (and other) workshops and reports have identified the challenges in synthesis and processing that are most relevant to next-generation energy technologies. In particular, the Grand Challenges for the field include the ability to control and design materials with tailored and revolutionary properties through energy efficient processes and precise control even under far-from-equilibrium conditions. The Synthesis and Processing Science activity is encouraging hypothesis-driven proposals that integrate a creative experimental methodology with a first-principles theoretical-based approach that will accelerate progress in understanding unifying principles for synthesis and discovery of new materials.

Over the past few years, the activity has developed an increasing interest in understanding nanoscale morphology, defect and dopant control in deposition processes, and complex chemical and structural materials growth. Over the next several years, these directions are expected to continue with a stronger focus on investigating fundamental mechanisms for bulk materials growth, new deposition techniques for organic and inorganic films, and organization of mesoscopic assemblies across a range of length scales, especially relating to use-inspired clean energy research.

Subprogram Contact: Bonnie Gersten, (301) 903-0002, <u>bonnie.gersten@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/mse/research-areas/synthesis-and-processing-science/</u>

## (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, and nanoscale systems. The program also supports research that involves characterization of 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 support the search for new material systems with which to explore the central scientific themes. The portfolio will continue support research on electronic structure of materials in bulk and thin film form, at interfaces, and in reduced dimensionality, as well as the development of experimental techniques that enable such studies. Efforts will continue to strengthen research in unconventional superconductivity, including the high-temperature cuprate superconductors, heavy fermion superconductors, and iron-arsenide superconductors. Continued growth in support is expected for spin physics, nanomagnetism, topological states of matter, and cold atom research to provide insights into open questions about correlated electron behavior in condensed matter systems.

Subprogram Contact: James Horwitz, (301) 903-4894, james.horwitz@science.doe.gov Website: <u>http://science.energy.gov/bes/mse/research-areas/experimental-condensed-matter-physics/</u>

## (e) Theoretical Condensed Matter Physics

This activity supports Theoretical Condensed Matter Physics with an emphasis on electron correlation, electron and phonon transport, fundamental research in materials related to energy technologies, and theory relevant to the interpretation of experimental results at BES user facilities. Suitable topics include strongly correlated electron systems, quantum phase transitions, magnetism, superconductivity, optical response, thermoelectric materials, and neutron and photon scattering. Novel, physics based computational techniques and algorithms are supported along with techniques relevant to the discovery and design of new materials.

The program will continue to emphasize the development of our understanding of matter at atomistic length scales expanding to include properties at the mesoscale. 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 properties (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.

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. There is increasing emphasis in plasmonics, metamaterials and organic electronic materials. 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, <u>refik.kortan@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/mse/research-areas/physical-behavior-of-materials/</u>

## (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. In addition to traditional structural materials, it is also important to understand deformation and failure mechanisms in other materials used in energy systems (e.g. membranes, coating materials, electrodes) so this will become an increasing part of the portfolio.

The long-term goals of this program 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. This can be accomplished by taking 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 can be used as both a tool and a probe to gain a greater understanding of fundamental atomistic behavior of materials.

Subprogram Contact: John Vetrano, (301) 903-5976, john.vetrano@science.doe.gov

Website: http://science.energy.gov/bes/mse/research-areas/mechanical-behavior-and-radiationeffects/

# (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, across the full electromagnetic spectrum, including research aimed at manipulating and detecting ultrafast transient physical phenomena in materials (especially at excitation levels consistent with energy conversion and transport), 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 expand capabilities at the DOE facilities by providing support for independent external researchers who motivate and lead new instrumentation and technique development at those facilities. A continuing theme in the scattering program will be the integration and support of materials preparation, especially when coupled to *in-situ* and in operation investigation of materials processing and energy related realistic materials environments. New investments in ultrafast science will focus on research that uses radiation sources associated with BES facilities and beam lines but also includes research performed with ultra-short pulse radiation probes created by tabletop laser sources.

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

# (i) Neutron Scattering

This activity supports basic research on the unique 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. Main emphasis is on the application of neutron scattering, spectroscopy, and imaging as major tools for transformational research, primarily at BES-supported user facilities. Development of next-generation instrumentation concepts and advanced tools for neutron scattering and imaging for materials research are distinct aspects of this activity.

The 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. It will support research addressing the effects of interfaces on the collective behavior of multi-component systems consisting of hard and soft matter. This program supports the development of novel approaches that will exploit the unique aspects of neutron scattering/imaging and *in-situ* capabilities to investigate materials with hierarchical structures and excitations in a wide range of length and time scales.

Subprogram Contact: P. Thiyagarajan (Thiyaga), (301) 903-9706, <u>p.thiyagarajan@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/mse/research-areas/neutron-scattering/</u>

## (j) Electron and Scanning Probe Microscopies

This activity supports basic research in materials sciences using advanced electron and scanning probe microscopy and related spectroscopy techniques to understand the atomic, electronic, and magnetic structures and properties of materials. This activity also supports the development of new instrumentation concepts and quantitative techniques, including ultrafast electron diffraction and imaging techniques, to advance basic science and materials characterizations for energy applications. The goal is to develop a fundamental understanding of materials through advanced microscopy and spectroscopy.

Significant improvements in resolution and sensitivity will provide an array of opportunities for groundbreaking science. This activity will continue to support on the development and use of advanced microscopy instrumentation and techniques, and the associated theoretical tools to understand the experiments, for research on imaging the functional aspects of materials and understanding the electronic structure, spin dynamics, magnetism, and transport properties from atomistic to mesoscopic scales; understanding the interplay between charge, orbital, spin and lattice structures in complex materials; correlation of structure and properties of nanostructured materials for energy applications; combining multiple probes in a single experiment; high resolution analyses of energy-relevant soft matter; and quantitative *in-situ* analysis capabilities under perturbing parameters such as temperature, stress, chemical environment, and magnetic and electric fields.

Subprogram Contact: Jane Zhu, (301) 903-3811, jane.zhu@science.doe.gov Website: <u>http://science.energy.gov/bes/mse/research-areas/electron-and-scanning-probe-</u> microscopies/

#### **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.

CSGB Division 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 the development and application of novel, ultrafast optical probes of matter; the interactions of atoms and molecules with intense electromagnetic fields; and quantum control of atomic and 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, strong-field, 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.

Subprogram Contact: Jeffrey Krause, (301) 903-5827, <u>jeff.krause@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/atomic-molecular-and-optical-</u> science/

#### (I) Gas Phase Chemical Physics

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

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

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

Subprogram Contact: Wade Sisk, (301) 903-5692, <u>wade.sisk@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/gas-phase-chemical-physics/</u>

#### (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.

Subprogram Contact: Mark Pederson, (301) 903-9956, <u>mark.pederson@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/computational-and-theoretical-</u> chemistry/

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

This activity emphasizes basic research of energy relevance at the interface of chemistry and physics, pursuing a molecular understanding of chemical, physical, and electron- and photondriven processes in aqueous media and at interfaces. 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. Experimental and theoretical investigations in the gas phase, condensed phase, and at interfaces aim at elucidating the molecular-scale chemical and physical properties and interactions that govern chemical reactivity, solute/solvent structure and transport. Studies of reaction dynamics at wellcharacterized metal and metal-oxide surfaces and clusters lead to the development of theories on the molecular origins of surface-mediated catalysis and heterogeneous chemistry; included is the development of a structural basis for gas/surface interactions, encouraging site-specific studies that measure local behavior at defined sites. Studies of model condensed-phase systems target first-principles understandings of molecular reactivity and dynamical processes in solution and at interfaces; included are studies of the molecular origins of condensed phase behavior and the nature and effects of non-covalent interactions including hydrogen bonding and proton transport. 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.

Basic research is also supported to develop new experimental and theoretical tools that push the horizon of joint space-time resolution needed to probe chemical behavior selectively at interfaces and in solution. For example, a long-term emphasis has been the investigation of interfacial chemical dynamics and charge transfer with a high degree of temporal resolution using advances in chemical imaging at the molecular level. The transition from molecular-scale chemistry to collective phenomena in complex systems is also supported, including the effects of solvation on chemical structure and reactivity. The desired evolution for CPIMS-supported research is toward predictive capabilities that span the microscopic to mesoscale domains enabling the computation of individual molecular interactions as well as their role in complex, collective behavior in real-world devices.

With its foundation in chemical physics, the CPIMS program does not fund research in bulk fluid mechanics or fluid dynamics, applications such as the development of micro-scale devices, and research that is of principle importance to medical applications.

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#### (o) Catalysis Science

This activity develops the fundamental scientific principles enabling rational catalyst design and chemical transformation control for novel reactions of relevance to the DOE's energy mission. This activity does not support the study of reactions relevant to medical applications. 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 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 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. This activity supports innovative approaches to discovering new science from the wealth of experimental information 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 than with current approaches. 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 as a means to derive new 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 and multifunctional molecules will continue to receive attention. The activation and reaction of certain small molecules, such as  $NO_x$ ,  $CO_2$  and water, however, are not covered under this activity, and receive more attention elsewhere. 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 complex molecules into chemicals and fuels.

Subprogram Contact: Raul Miranda, (301) 903-8014, <u>raul.miranda@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/catalysis-science/</u>

#### (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 manipulate 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.

Based on programmatic priorities, this activity does not support engineering or scale up of narrowly defined processes, devices or sensors, activities directed at lab-on-a-chip development, or research directed toward medical applications; as these areas are more appropriately supported through other federally funded programs.

Subprogram Contact: Larry Rahn, (301) 903-2508, <u>larry.rahn@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/separations-and-analysis/</u>

# (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. Fundamental understanding of the chemistry of radioactive species is required to accurately predict their chemical behavior during the entire nuclear fuel cycle, from fuel fabrication to waste separation and disposition.

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 environmental transport 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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#### (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 smallscale 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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#### (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, high-value chemicals, 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,  $NH_3$  in the fixation of nitrogen, 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 and other valued chemicals.

Research areas concerned with separation of charge that might result in electricity include multibandgap, multilayer cascade-type semiconductors, photosensitized nanoparticulate solids. 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, including both aqueous and non-aqueous solutions. 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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#### (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. Such research brings together molecular biology, biochemistry, chemistry, and biophysics in a multidisciplinary effort to uncover the fundamental science of biological capture of sunlight and its conversion to and storage as chemical energy. Topics of study include light harvesting, exciton transfer, charge separation, transfer of reductant to carbon dioxide, as well as carbon fixation, metabolism, and storage. In addition, research is supported in the areas of self-assembly of photosynthetic components, efficient photon capture and charge separation, self-regulating/repairing systems, and processes and mechanisms of photosynthetic redox reactions.

Such research will lead to greater knowledge of the structural and mechanistic features of photosynthetic complexes; insight into factors that enhance photosynthetic energy production; 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; and discovery of the physical and chemical rules that underlie biological mechanisms of repair and photo-protection. This multidisciplinary approach is viewed as a key strength of Photosynthetic Systems and will allow a multidimensional understanding of photosynthesis and how it is coupled to related processes

such as carbon fixation and central 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 in: 1) prokaryotic systems related to human/animal health or disease; 2) development or optimization of devices/processes; 3) development or optimization of microbial strains or plant varieties for biofuel/biomass production. Projects should ideally be hypothesis-driven; projects that develop high-throughput screening approaches will not be supported nor will theory/modeling projects that lack experimental verification.

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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#### (u) Physical Biosciences

This activity supports basic research that combines tools from the physical sciences with biochemical and molecular biological 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 the active site chemistries of multi-electron redox reactions, the assembly and maintenance of energy transduction systems, the processes that regulate energy-relevant chemical reactions within the cell and the underlying biochemical and biophysical principles that determine the architecture of biopolymers including the biosynthesis of the plant cell wall.

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 structural and mechanistic properties of biological reactions that could provide a basis for the design of highly selective and efficient bioinspired catalysts. Critical foundational knowledge needed to achieve this goal will come from studies of multi-electron redox reactions, in particular the poorly understood yet highly effective mechanisms of electron gating and proton coupling/channeling. Of interest in this regard are enzymes and their affiliated co-factors involved in nitrogen reduction, carbon-carbon bond formation, and carbon dioxide assimilation and reduction (including *Archaeal* systems). Other supported areas of research include studies of the roles played by ion gradients in storing energy and driving transport processes and investigations of the structure and dynamics of suprastructures such as cell walls, cytoskeletal components and multi-enzyme (non-photosynthetic) assemblies involved in energy capture, transduction, and storage.

Physical Biosciences does not fund research in: 1) animal systems; 2) prokaryotic systems related to human/animal health or disease; 3) development or optimization of devices/processes; 4) development or optimization of microbial strains or plant varieties for biofuel/biomass production; 5) cell wall breakdown or deconstruction. Projects should ideally be hypothesis-

driven; projects that develop or rely primarily on high-throughput screening approaches will not be supported nor will theory/modeling projects that lack experimental verification.

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

Subprogram Contact: Robert Stack, (301) 903-5652, <u>robert.stack@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/csgb/research-areas/physical-biosciences/</u>

## **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.

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

## (v) BES Accelerator and Detector Research

This program supports research that advances the instruments, techniques, and capabilities of the existing and/or future scientific user facilities. Research includes studies on creating, manipulating, transporting, and performing diagnostics of ultrahigh brightness electron beams, studies of the properties of cathodes materials and factors that limit cathode lifetime, and modeling of ultrashort electron beam dynamics. Research is supported that aims at developing techniques that will strongly benefit the next generation of free electron lasers (FELs), in particular seeding techniques enhancing temporal control of X-ray FELs. Development studies of loss control methods in high-intensity proton sources used for neutron spallation facilities are also supported.

To fully exploit the fluxes delivered by all these sources, new detectors capable of acquiring data several orders of magnitude faster than current rates are required. Detector developments are sought that allow highly efficient use of X-rays and neutrons produced by the sources. Improved detectors are especially important in the study of multi-length-scale systems such as proteinmembrane interactions as well as nucleation and crystallization in nanophase materials.

Advanced X-ray optics developments and modeling are needed to respond to increasing requirements of higher energy resolution, focusing, and preservation of coherence. Innovative and precise optical elements are required to transport and manipulate nearly diffraction and Fourier limited X-ray beams.

This program strongly interacts with BES research divisions that make use of synchrotron radiation and neutron sources.

Subprogram Contact: Eliane Lessner, (301) 903-9365, <u>eliane.lessner@science.doe.gov</u> Website: <u>http://science.energy.gov/bes/suf/accelerator-and-detector-research/</u>

## 3. Biological and Environmental Research (BER)

Program Website: http://science.energy.gov/ber/

The mission of the Biological and Environmental Research (BER) program is to support fundamental research focused on three scientific drivers: exploring the frontiers of genomeenabled biology; discovering the physical, chemical, and biological drivers and environmental impacts of climate change; and seeking the geological, hydrological, and biological determinants of environmental sustainability and stewardship.

The BER subprograms and their objectives follow:

## (a) Biological Systems Science

Research is focused on using DOE's unique resources and facilities to achieve a predictive systems-level understanding of complex biological systems to advance DOE missions in energy and the environment. By integrating genome science with advanced computational and experimental approaches, the Division seeks to gain a predictive understanding of living systems, from microbes and microbial communities to plants and other whole organisms. This foundational knowledge serves as the basis for the confident redesign of microbes and plants for sustainable biofuel production, improved carbon storage and contaminant remediation.

The major objectives are:

- to develop the experimental and computational resources needed to understand and predict complex behavior of complete biological systems, principally plants, microbes, and microbial communities; Joe Graber, (301) 903-1239, joseph.graber@science.doe.gov, http://science.energy.gov/ber/research/bssd/genomic-science/;
- 2. to take advantage of the remarkable high throughput DNA sequencing capacity at the Joint Genome Institute to meet the genome sequencing and analysis needs of the scientific community; Dan Drell, (301) 903-4742, <u>daniel.drell@science.doe.gov</u>, <u>http://science.energy.gov/ber/research/bssd/doe-joint-genome-institute/;</u>
- 3. to understand and characterize the risks to human health from exposures to low levels of ionizing radiation; Noelle Metting, (301) 903-8309, <u>noelle.metting@science.doe.gov</u>, <u>http://science.energy.gov/ber/research/bssd/low-dose-radiation/;</u>
- 4. to operate experimental biological stations at synchrotron and neutron sources; Roland Hirsch, (301) 903-9009, <u>roland.hirsch@science.doe.gov</u>, http://science.energy.gov/ber/research/bssd/structural-biology/; and
- 5. to develop radiochemistry and advanced technologies for imaging and high throughput characterization and analysis for BER missions in bioenergy, subsurface, and climate change;

Prem Srivastava, (301) 903-4071, <u>prem.srivastava@science.doe.gov</u>, http://science.energy.gov/ber/research/bssd/radiochemistry-and-imaging-instrumentation/

Subprogram Contact: Todd Anderson, (301) 903-3213, <u>todd.anderson@science.doe.gov</u>, Website: <u>http://science.energy.gov/ber/research/bssd/</u>

## (b) Climate and Environmental Sciences

Research is focused on using DOE's unique resources and facilities to understand the basic physical, chemical, and biological processes of the Earth's System and how these processes may be affected by energy production and use. Research is designed to provide data to enable an objective, scientifically based assessment of the potential for, and the consequences of, human-induced climate change at global and regional scales. The program also provides data and models to enable assessments of mitigation options to prevent such change.

The major objectives are:

 understanding and simulating the radiation balance from the surface of the Earth to the top of the atmosphere, including the effect of clouds, water vapor, trace gases, and aerosols. (The Atmospheric Radiation Measurement Climate Research Facility provides key observational data to the climate research community on the radiative properties of the atmosphere, especially clouds and aerosols. This national user facility includes highly instrumented ground stations, mobile facilities, and an aerial vehicles program.); Wanda Ferrell (ARM), (301) 903-0043, <u>wanda.ferrell@science.doe.gov</u>, http://science.energy.gov/ber/research/cesd/arm-climate-research-facility/; Ashley

Williamson (Atmospheric System Research), (301) 903-3120, ashley.williamson@science.doe.gov,

http://science.energy.gov/ber/research/cesd/atmospheric-system-research-program/;

- enhancing and evaluating the quantitative models necessary to predict natural climatic variability and possible human-caused climate change at global and regional scales; Dorothy Koch (Earth System Modeling), (301) 903-0105, <u>dorothy.koch@science.doe.gov</u>, <u>http://science.energy.gov/ber/research/cesd/earth-system-modeling-program/</u>; Renu Joseph (Regional Modeling), (301) 903-9237, <u>renu.joseph@science.doe.gov</u>, <u>http://science.energy.gov/ber/research/cesd/regional-and-global-modeling/</u>;
- improving the understanding and representation of terrestrial ecosystem processes in Earth system models, thereby improving the quality of climate model projections and providing the scientific foundation needed to inform DOE's energy decisions; Mike Kuperberg, (301) 903-3511, <u>michael.kuperberg@science.doe.gov</u>,; Dan Stover, (301) 903-0289, <u>daniel.stover@science.doe.gov</u>, <u>http://science.energy.gov/ber/research/cesd/terrestrialecosystem-science/;</u>
- improving approaches to integrated assessments of effects of, and options to mitigate, climatic change; Bob Vallario, (301) 903-5758, <u>robert.vallario@science.doe.gov</u>, <u>http://science.energy.gov/ber/research/cesd/integrated-assessment-of-global-climate-change/;</u>
- subsurface biogeochemical research to understand and predict subsurface contaminant fate and transport; David Lesmes, (301) 903-2977, <u>david.lesmes@science.doe.gov</u>, <u>http://science.energy.gov/ber/research/cesd/subsurface-biogeochemical-research/;</u> and

6. supporting research that take advantage of a second national user facility, the Environmental Molecular Sciences Laboratory (EMSL), that houses an unparalleled collection of state-of-the-art capabilities, including a supercomputer and over 60 major instruments, providing integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences. EMSL also contributes to systems biology by providing leading edge capabilities in proteomics; Paul Bayer, (301) 903-5324, paul.bayer@science.doe.gov, http://science.energy.gov/ber/research/cesd/environmental-molecular-sciences-laboratory/.

Subprogram Contact: Gary Geernaert, (301) 903-3281, <u>Gerald.Geernaert@science.doe.gov</u> Website: <u>http://science.energy.gov/ber/research/cesd/</u>

#### 4. Fusion Energy Sciences (FES)

Program Website: http://science.energy.gov/fes/

The mission of the Fusion Energy Sciences (FES) program is to expand the fundamental understanding of matter at very high temperatures and densities and to build the scientific foundation needed to develop a fusion energy source. This is accomplished by studying plasma and its interaction 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 advances 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 addresses scientific challenges by developing and continually improving the hardware, materials, and technology that are incorporated into existing and next-generation fusion research facilities, thereby enabling these facilities to achieve higher levels of performance and flexibility, and consequently allowing the exploration of new scientific regimes.

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 & AT Optimization

The ITER & 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, <u>Mark.Foster@science.doe.gov</u> Website: <u>http://science.energy.gov/fes/research/</u>

# (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 multi-scale, 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 multi-scale and multi-physics 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 simulation sof 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, <u>John.Mandrekas@science.doe.gov</u> Website: <u>http://science.energy.gov/fes/research/</u>

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

The Targeted Validation Platforms 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. Validation Platforms 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 Validation Platform experiments, and several small topic-specific investigations.

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

#### (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, corresponding 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 electron volts) can have pressures as low as 0.1 Mbar and are also considered high-energy-density plasmas. Scientific explorations of high-energy-density states of matter are being supported in this program.

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

#### (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. Since many of these research topics are covered under the regular annual solicitation of the NSF/DOE Partnership in Basic Plasma Science and Engineering, it is advisable to also check with this program.

Subprogram Contact: Nirmol Podder, (301) 903-9536, <u>Nirmol.Podder@science.doe.gov</u> Websites: <u>http://science.energy.gov/fes/research/</u> http://www.nsf.gov/funding/pgm\_summ.jsp?pims\_id=5602

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

The materials used to confine burning plasma are exposed to extreme environments with respect to bombardment by highly energetic particles, damaging heat loads, and chemical attack. Hence, a major goal of the FES program is to support the development of the scientific understanding required to design and deploy the materials needed to withstand a burning plasma environment. In addition, the Materials Science and Enabling Technologies program supports research in: plasma heating and fueling, superconducting magnets, plasma neutronics, and tritium management. The materials science and related research also helps to (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; and (4) explore the science underlying these technological advances.

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

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

Diagnostics—the scientific instruments used to make detailed measurements of the behavior of plasmas—are key to advancing our abilities to predict and control the behavior of fusion plasmas in a variety of device configurations. New observations leading to scientific breakthroughs are often enabled by the development of a diagnostic technique or methodology with higher resolution, higher reliability, reduced complexity, or access to previously unmeasured parameters. 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, <u>Francis.Thio@science.doe.gov</u> Website: <u>http://science.energy.gov/fes/research/</u>

# 5. High Energy Physics (HEP)

Program Website: <u>http://science.energy.gov/hep</u>

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 to provide precision measurements of these phenomena; and
- *The Cosmic Frontier*, where non-accelerator-based experiments observe the cosmos and detect cosmic particles, making measurements of natural phenomena that can provide information about the nature of dark matter, dark energy, and other fundamental properties of the Universe that impact our understanding 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 four cross-cutting research areas that enable new scientific opportunities by developing the necessary tools and methods for discoveries:

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

The scientific objectives and priorities for the field recommended by the High Energy Physics Advisory Panel are detailed in the long-range plan available at: <u>http://science.energy.gov/~/media/hep/pdf/files/pdfs/p5\_report\_06022008.pdf</u> Applications in response to this open solicitation may propose activities *in support of* HEP research, which include, but are not limited to: conferences, experimental operations, conceptual research and development (R&D), design or fabrication directed towards a specific project within the HEP scientific program.

Applicants addressing *specific HEP research or technology development* activities in one or more of the six research subprograms (as in the examples given below, excluding Computational Research in High Energy Physics), are *strongly encouraged* to submit applications to either the annual HEP Comparative Review Funding Opportunity Announcement and/or to the annual Early Career Research Program Funding Opportunity Announcement, each available through <u>http://www.grants.gov</u>. Applications that are in direct support of HEP research activities in the six subprograms may be submitted to this open solicitation but will likely be assigned a lower programmatic priority than those from the comparative review process.

Applications submitted to this open solicitation for support of *generic particle detector R&D* efforts should be directed to the Particle Detector Research and Development research area described below. However, applicants proposing physics studies and pre-conceptual R&D efforts directed towards a *specific experiment* within an experimental frontier should submit their application to the relevant HEP scientific frontier research area.

#### (a) Experimental Research at the Energy Frontier in High Energy Physics

This research area 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 data being collected at the Large Hadron Collider (LHC) by the ATLAS and CMS experiments and for analyses using data collected at the Fermilab Tevatron collider. This research area also provides graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities. Applications addressing physics studies and pre-conceptual R&D directed towards specific future Energy Frontier experiments are also accepted. Support for Heavy Ion Physics research is <u>not</u> provided under this research area.

Subprogram Contact: Abid Patwa, (301) 903-0408, <u>abid.patwa@science.doe.gov</u> Website: <u>http://science.energy.gov/hep/research</u>

#### (b) Experimental Research at the Intensity Frontier in High Energy Physics

This research area 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 research area 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 research area includes searches for proton decay. This program also provides graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities. Applications addressing physics studies and pre-conceptual R&D directed towards specific future Intensity Frontier experiments are also accepted. Support for LHCb research is <u>not</u> provided under this research area.

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

# (c) Experimental Research at the Cosmic Frontier in High Energy Physics

This research area includes efforts in direct support of experimental HEP using naturally occurring cosmic particles and observations of the cosmos. Studies of the nature of dark energy and direct-detection searches for dark matter particles are major activities in this program. This area also uses cosmic rays and photons to search for indirect signals of dark matter, the presence of primordial antimatter and other fundamental phenomena related to the properties of particles, space and matter; and measurements of the cosmic microwave background to explore the nature of inflation in the early universe. This program also provides graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities. Applications addressing physics studies and pre-conceptual R&D directed towards specific future Cosmic Frontier experiments are also accepted.

Studies of gravitational physics, classical astrophysics phenomena, or fundamental symmetries are <u>not</u> included in this research area.

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

#### (d) Theoretical Research in High Energy Physics

This research area 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 verify such predictions. Topics studied in theoretical high energy physics research include, but are not limited to: phenomenological and theoretical studies that support experimental HEP research at the Energy, Intensity and Cosmic Frontiers, both in understanding the data and in finding new directions for experimental exploration; development of analytical and numerical computational techniques for these studies; and construction and exploration of theoretical frameworks for understanding fundamental particles and forces at the deepest level possible. This research area 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) Computational Research in High Energy Physics

This research area currently supports partnership (SciDAC - Scientific Discovery through Advanced Computing) projects and specific computational tools (Scientific Computing) that target the cross-cutting needs of HEP. Sponsored support within this area is confined to computational science and simulations that broadly advance scientific discovery aligned with the HEP mission, and research on computing and data management tools that benefit multiple parts of the program.

This subprogram does <u>not</u> support computing research and/or activities specific to individual projects in any of the other six research and technology R&D subprograms described in this open solicitation. Support for specific operation efforts and/or hardware requests in each of the other subprograms are also outside the scope of this area. Applicants proposing such activities should submit their application to the relevant subprogram.

Subprogram Contact: Lali Chatterjee, (301) 903-0435, <u>lali.chatterjee@science.doe.gov</u> Website: <u>http://science.energy.gov/hep/research</u>

#### (f) Accelerator Science and Technology Research & Development in High Energy Physics

The accelerator science and technology R&D research area develops the next generation of particle accelerators and related technologies for discovery science; and also for possible applications in industry, medicine and other fields. This research area supports world-leading research in the physics of particle beams and long-range, exploratory research aimed at developing new concepts. This research area also provides graduate and postdoctoral research training, equipment for experiments and related computational efforts.

Topics studied in the accelerator science and technology R&D research area include, but are not limited to: accelerator and beam physics, including analytic and computational techniques for modeling particle beams and simulation of accelerator systems; novel acceleration concepts; the science of high gradients in accelerating cavities and structures; high-power radio frequency sources; high-brightness beam sources; and beam instrumentation. Also of interest are superconducting materials and conductor development; innovative magnet design and development of high-field superconducting magnets; as well as associated testing and cryogenic systems. Muon collider and neutrino factory R&D is coordinated through the Muon Accelerator Program (MAP) and is outside the scope of this FOA.

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

#### (g) Particle Detector Research and Development in High Energy Physics

The particle detector R&D research area develops the next generation of detectors for particle physics and supports research leading to fundamental advances in the science of particle

detection and instrumentation. This is typically long-term, "generic" research on the physics of particle detection that has potential for wide applicability and/or high impact.

Topics studied in the particle detector R&D research area include, but are not limited to: lowmass, 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 research area develops next-generation computational tools and techniques in support of experimental HEP research. This research area also provides graduate and postdoctoral research training, equipment for experiments and related computational efforts. Support for engineering and other technical efforts and equipment required for experimental detector R&D and fabrication is included in this research area.

Subprogram Contact: Glen Crawford, (301) 903-4829, <u>glen.crawford@science.doe.gov</u> Website: <u>http://science.energy.gov/hep/research</u>

#### 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. It is one of the enduring mysteries of the universe: What, really, is matter? What are the units that matter is made of, and how do they fit together to give matter the properties we observe?

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 Nuclear Physics subprogram focuses primarily on experimental tests of the mathematical description of how quarks and gluons in nuclear matter interact, referred to as Quantum Chromodynamics (QCD) and in particular, the behavior of quarks inside protons and neutrons. Specific questions addressed include: What is the internal landscape of the protons and neutrons (collectively known as 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? Various experimental approaches are pursued to determine the distribution of up, down, and strange quarks (and implicitly their antiquarks) in nucleons, as well as the roles of the gluons that bind the quarks; the effects of the quark and gluon spins within the nucleon; and the effect of the nuclear environment on the quarks and gluons. The subprogram also produces and studies higher-mass "excited states" of hadrons (composite particles, including nucleons, made of quarks, antiquarks, and gluons) predicted by QCD in order to determine how the theory leads to the observed properties of these strongly interacting particles. In pursuing these goals, the Medium Energy subprogram supports experimental research primarily at the Thomas Jefferson National Accelerator Facility (TJNAF) and the Relativistic Heavy Ion Collider (RHIC).

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

# (b) Heavy Ion Nuclear Physics

The Heavy Ion Nuclear Physics subprogram focuses on studies of nuclear matter at extremely high densities and temperatures that are directed primarily at answering the overarching questions defining one of the three nuclear physics frontiers—Quantum Chromodynamics (QCD). 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 space-time? With careful measurements, scientists are accumulating data which offers insights into the processes early in the creation of the universe, and how protons, neutrons, and other bits of normal matter developed from that plasma. Important avenues of investigation are directed at learning more about the physical characteristics of the quark-gluon plasma including exploring the energy loss mechanism for quarks and gluons traversing the plasma, determining the speed of sound in the plasma and locating the critical point for the transition between the plasma and normal matter. 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: James Sowinski, (301) 903-7587, james.sowinski@science.doe.gov Website: <u>http://science.energy.gov/np/research/</u>

#### (c) Low Energy Nuclear Physics

The Low Energy Nuclear Physics subprogram is the most diverse within the NP portfolio, supporting research activities aligned with scientific thrusts focusing primarily on answering the overarching questions associated with two science frontiers: Nuclei and Nuclear Astrophysics, and Fundamental Symmetries and Neutrinos. Questions associated with the Nuclei and Nuclear Astrophysics frontier include: What is the nature of the nuclear force that binds protons and neutrons into stable nuclei and rare isotopes? 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? One major goal of this subprogram is to develop a comprehensive description of nuclei using beams of stable and rare isotopes to yield new insights and reveal new nuclear phenomena. A second is to measure the cross sections of nuclear reactions powering stars and resulting in spectacular stellar explosions responsible for the synthesis of the elements. Questions addressed in the Fundamental Symmetries and Neutrinos frontier, which uses neutrinos and neutrons as primary probes, 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 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? This subprogram also seeks to measure or set a limit on the neutrino mass and to determine if the neutrino is its own anti-particle (a Majorana particle). Neutrino properties are believed to play an important role in the evolution of the cosmos. Beams of cold and ultracold neutrons are used to study fundamental properties of neutrons. Precision studies to observe or set a limit on violation of time-reversal invariance in nucleonic, nuclear, and atomic systems investigate the origin of dominance of matter over antimatter in the universe, addressing fundamental questions in nuclear and particle physics, astrophysics, and cosmology.

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

#### (d) Nuclear Theory

The Nuclear Theory subprogram provides the theoretical support needed to interpret the wide range of data obtained from the experimental nuclear science subprograms, and to advance new ideas and hypotheses that identify potential areas for future experimental investigations. Nuclear Theory addresses all three of NP's scientific frontiers. One major theme of theoretical research is the development of an understanding of the mechanisms and effects of quark confinement and deconfinement. A quantitative description of these phenomena, QCD, is one of this subprogram's greatest intellectual challenges. New theoretical and computational tools are also being developed to describe nuclear many-body phenomena; these approaches will likely also see important applications in condensed matter physics and in other areas of the physical sciences. Another major research area is nuclear astrophysics, which includes efforts to understand the origins of the elements (e.g., via supernovae) and the consequences that neutrino masses have for nuclear astrophysics and for the current Standard Model of elementary particles and forces.

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

#### (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 E. (Ted) Barnes, (301) 903-3212, <u>ted.barnes@science.doe.gov</u> Website: <u>http://science.energy.gov/np/research/</u>

#### (f) Isotope Development and Production for Research and Applications

The Isotope Development and Production for Research and Applications subprogram supports the production, distribution, and development of production techniques for radioactive and enriched isotopes in short supply and critical to the Nation. Isotopes are commodities of strategic importance for the Nation that are essential for energy exploration and innovation, medical applications, national security, and basic research. An important goal of the program is to make key isotopes more readily available to meet U.S. needs. To achieve this goal, 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. 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 to develop new or improved production or separation techniques for high priority isotopes in short supply. Examples for planned research include the need for positron-emitting radionuclides to support the rapidly growing area of medical imaging using positron emission tomography (PET), development of isotopes that support medical research used to diagnose and treat diseases spread through acts of bioterrorism, development of production methods for alpha-emitting radionuclides that exhibit great potential in disease treatment, development and use of research isotopes for various biomedical applications, development of stable isotope enrichment technologies, and the need for alternative isotope supplies for national security applications and advanced power sources. One of the high priorities is to conduct R&D aimed at re-establishing a domestic capability for stable isotope enrichment in the U.S. All R&D activities are peer reviewed. Another high priority is to provide opportunities for workforce development in the areas of nuclear chemistry and radiochemistry. These disciplines are essential to the long-term health of the fields of radioisotope production and applications.

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

# (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 Facility for Rare Isotope Beams (FRIB).

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

# Section II – AWARD INFORMATION

# A. TYPE OF AWARD INSTRUMENT

DOE anticipates awarding grants and cooperative agreements under this 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.

DOE will consider funding multi-institution collaborations under this FOA.

# **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 2014, subject to the availability of FY 2014 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.

DOE is under no obligation to pay for any costs associated with preparation or submission of applications. 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

(See B. Estimated Funding Section above.)

The award size will depend on the number of meritorious applications and the availability of appropriated funds.

Ceiling None

Floor None

# **D. EXPECTED NUMBER OF AWARDS**

(See B. Estimated Funding Section above.)

The number of awards is subject to availability of FY 2014 appropriated funds. Historically, applications that arrive in response to the open solicitation for applications have resulted in 200 to 350 new awards per year.

The exact number of awards will depend on the number of meritorious applications and the availability of appropriated funds.

# E. ANTICIPATED AWARD SIZE

(See B. Estimated Funding Section above.)

N/A

# F. PERIOD OF PERFORMANCE

(See B. Estimated Funding Section above.)

N/A

# G. TYPE OF APPLICATION

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

# Section III – ELIGIBILITY INFORMATION

# A. ELIGIBLE APPLICANTS

All types of applicants are eligible to apply, except Federally Funded Research and Development Center (FFRDC) Contractors, and nonprofit 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. ELIGIBLE INDIVIDUALS**

Individuals with the skills, knowledge, and resources necessary to carry out the proposed research as a Program Director/Principal Investigator are invited to work with their organizations to develop an application for assistance. Individuals from underrepresented groups as well as individuals with disabilities are always encouraged to apply for assistance.

# Section 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 <u>http://www.grants.gov</u>, select "Apply for Grants", and then select "Download Application Package." Enter the CFDA number (81.049) and/or the funding opportunity number (DE-FOA-0000995) shown on the cover of this FOA and then follow the prompts to download the application package.

Applications submitted through <u>www.FedConnect.net</u> will not be accepted.

# **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 APPLICATION FORMS

You must complete the mandatory forms and any applicable optional forms (e.g., Disclosure of Lobbying Activities (SF-LLL)) 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 announcement.

#### APPLICATIONS FOR NEW AWARDS

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.

#### APPLICATIONS FOR RENEWAL AWARDS

Renewal applications are requests for additional funding for a period subsequent to that provided by a current award. 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:

- Include under the project description section information on any changes that affect the overall direction of the research being pursued.
- Include an estimate of anticipated unexpended funds that will remain at the end of the current project period.
- 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.

# APPLICATIONS FOR SUPPLEMENTAL AWARDS

Two types of supplemental applications may be submitted:

- 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.
- If the awardee needs additional funds:
  - for increased costs that could not have been predicted when the application was originally approved; or
  - 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 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.

# 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 is available 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.

#### CERTIFICATIONS AND REPRESENTATIONS

By submitting an application in response to this FOA the Applicant makes the following representations and certifications:

- It is **not** a corporation that has been convicted (or had an officer or agent of such corporation acting on behalf of the corporation convicted) of a felony criminal violation under **any** Federal law within the preceding 24 months.
- No officer or agent of the corporation have been convicted of a felony criminal violation for an offense arising out of actions for or on behalf of the corporation under Federal law in the past 24 months.
- It is **not** a corporation that has any unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or have lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability.
- If chosen for a grant award in excess of \$1,000,000, it will, by the end of the Federal Government's fiscal year, upgrade the efficiency of its facilities by replacing any incandescent lighting of the type for which section 325 of the Energy Policy and Conservation Act (42 USC 6295) establishes a standard that does not meet or exceed the energy efficiency standard for incandescent light bulbs set forth in that section with a lamp that meets or exceeds the standards for lamps established in or pursuant to that section.

#### PUBLIC POLICY REQUIREMENTS

The applicant assures DOE of its compliance with applicable public policy requirements, including the following:

Animal Welfare Act	7 USC 2131 et seq., 10 CFR 600, 10 CFR 602
Buy American Act	41 USC 10 et seq.
Cargo Preference Act	46 USC 55305, 46 CFR 381.7
Civil Rights Protections	10 CFR 1040, 10 CFR 600
Debarment and Suspension	10 CFR 600, 2 CFR 180, 2 CFR 901
Drug-Free Workplace Act	41 USC 701, 10 CFR 607
Environmental Protections	42 USC 7401, 33 USC 1251, 42 USC 4321, 10 CFR 600
False Claims Act	31 USC 3729, 18 USC 287, 18 USC 1001, 10 CFR 1013
Federal Funding Accountability and Transparency Act	P.L. 109-282, 2 CFR 170
Fly America Act	49 USC 40118
Hatch Act	5 USC 1501 et seq., 10 CFR 600
Human Research Subjects Protections	10 CFR 745, 10 CFR 600
Lobbying Disclosure Act	2 USC 1601 et seq.
Lobbying Prohibitions	31 USC 1352, 10 CFR 601
Metric System use	EO 12770
Non-delinquency on Federal Debt	28 USC 3201
Prohibition on benefitting Members of Congress	41 USC 6306
Seat Belt Use	EO 13043
Terrorist Financing	EO 13224, 66 FR 49079
Text Messaging While Driving	EO 13513, 74 FR 51225
Trafficking in Persons	22 USC 7104, 2 CFR 175

# 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 is a summary of the proposed activity suitable for distribution to the public and sufficient to permit potential reviewers to identify conflicts of interest. It must be a self-contained document. Provide the name of the applicant, the project title, the project director/principal investigator(s) (PD/PI) and the PD/PI's institutional affiliation, any coinvestigators and their institutional affiliations, the objectives of the project, a description of the project, including methods to be employed, and the potential impact of the project (i.e., benefits, outcomes). A sample is provided below:

A Really Great Idea A. Smith, Lead Institution (Principal Investigator) A. Brown, Institution 2 (Co-Investigator) A. Jones, Institution 3 (Co-Investigator)

Text of abstract

The project summary must not exceed 1 page when printed using standard 8.5" by 11" paper with 1" margins (top, bottom, left and right) with font not smaller than 11 point. To attach a Project Summary/Abstract, click "Add Attachment."

- Do not include any proprietary or sensitive business information.
- DOE may use the abstract may to prepare public reports about supported research.

# DOE COVER PAGE

(PART OF PROJECT NARRATIVE ATTACHED TO FIELD 8 ON THE FORM)

The application narrative should begin with a cover page. The cover page must include the following items:

- The project title
- Applicant/Institution:
- Street Address/City/State/Zip:
- Postal Address:
- Lead PI name, telephone number, email:
- Administrative Point of Contact name, telephone number, email:
- Funding Opportunity FOA Number: DE-FOA-0000995
- DOE/Office of Science Program Office:
- DOE/Office of Science Program Office Technical Contact:
- DOE Award Number (if Renewal or Supplemental Application):
- Research area or areas as identified in Section I of this FOA (if applicable) :

#### COVER PAGE SUPPLEMENT FOR COLLABORATIONS

#### (PART OF PROJECT NARRATIVE ATTACHED TO FIELD 8 ON THE FORM)

Collaborative applications submitted from different institutions must 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 abstract, narrative, and all required appendices and attachments, must be identical with one exception: Each application must 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.

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

The Office of Science will use the multiple applications associated with a collaborative group to create one consolidated document for merit review that consists of the common, identical application materials combined with a set of detailed budgets from the partner institutions. It is very important that every application in the collaborative group be identical (including the title) with the exception of the budget and budget justification pages.

If the project is a collaboration, provide the following information on a separate page as a supplement to the cover page.

- List all collaborating institutions by name with each institution's principal investigator on the same line.
- Indicate the lead PI who will be the point of contact and coordinator for the combined research activity.
- Provide a statement explaining the leadership structure of the collaboration.
- Include a description of each collaborating institution's facilities, equipment, and resources that will be made available to the collaborative group.
- If applicable, explain how students and junior researchers will be trained and mentored by the collaborators.
- Include a table modeled on the following chart providing summary budget information from all collaborating institutions. Provide the total costs of the budget request in each year for each institution and totals for all rows and columns.

Collaborative Application Information						
	Name	Institution	Year 1 Budget	•••	Year N Budget	Total Budget
Lead			Duuget		Duuget	Duuget
PI						
Co-PI						
Co-PI						
Co-PI						

Example budget table (\$ in thousands)

\* Note that collaborating applications must be submitted separately.

#### PROJECT NARRATIVE (FIELD 8 ON THE FORM)

The project narrative consists of technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right). The font must not be smaller than 11 point.

Do not include any Internet addresses (URLs) that provide supplementary or additional information that constitutes a part of the application. Merit reviewers are not required to access Internet sites. See Part VIII.D for instructions on how to mark proprietary application information. To attach a Project Narrative, click "Add Attachment."

The Project Narrative comprises the research plan for the project. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. 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 also indicate which project personnel will be responsible for which activities. There should be no ambiguity about which personnel will perform particular parts of the project.

**For Collaborative Proposals Only**: Each collaborating institution must submit an identical common narrative. The common narrative must identify which tasks and activities will be performed by which of the collaborating institutions in every budget period of the proposed project. The budget and the budget justification which are unique to each collaborating institution—may refer to parts of the common narrative to further identify each collaborating institution's activities in the joint project. There should be no ambiguity about each institution's role and participation in the collaborative group.

The Office of Science will use the multiple applications associated with a collaborative group to create one consolidated document for merit review that consists of the common, identical application materials combined with a set of detailed budgets from the partner institutions. It is very important that every application in the collaborative group be identical (including the title) with the exception of the budget and budget justification pages.

#### APPENDIX 1: BIOGRAPHICAL SKETCH

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 (curriculum vitae) for each person must not exceed 2 pages when printed on 8.5" by 11" paper with 1 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 5 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. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the Principal Investigator interacted on a regular basis while the research was being done. 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). Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates during the past 5 years.

**Personally Identifiable Information**: Do not include sensitive personally identifiable information such as a Social Security Number, date of birth, or city of birth. Do not include information that a merit reviewer should not make use of.

#### 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. Concurrent submission of an application to other organizations for simultaneous consideration will not prejudice its review.

• Do not attach a separate file.

#### APPENDIX 3: BIBLIOGRAPHY & REFERENCES CITED

Provide a bibliography of any references cited in the Project Narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. For research areas where there are routinely more than ten coauthors of archival publications, you may use an abbreviated style such as the Physical Review Letters (PRL) convention for citations (listing only the first author). For example, your paper may be listed as, "A Really Important New Result," A. Aardvark et. al. (MONGO Collaboration), PRL 999. Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the application. Provide the Bibliography and References Cited information as an appendix to your project narrative.

• Do not attach a separate file.

#### APPENDIX 4: FACILITIES & OTHER RESOURCES

This information is used to assess the capability of the organizational resources, including subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. Please 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 ATTACHMENT

If you need to elaborate on your responses to questions 1-6 on the "Other Project Information" document, please provide the Other Attachment information as an appendix to your project narrative. Information not easily accessible to a reviewer may be included in this appendix, but do not use this appendix to circumvent the page limitations of the application. Reviewers are not required to consider information in this appendix.

• 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. Follow the above instructions to include the information as appendices to the project narrative file.

#### 3. Research And Related Budget

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

Section A Senior/Key Person	For each Senior/Key Person, enter the requested information. List personnel, base salary, the number of months that person will be allocated to the project, requested salary fringe benefits, and the total funds requested for each person. The requested salary must be the product of the base salary and the effort. Include a written narrative in the budget justification that justifies the
Section B Other Personnel	need for requested personnel.List personnel, the number of months that person will be allocated to the project, requested salary fringe benefits, and the total funds requested for each person.Include a written narrative in the budget justification that fully justifies
	the need for requested personnel.
Section C Equipment	For the purpose of this budget, equipment is designated as an item of property that has an acquisition cost of \$5,000 or more and an expected service life of more than one year. (Note that this designation applies for proposal budgeting only and differs from the DOE definition of capital equipment.) List <b>each</b> item of equipment separately and justify each in the budget justification section. Do not aggregate items of equipment. Allowable items ordinarily will be limited to research equipment and apparatus not already available for the conduct of the work. General-

Budget Fields

	purpose office equipment is not eligible for support unless primarily or		
	exclusively used in the actual conduct of scientific research.		
Section D	For purposes of this section only, travel to Canada or to Mexico is		
Travel	considered domestic travel. In the budget justification, list each trip's		
Tiuvei	destination, dates, estimated costs including transportation and		
	subsistence, number of staff traveling, the purpose of the travel, and how		
	it relates to the project. Indicate the basis for the cost estimate (quotes		
	from vendors or suppliers, past experience of similar items, or some other		
	basis). To qualify for support, attendance at meetings or conferences must		
	enhance the investigator's capability to perform the research, plan		
	extensions of it, or disseminate its results. Domestic travel is to be		
	justified separately from foreign travel.		
Section E	If applicable, submit training support costs. Educational projects that		
Participant/Trainee	intend to support trainees (precollege, college, graduate and post		
Support Costs	graduate) must list each trainee cost that includes stipend levels and		
Support Costs	amounts, cost of tuition for each trainee, cost of any travel (provide the		
	same information as needed under the regular travel category), and costs		
	for any related training expenses. Participant costs are those costs		
	associated with conferences, workshops, symposia or institutes and		
	breakout items should indicate the number of participants, cost for each		
	participant, purpose of the conference, dates and places of meetings and		
	any related administrative expenses.		
	Indicate the basis for the cost estimate (quotes from vendors or suppliers,		
	past experience of similar items, or some other basis).		
Section F	<ul> <li>Materials and Supplies: Enter total funds requested for materials</li> </ul>		
Other Direct Costs	and supplies in the appropriate fields. In the budget justification,		
Other Direct Costs	indicate general categories such as glassware, and chemicals,		
	including an amount for each category (items not identified under		
	"Equipment"). Categories less than \$1,000 are not required to be		
	itemized. Indicate the basis for the cost estimate (quotes from		
	vendors or suppliers, past experience of similar items, or some		
	other basis).		
	<ul> <li>Publication Costs: Enter the total publication funds requested. The</li> </ul>		
	proposal budget may request funds for the costs of documenting,		
	preparing, publishing or otherwise making available to others the		
	findings and products of the work conducted under the award. In		
	the budget justification, include supporting information. Indicate		
	the basis for the cost estimate (quotes from vendors or suppliers,		
	past experience of similar items, or some other basis).		
	<ul> <li>Consultant Services: Enter total funds requested for all consultant</li> </ul>		
	services. In the budget justification, identify each consultant, the		
	services in the budget justification, identify each consultant, the services he/she will perform, total number of days, travel costs, and		
	total estimated costs. Indicate the basis for the cost estimate (quotes		
	from vendors or suppliers, past experience of similar items, or some		
	other basis).		
	<ul> <li>ADP/Computer Services: Enter total funds requested for</li> </ul>		
	- infreemputer services. Enter total funds requested for		

	<ul> <li>ADP/Computer Services. The cost of computer services, including computer-based retrieval of scientific, technical and education information may be requested. In the budget justification, include the established computer service rates at the proposing organization if applicable. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).</li> <li>Subawards/Consortium/Contractual Costs: Enter total costs for all subawards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details.</li> <li>Equipment or Facility Rental/User Fees: Enter total funds requested for Equipment or Facility Rental/User Fees. In the budget justification, identify each rental/user fee and justify. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).</li> <li>Alterations and Renovations: Enter total funds requested for Alterations and Renovations. In the budget justification, itemize by category and justify the costs of alterations and renovations, including repairs, painting, removal or installation of partitions, shielding, or air conditioning. Where applicable, provide the square footage and costs.</li> <li>Other: Add text to describe any other Direct Costs not requested above. Enter costs associated with "Other" item(s). Use the budget justification to further itemize and justify.</li> </ul>
Section G	This represents Total Direct Costs (Sections A through F)
Direct Costs	
Section H	Enter the Indirect Cost information for each field. Only four general
Other Indirect Costs	categories of indirect costs are allowed/requested on this form, so please
	consolidate if needed. Include the cognizant Federal agency and contact
Castian I	information if using a negotiated rate agreement.
Section I	This is the total of Sections G and H
Total Direct and Indirect Costs	
manoet costs	

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; materials 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 Subawardees, other than DOE FFRDC Contractors**: You must provide a separate cumulative R&R budget for each subawardee 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 subawardees (See Section IV.D for submission of Subawardees' multi-year budgets). Download the R&R Budget Attachment from the R&R SUBAWARD BUDGET ATTACHMENT(S) FORM and e-mail it to each subawardee that is required to submit a separate budget. After the subawardee has e-mailed its completed budget back to you, attach it to one of the blocks provided on the form. Use up to 10 letters of the subawardee'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 2 digit state code followed by a dash and a 3 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. Summary of Required Forms/Files

Your application must include the following items:

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
<b>RESEARCH &amp; RELATED BUDGET</b>	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**

None

# 2. Pre-application Due Date

None

# **3. Application Due Date**

This FOA will remain open until September 30, 2014, 11:59 PM Eastern Time, or until it is succeeded by another issuance, whichever occurs first. This Annual FOA DE-FOA-0000995 succeeds FOA DE-FOA-0000768, which was published September 30, 2012.

Applications for conference or workshop support must be submitted at least six months before the meeting date and no later than April 1, 2014, to be considered for FY 2014 funding.

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.

# F. INTERGOVERNMENTAL REVIEW

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

# G. FUNDING RESTRICTIONS

Funding for all awards and future budget periods are contingent upon the availability of funds appropriated by Congress for the purpose of this program and the availability of future-year budget authority.

**Cost Principles**: Costs must be allowable, allocable and reasonable in accordance with the applicable Federal cost principles referenced in 10 CFR 600. The cost principles for commercial organization are in FAR Part 31.

**Pre-award Costs**: Recipients may charge to an award resulting from this announcement preaward 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 600 and 2 CFR 215. 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 <u>www.Grants.gov</u>. 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 <u>support@grants.gov</u>.

Please ensure that you have read the applicable instructions, guides, help notices, frequently asked questions, and other forms of technical support on grants.gov.

# 2. Registration Process

#### **ONE-TIME REGISTRATION PROCESS**

You must complete the one-time registration process (all steps) before you can submit your first application through Grants.gov (See <u>http://www.grants.gov/web/grants/applicants/grant-application-process.html</u>). We recommend that you start this process at least six weeks before the application due date. It may take 44 days or more to complete the entire process. Use the Grants.gov Organizational Registration Checklists at

<u>http://www.grants.gov/web/grants/applicants/organization-registration.html</u> to guide you through the process. IMPORTANT: During the SAM 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).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

#### **3. Viewing Submitted Applications**

Each Grants.gov application submitted to the DOE Office of Science (SC) automatically transfers into PAMS and is subsequently assigned to a program manager. At the time of program manager assignment, the three people listed on the SF-424 (R&R) cover page will receive an email with the subject line, "Receipt of Proposal 0000xxxxx by the DOE Office of Science." These three people are the Principal Investigator (Block 14), Authorized Representative (Block 19), and Point of Contact (Block 5). In PAMS notation, applications are known as proposals, the Principal Investigator is known as the PI, the Authorized Representative is known as the Sponsored Research Officer/Business Officer/Administrative Officer (SRO/BO/AO), and the Point of Contact is known as the POC.

There will be a period of time between the application's receipt at grants.gov and its assignment to a DOE Office of Science program manager. Program managers are typically assigned two weeks after applications are due at grants.gov: please refrain from attempting to view the proposal in PAMS until you receive an email providing the assignment of a program manager.

Once the email is sent, the PI, SRO/BO/PO, and POC will each be able to view the submitted proposal in PAMS. Viewing the proposal is optional.

You may use the Internet Explorer, Firefox, Google Chrome, or Safari browsers to access PAMS.

Following are two sets of instructions for viewing the submitted proposal, one for individuals who already have PAMS accounts and one for those who do not.

If you already have a PAMS account, follow these instructions:

- 1. Log in to PAMS at <u>https://pamspublic.science.energy.gov/</u>.
- 2. Click the "Proposals" tab and click "Access Previously Submitted Grants.gov Proposal."
- 3. Enter the following information:
  - Proposal ID: Enter the ten-digit PAMS proposal ID, including the leading zeros (e.g., 00002xxxx). Do not use the Grants.gov proposal number. Use the PAMS number previously sent to you in the email with subject line, "Receipt of Proposal ...".
  - Email (as entered in Grants.gov proposal): Enter your email address as it appears on the SF424(R&R) Cover Page.

- Choose Role: Select the radio button in front of the role corresponding to the SF-424 (R&R) cover page. If your name appears in block 19 of the SF-424 (R&R) cover page as the authorizing representative, select "SRO/BO/AO (Sponsored Research Officer/Business Officer/Administrative Officer)." If your name appears in block 14 of the SF424 R&R cover page as the PI, select "Principal Investigator (PI)." If your name appears in block 5 of the SF424 R&R as the point of contact, select "Other (POC)."
- 4. Click the "Save and Continue" button. You will be taken to your "My Proposals" page. The Grants.gov proposal will now appear in your list of proposals. Click the "Actions/Views" link in the options column next to this proposal to obtain a dropdown list. Select "Proposal" from the dropdown to see the proposal. Note that the steps above will work only for proposals submitted to the DOE Office of Science since May 2012.

If you do not already have a PAMS account, follow these instructions:

- 1. To register, click the "Create New PAMS Account" link on the website <u>https://pamspublic.science.energy.gov/</u>.
- 2. Click the "No, I have never had an account" link and then the "Create Account" button.
- 3. You will be prompted to enter your name and email address, create a username and password, and select a security question and answer. Once you have done this, click the "Save and Continue" button.
- 4. On the next page, enter the required information (at least one phone number and your mailing address) and any optional information you wish to provide (e.g., FAX number, website, mailstop code, additional email addresses or phone numbers, Division/Department). Click the "Create Account" button.
- 5. Read the user agreement and click the "Accept" button to indicate that you understand your responsibilities and agree to comply with the rules of behavior for PAMS.
- 6. You will be taken to the Register to Institution page. Select the link labeled, "Option 1: My institution has submitted a proposal in Grants.gov. I am here to register as an SRO, PI, or POC (Sponsored Research Officer, Principal Investigator, or Point of Contact)."
- 7. Enter the following information:
  - Proposal ID: Enter the ten-digit PAMS proposal ID, including the leading zeros (e.g., 00002xxxx). Do not use the Grants.gov proposal number. Use the PAMS number previously sent to you in the email with subject line, "Receipt of Proposal ...".
  - Email (as entered in Grants.gov proposal): Enter your email address as it appears on the SF424(R&R) Cover Page.
  - Choose Role: Select the radio button in front of the role corresponding to the SF-424 (R&R) cover page. If your name appears in block 19 of the SF-424 (R&R) cover page as the authorizing representative, select "SRO/BO/AO (Sponsored Research Officer/Business Officer/Administrative Officer)." If your name appears in block 14 of the SF424 R&R cover page as the PI, select "Principal Investigator (PI)." If your name appears in block 5 of the SF424 R&R as the point of contact, select "Other (POC)."
- 8. Click the "Save and Continue" button. You will be taken to your "My Proposals" page. The Grants.gov proposal will now appear in your list of proposals. Click the "Actions/Views" link in the options column next to this proposal to obtain a dropdown list. Select "Proposal" from the dropdown to see the proposal.

If you were listed as the PI on a prior submission but you have not previously created an account, you may already be listed in PAMS. If this is the case, you will be taken to the PAMS home page after agreeing to the Rules of Behavior. If that happens, follow the instructions listed above under "If you already have a PAMS account..." to access your Grants.gov proposal.

The steps above will work only for proposals submitted to the DOE Office of Science since May 2012.

For help with PAMS, click the "External User Guide" link on the PAMS website, <u>https://pamspublic.science.energy.gov/</u>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: <u>sc.pams-helpdesk@science.doe.gov</u>. All submission and inquiries about this Funding Opportunity Announcement should reference **DE-FOA-0000995**.

# Section 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; (4) the proposed project is responsive to the objectives of the funding opportunity announcement, and (5) the proposed project is not duplicative of programmatic work. 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 criteria, listed in descending order of importance as found in 10 CFR 605.10 (d), the Office of Science Financial Assistance Program Rule.

- Scientific and/or Technical Merit of the Project;
- Appropriateness of the Proposed Method or Approach;
- Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
- 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 agency's 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.

The questions below are provided to the merit reviewers to elaborate the criteria established by regulation:

#### SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROPOSED RESEARCH

What is the scientific innovation of proposed research? What is the likelihood of achieving valuable results? How might the results of the proposed research impact the direction, progress, and thinking in relevant scientific fields of research? How does the proposed research compare with other research in its field, both in terms of scientific and/or technical merit and originality?

#### APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

How logical and feasible are the research approaches? Does the proposed research employ innovative concepts or methods? Are the conceptual framework, methods, and analyses well justified, adequately developed, and likely to lead to scientifically valid conclusions? Does the applicant recognize significant potential problems and consider alternative strategies?

#### COMPETENCY OF APPLICANT'S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES

What are the past performance and potential of the Principal Investigator (PI)? How well qualified is the research team to carry out the proposed research? Are the research environment and facilities adequate for performing the research? Does the proposed work take advantage of unique facilities and capabilities?

#### REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET

Are the proposed budget and staffing levels adequate to carry out the proposed research? Is the budget reasonable and appropriate for the scope?

# **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 605.10(d) in accordance with the guidance provided in the "Office of Science Merit Review System for Financial Assistance," which is available at: <u>http://www.sc.doe.gov/grants/merit.asp</u>.

#### 2. Selection

The Selection Officials will consider the following items, listed in no order of significance:

- Merit review of the proposed activity
- Availability of funds
- Relevance of the proposed activity to Office of Science priorities
- Ensuring an appropriate balance of activities within Office of Science programs
- Previous performance

#### 3. Discussions and Award

The Government may enter into discussions with a selected applicant for any reason deemed necessary, including but not limited to the following: (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 600 and 10 CFR 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 the application is received.

# Section 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 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, the following items: (1) Special Terms and Conditions; (2) Applicable program regulations, if any; (3) Application as approved by DOE; (4) DOE assistance regulations at 10 CFR 600, or, for Federal Demonstration Partnership (FDP) institutions, the FDP terms and conditions; (5) National Policy Assurances To Be Incorporated As Award Terms; (6) Budget Summary; and (7) Federal Assistance Reporting Checklist, which identifies the reporting requirements.

# **B. ADMINISTRATIVE AND NATIONAL POLICY REQUIREMENTS**

#### **1. Administrative Requirements**

The administrative requirements for DOE grants and cooperative agreements are contained in 10 CFR 600 and 10 CFR 605. Grants and cooperative agreements made to universities, non-profits and other entities subject to 2 CFR 215 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.

#### **REGISTRATION REQUIREMENTS**

Additional administrative requirements for DOE grants and cooperative agreements are contained in 2 CFR 25 (See: <u>http://www.ecfr.gov</u>). Prime awardees must keep their data at the System for Award Management (SAM) current at <u>http://www.sam.gov</u>. SAM is the government-wide system that replaced the Central Contractor Registry (CCR). If you had an active registration in the CCR, you have an active registration in SAM. 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 170. (See: <a href="http://www.ecfr.gov">http://www.ecfr.gov</a>). 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 System for Award Management (SAM).

#### PROHIBITION ON LOBBYING ACTIVITY

By accepting funds under this award, you agree that none of the funds obligated on the award shall be expended, directly or indirectly, to influence congressional action on any legislation or appropriation matters pending before Congress, other than to communicate to Members of Congress as described in 18 USC 1913. This restriction is in addition to those prescribed elsewhere in statute and regulation.

#### 2. Terms and Conditions

The DOE Special Terms and Conditions for Use in Most Grants and Cooperative Agreements are located at <u>http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms</u> under Award Terms.

The standard DOE financial assistance intellectual property provisions applicable to various types of recipients are located at: <a href="http://energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards">http://energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards</a>

# **3. National Policy Assurances**

The National Policy Assurances To Be Incorporated As Award Terms are located at <a href="http://www.nsf.gov/bfa/dias/policy/rtc/appc.pdf">http://www.nsf.gov/bfa/dias/policy/rtc/appc.pdf</a> and at <a href="http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms">http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms</a> under Award Terms.

#### 4. Statement of Substantial Involvement

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

# **C. REPORTING**

Reporting requirements are identified on the Federal Assistance Reporting Checklist, DOE F 4600.2, attached to the award agreement. The checklist is available at <a href="http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance/financial-assistance-forms">http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms</a> under Award Forms.

# Section VII - QUESTIONS/AGENCY CONTACTS

#### **A. QUESTIONS**

Questions relating to the grants.gov 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 <u>support@grants.gov</u>. DOE cannot answer these questions.

Please contact the grants.gov help desk for questions related to grants.gov.

For help with PAMS, click the "External User Guide" link on the PAMS website, <u>https://pamspublic.science.energy.gov/</u>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: <u>sc.pams-helpdesk@science.doe.gov</u>. All submission and inquiries about this Funding Opportunity Announcement should reference **DE-FOA-0000995**. Please contact the PAMS help desk for technological issues with the PAMS system.

Questions regarding the specific program areas and technical requirements may be directed to the technical contacts listed for each program within the FOA or below.

Please contact the program staff with all questions not directly related to the grants.gov or PAMS systems.

Grants.gov	800-518-4726 (toll-free)
Customer Support	support@grants.gov
PAMS	855-818-1846 (toll-free)
Customer Support	301-903-9610
	sc.pams-helpdesk@science.doe.gov
Program Manager	Questions regarding the specific program areas/technical
Scientific Contact	requirements should be directed to the point of contact listed for
	each program office within the FOA

# **B. AGENCY CONTACTS**

# Section 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 FOA 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 FOAs. More information is available at <u>http://www.fedconnect.net</u>.

# **B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE**

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

# C. COMMITMENT OF PUBLIC FUNDS

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

# **D. PROPRIETARY APPLICATION INFORMATION**

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

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

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

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

#### E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL

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

# F. INTELLECTUAL PROPERTY DEVELOPED UNDER THIS PROGRAM

**Patent Rights:** The government will have certain statutory rights in an invention that is conceived or first actually reduced to practice under a DOE award. 42 USC 5908 provides that title to such inventions vests in the United States, except where 35 USC 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. For more information, see <a href="http://energy.gov/gc/patents-licensing-and-patent-waivers">http://energy.gov/gc/patents-licensing-and-patent-waivers</a>.

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 scientific and technical aspects of specific energy technologies, 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.