# FINANCIAL ASSISTANCE FUNDING OPPORTUNITY ANNOUNCEMENT



U. S. Department of Energy Office of Science

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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 are encouraged to 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

https://www.sam.gov/sam/transcript/Quick\_Guide\_for\_Grants\_Registrations\_v1.7.pdf.

Applicants must register with FedConnect at <u>www.fedconnect.net</u>. If an award is made, the full and binding version of the assistance agreement between your institution and DOE 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. There are 3 steps to this process.

- 1. The Authorized Organizational Representative (AOR) must register at: <u>https://apply07.grants.gov/apply/OrcRegister</u>
- 2. An email is sent to the E-Business (E-Biz) POC listed in SAM. The E-Biz POC must approve the AOR registration using their MPIN from their SAM registration.
- 3. AOR verifies that registration was completed at: http://grants.gov/applicants/applicant\_profile.jsp.

More information about the above steps is provided at: <u>http://www.grants.gov/applicants/organization\_registration.jsp</u>.

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 **support@grants.gov**.

**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.

The DOE Office of Science performs many functions for grants and cooperative agreements in PAMS, which is available at <u>https://pamspublic.science.energy.gov</u>.

There are many activities that you can perform in PAMS, and more functionality will be added throughout the near future. Most significantly, you can "register to" your application: You can link yourself to the application after it has been submitted through grants.gov and processed by DOE. You will submit pre-applications and letters of intent through PAMS.

You must register in PAMS to submit a pre-application or a letter of intent.

To access PAMS, you may use the Internet Explorer, Firefox, Google Chrome, or Safari browsers.

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. (Note: If you reviewed for or were listed as PI on a prior submission to the Office of Science but have not previously created an account, you may already be linked to an institution in PAMS. If this is the case, PAMS will take you 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 need not enter the exact name of the institution, but you should enter a word or phrase contained within the institution name. (Hint: If your institution has an acronym, such as ANL for Argonne National Laboratory or UCLA for the Regents of the University of California, Los Angeles, you may 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-0000958**.

# Section I – FUNDING OPPORTUNITY DESCRIPTION

# GENERAL INQUIRIES ABOUT THIS FOA SHOULD BE DIRECTED TO:

#### **Technical/Scientific Program Contact:**

Questions regarding the specific program areas/technical requirements can be directed to the program managers listed for each program within the FOA.

# Administrative Contact (questions about program rules):

Questions about program rules should be sent to <u>early.career@science.doe.gov</u>

# 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 invites grant applications for support under the Early Career Research Program in the following program areas: Advanced Scientific Computing Research (ASCR); Biological and Environmental Research (BER); Basic Energy Sciences (BES), Fusion Energy Sciences (FES); High Energy Physics (HEP), and Nuclear Physics (NP). The purpose of this program is to support the development of individual research programs of outstanding scientists early in their careers and to stimulate research careers in the areas supported by the DOE Office of Science.

# SUPPLEMENTARY INFORMATION

# Office of Science Website: http://science.energy.gov/

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.

Early Career Research Program opportunities exist in the following Office of Science research programs. Additional details about each program, websites, and technical points of contacts are provided in the materials that follow.

# I. Advanced Scientific Computing Research (ASCR)

- (a) Applied Mathematics
- (b) Computer Science

#### **II. Biological and Environmental Research (BER)**

- (a) Systems Biology Enabled Research on the Role of Microbial Communities in Carbon Cycling
- (b) Water Cycle

#### **III. 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 (GPCP)
- (m) Computation and Theoretical Chemistry
- (n) Condensed Phase and Interfacial Molecular Science (CPIMS)
- (o) Catalysis Science
- (p) Separations and Analysis
- (q) Heavy Element Chemistry (HEC)
- (r) Geosciences Research
- (s) Solar Photochemistry
- (t) Photosynthetic Systems
- (u) Physical Biosciences
- (v) Nanoscale Science Research Centers and Electron-Beam Microcharacterization Centers Research
- (w) Accelerator and Detector Research
- (x) X-ray Instrumentation and Technique Development
- (y) Neutron Scattering Instrumentation and Technique Development

# **IV. Fusion Energy Sciences (FES)**

- (a) Magnetic Fusion Energy Science Experimental Research
- (b) Magnetic Fusion Energy Science Theory and Simulation
- (c) High-Energy-Density Plasma Science and Inertial Fusion Energy Science
- (d) General Plasma Science Experiment and Theory
- (e) Materials Science and Enabling Technologies for Fusion

# V. 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) Accelerator Science and Technology Research & Development in High Energy Physics
- (f) Particle Detector Research and Development in High Energy Physics

# VI. 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) Accelerator Research and Development for Current and Future Nuclear Physics Facilities
- (g) Isotope Development and Production for Research and Applications
- (h) Applications of Nuclear Science and Technology
- (i) Advanced Detector Technology Research and Development in Nuclear Physics

# I. 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. A particular challenge of this program is fulfilling the science potential of emerging computing systems and other novel computing architectures, which will require numerous and significant modifications to today's tools and techniques to deliver on the promise of exascale science.

Some priority areas for ASCR are listed below:

- To develop mathematical descriptions, models, methods and algorithms to accurately describe and understand the behavior of complex systems involving processes that span vastly different time and/or length scales.
- To develop the underlying concepts and software to make effective use of computers at extreme scales
- To transform extreme scale data from experiments and simulations into scientific insight.

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 algorithms, software tools, the software libraries 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 and implements a broad base research

portfolio to solve complex problems on computational resources that are on a trajectory to reach well beyond a petascale within a few years.

For the purposes of the Early Career Research Program, proposed research must be in either Applied Mathematics or Computer Science and be responsive to their respectively specified topic areas.

# (a) Applied Mathematics Technical Contact: Sandy Landsberg, 301-903-8507, <u>sandy.landsberg@science.doe.gov</u>

This program supports basic research leading to fundamental mathematical advances and computational breakthroughs across DOE and Office of Science missions. Applied Mathematics research includes and supports efforts to develop robust mathematical models, algorithms and numerical software for enabling predictive scientific simulations of DOE-relevant complex systems. For this solicitation, the specific topic areas of interest are listed here:

- Scalable solvers for next-generation high-performance computing: basic research in the design, synthesis, analysis, and demonstration of algorithms that provide numerical solutions to mathematical models of physical systems with relevance to the DOE missions. Solver research opportunities include new classes of algorithms that need to be developed: communication/synchronization hiding and reducing algorithms; mixed-precision-arithmetic algorithms; fault-tolerant and resilient algorithms; energy-efficient algorithms; stochastic algorithms; algorithms with reproducibility. A key research characteristic is that the results will also be useful for exascale simulations.
- 2. Rigorous mathematical and computationally efficient approaches for analyzing and extracting information and insight from large-scale datasets relevant to the DOE missions. Of particular interest are (a) algorithms for data-driven modeling and validation, model reduction, and data-driven control, (b) robust algorithms for sparse and noisy data, and (c) mathematical techniques for data reduction of streaming data;
- 3. Innovative mathematics research to improve the fidelity and predictability of continuous and/or distributed complex systems that accurately capture the physics and/or subcomponent interactions across vastly different time and length scales.

The pre-proposal's and proposal's responsiveness to this solicitation in these topic areas will be based on addressing all of the following criteria: (a) advances and innovations in mathematical models, methods and/or numerical algorithms, (b) mathematical and algorithmic challenges arising in simulations at scale, and (c) relevance of proposed research to DOE missions and/or scientific grand challenges. In addition, pre-proposals and proposals focused on any of the following will be considered out of scope: (1) tailoring or implementation of existing numerical methods for specific scientific problems; (2) HPC implementation or "framework" for scientific or engineering calculations that are based on specific programming models (for example, "OpenCL", "CUDA") or architectures (such as "GPGPU", "MIC", or variants); or (3) solutions for specific scientific or engineering problems that are not applicable to a broader class of problems.

# (b) Computer Science Technical Contact: Sonia R. Sachs, 301-903-0060, <u>sonia.sachs@science.doe.gov</u>

This program supports research to advance the development, operation and systems management of Leadership Class and production high performance computing facilities at DOE National Labs, application software development for scientific modeling and simulation at petascale to exascale, high performance computing systems architecture and software, and scientific data management and analysis at scale.

Topics of interest for this solicitation are focused on the following key research challenges for exascale platforms, namely:

- 1. Resilience for extreme-scale scientific applications in the context of leadership-class computing platforms, including research aimed at improving understanding of the causes, frequency, and impact of various types of hard and soft faults and the detection and mitigation thereof;
- 2. Correctness and debugging tools that complement exascale software stack solutions currently being developed;
- 3. Methods needed to advance the state-of-the-art of the joint modeling of performance, reliability, and power and that can accurately predict application behavior in view of dynamic and adaptive executions in future platforms;
- 4. Scientific data management, analysis and visualization, including knowledge representation to facilitate scientific data management, integration, and analysis; data provenance representation, capture, and analysis; data interoperability across scientific disciplines and platforms; scientific workflow systems that support data triage or down-selection, data analysis and visualization for petabyte to exabyte data sets from simulations and/or experimental platforms, including visualization of HPC system behavior and/or software visualization for highly parallel HPC codes; and methods to support creation of skeletal versions or mini-apps of data management, analysis and visualization applications for the purposes of extreme-scale system modeling and codesign.

Pre-proposals and proposals must explain their relevance to current and future high performance computing platforms as well as their relevance to the mission of the Office of Science and the Advanced Scientific Computing Research programs. Topics that are out of scope for this program include hardware architecture, all aspects of quantum computing, networking, computer-supported collaboration, social computing, natural language processing / understanding / generation and/or analysis, generalized research in human-computer interaction, discipline-specific data analytics and informatics, research focused on the World Wide Web and/or Internet, and research that is only applicable to hand-held, portable, desktop, embedded or cloud computing.

# II. Biological and Environmental Research (BER)

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

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.

#### **Biological Systems Science**

Biological Systems Science at DOE focuses on fundamental research and technology development to achieve a predictive systems-level understanding of complex biological systems to advance DOE missions in energy, climate, and the environment. By integrating genome enabled science with advanced computational and experimental biology approaches, DOE Biological Systems Science seeks to gain a predictive understanding of living systems including microbes, plants, and complex communities of organisms.

In support of DOE mission goals in understanding the biological processes involved in terrestrial carbon cycling and how these processes will be impacted by climate change, DOE Biological Systems Science brings the -omics driven tools of modern system biology (e.g. genomics, transcriptomics, proteomics, metabolomics, and meta-omics approaches) to bear on analyzing interactions between organisms that form biological communities and with their surrounding environments. Understanding the relationships between molecular-scale functional biology and ecosystem-scale environmental processes illuminates the basic mechanisms that drive biogeochemical cycling of elements, carbon biosequestration, and greenhouse gas emissions in terrestrial ecosystems.

BER is only seeking Biological Systems Science research in the following area:

# (a) Systems Biology Enabled Research on the Role of Microbial Communities in Carbon Cycling

Program Manager: Pablo Rabinowicz, 301-903-0379, pablo.rabinowicz@science.doe.gov

Applications are requested for –omics driven systems biology research on the roles of microbial communities in large scale biogeochemical carbon cycle processes of terrestrial ecosystems and potential impacts of climate change variables on relevant functional processes. Research should focus on (i) characterization of functional properties and underlying regulatory and metabolic networks of microbes, microbial consortia, and microbe-plant interactions involved in biogeochemical cycling of carbon, and/or (ii) development of novel –omics enabled approaches for in situ analysis and modeling of microbially mediated functional processes involved in carbon cycling in terrestrial ecosystems (either at field sites or using laboratory micro/mesocosms representing environments of interest). Key environments of interest include permafrost systems, soils of grasslands and forests, and agricultural systems focused on bioenergy production.

Applications focusing on marine systems or agricultural food production systems will not be considered.

#### **Climate and Environmental Sciences**

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

BER is only seeking Climate and Environmental Sciences research in the following area:

#### (b) Water Cycle Program Manager: Sally McFarlane, 301-903-0943, <u>sally.mcfarlane@science.doe.gov</u>

Water is a key component of the Earth and human systems due to its strong interactions with the energy cycle and its vital roles in the energy-water-land system. Uncertainties in predicting the Earth's hydrological cycle limits our ability to address future energy and environmental challenges. Due to the multiple interactions among systems and processes, improved understanding of the hydrological cycle requires research on cloud, aerosol, terrestrial ecosystem and subsurface processes, as well as climate, Earth system, and integrated assessment modeling and analysis.

Applications are sought that will reduce the uncertainty in model predictions of the hydrological cycle by making substantial progress on one or more of the specific topics below. Applications that propose process-level experimental, analysis, or modeling studies must indicate a clear path toward the incorporation of the improved process level understanding into Earth system models. As water cycle processes span a wide range of temporal and spatial scales, applicants are encouraged to address important multi-scale interactions associated with the specific topics and to utilize a hierarchy of models, as needed. Applications should also address uncertainty characterization of the measurements and/or model components and systems being studied.

Applicants are encouraged to work with DOE-supported modeling systems and community models such as the Community Earth System Model, the Weather Research and Forecasting model, the Global Change Assessment Model, and the Integrated Global System Model.

Specific topics of interest include:

- Using data from the Atmospheric Radiation Measurement (ARM) facilities to improve understanding and model representation of microphysical processes of precipitation. Particular emphasis is placed on research characterizing the multi-scale nature of precipitation processes that bridges the scale gaps between in situ or remote sensing measurements and the next generation of high resolution regional and global climate models.
- Analysis of the multi-scale interactions of the coupled land-atmosphere system needed to enable better prediction of the water cycle at regional to global scales in climate and earth system models, including how errors/biases in one component of the system affect the other components.
- Multi-scale methods and approaches for high-resolution modeling of energy (production and use)-water-land system dynamics, with a particular focus on multiple stressors and/or extreme events.
- Improved understanding of surface water groundwater soil moisture interactions and the role of fine-scale topography, soil structure and vegetation dynamics (including roots and microbial interactions) controlling the multi scale hydrological and biogeochemical functioning of terrestrial ecosystems.

Proposed research that is focused primarily on aquatic systems and properties will not be considered.

# III. Basic Energy Sciences (BES)

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

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.

More detailed information about BES sponsored research can be found at the BES website listed above. There you will find BES-sponsored workshop reports that address the current status and possible future directions of some important research areas. Also, Principal Investigators' Meetings Reports contain abstracts of BES supported research in topical areas associated with Division-sponsored technical conferences. Finally, the websites of individual BES Divisions may also be helpful. The following web pages are listed for convenience: BES FY2011 Summary Report:

http://www.science.energy.gov/~/media/bes/pdf/reports/files/BES2011SR\_rpt.pdf

BES FY 2012 Research Descriptions:

http://science.energy.gov/~/media/bes/pdf/reports/files/bes\_fy2012\_research\_summaries.pdf Basic Research Needs Reports: http://science.energy.gov/bes/news-and-resources/reports/basic-research-needs/ BES Workshop Reports: http://science.energy.gov/bes/news-and-resources/reports/workshop-reports/ Materials Sciences and Engineering Division Principal Investigators' Meetings: http://science.energy.gov/bes/mse/principal-investigators-meetings/ Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings: http://science.energy.gov/bes/csgb/principal-investigators-meetings/ Scientific User Facilities Division web page: http://science.energy.gov/bes/suf/

Proposed research must be directed to one of the core research areas listed below:

# (a) Materials Chemistry Technical Contact: Michael Sennett, 301-903-6051, <u>Michael.Sennett@science.doe.gov</u>

This research activity supports basic research in chemical synthesis of materials and chemical control of material structures. The major programmatic focus is on the discovery, design and synthesis of novel materials with an emphasis on the *chemistry* and *chemical* control of composition and structure across the range of length scales from atomic to mesoscopic, and consequent materials properties. Major scientific areas of interest include: chemical synthesis of materials, assembly of hierarchical material structures and control of multi-scale material morphology; solid-state chemistry; synthesis and characterization of novel organic, inorganic and composite materials, synthesis and characterization of complex fluids, the study and control of surface and interfacial chemistry including electrochemistry, and the study of materials chemical environments.

Recent BES Basic Research Needs (and other) workshops and reports have articulated those areas of the materials sciences that are most relevant to energy. All of the reports variously identify the overarching goal of fundamental materials chemistry research as providing the *knowledge* needed to *design and produce* new materials with *tailored properties from first principles*. This program will therefore emphasize research on the chemistry-based discovery, synthesis and transformations of materials and/or morphologies with the goal of providing fundamental knowledge with the potential to enable the development next generation energy technologies, including energy conversion, energy storage and transport, and energy conservation.

The program particularly encourages hypothesis-driven proposals in the areas of solid state chemistry, organic magnetic materials, organic electrical conductors, fundamental studies of surface and interface chemistry, and chemistry of materials far from equilibrium; priority will be given to proposals focused on elucidating the chemistry of materials in reactive or operational environments (*in-situ, in-operando*), in energy-relevant applications including energy storage, transport and conversion.

The program will not support the following: Proposals aimed at *optimization* of material properties for any applications, proposals that have device fabrication and testing as a primary goal, proposals with a primary goal to synthesize nanoparticles, proposals related to energetic materials (i.e., propellants and explosives) or liquid crystal materials, and proposals focused on *developing* materials primarily for hydrogen storage or solid state lighting technologies.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

#### (b) Biomolecular Materials Technical Contact: Michael Markowitz, 301-903-6779, <u>mike.markowitz@science.doe.gov</u>

This activity supports basic research in the discovery, design and synthesis of functional materials and complex structures based on principles and concepts of biology. The major programmatic focus is on the creation of robust, scalable, energy-relevant materials and systems with collective behavior that work with the extraordinary effectiveness of molecules and processes of the biological world. Major scientific areas include: Harnessing or mimicking the energy-efficient synthesis approaches of biology to generate new, optimized materials capable of operating under a broad range of non-biological conditions; bioinspired self-assembly 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 for characterization of biomolecular and soft materials.

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 totally new properties for next-generation energy technologies. Biomolecular Materials research activity seeks to advance the ability for materials that can (i) self-repair; (ii) regulate, clean, and sequester impurities; and (iii) tolerate abuse. New pathways for bio-inspired materials discovery that link scalable physical and chemical processes with the synthesis and assembly strategies of biology to predictably create new polymeric, inorganic, and hybrid functional materials *in vitro* with controllable properties are sought. The activity will also expand research on creating materials optimized for non-biological conditions that can (i) respond to environmental stresses without losing function; (ii) self-repair without external input; (iii) spontaneously assemble and disassemble; (iv) coordinate collective behavior in response to multiple signals; and (v) self-replicate. Enhanced integration of theory and experiment leading to new design ideas and opportunities for discovery will also be emphasized.

Examples of research funded in this program can be found in Biomolecular Materials Principal Investigators' Meeting Reports at the link, <u>http://science.energy.gov/bes/mse/principal-investigators-meetings/</u>, under "Biomolecular Materials". BES-sponsored workshop reports outlining the current challenges and needs in this field can also be found on the following web page links: <u>http://science.energy.gov/~/media/bes/pdf/reports/files/OFMS\_rpt.pdf</u>, <u>http://science.energy.gov/~/media/bes/pdf/reports/files/gc\_rpt.pdf</u>, and <u>http://science.energy.gov/~/media/bes/pdf/reports/files/bm\_rpt.pdf</u>,

The program **will not** support projects aimed at optimization of materials properties, device fabrication, sensor development, tissue engineering, and biomedical research.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences & Engineering (MSE) Division funded programs at the laboratory of the applicant.

#### (c) Synthesis and Processing Science Technical Contact: Bonnie Gersten, 301-903-0002, <u>bonnie.gersten@science.doe.gov</u>

This activity supports fundamental research on the development of new techniques using physical means and approaches to scalable synthesis of energy-relevant materials with desired structure and tailored properties. An important element of this activity is the development of real-time monitoring tools, to provide information on the progression of structure and properties as a material is formed, in order to understand the underlying physical mechanisms and to gain atomic level control of material synthesis and processing. The focus of this activity on nanocomposite, bulk crystal and thin film synthesis and processing via physical means is complementary to the BES Materials Chemistry and Biomolecular Materials research activities.

Over the past few years, the activity has evolved an increasing interest in understanding nanoscale morphology, defect 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 -elucidating fundamental mechanisms for bulk materials growth, new deposition techniques for organic and inorganic films, and organization of nanoparticle assemblies across a range of length scales, especially relating to use-inspired clean energy research. Integration of experimental and theory/modeling activities to accelerate progress in understanding synthesis and discovery of new materials will be emphasized. The most recent summaries of the projects supported by this program can be found at: <a href="http://science.energy.gov/~/media/bes/pdf/reports/files/BES\_FY2012\_research\_summaries.pdf">http://science.energy.gov/~/media/bes/pdf/reports/files/BES\_FY2012\_research\_summaries.pdf</a>

The program **will not** support projects aimed at *optimization* of material properties for specific applications, device fabrication, nanoparticle synthesis as a primary goal, ion beam assisted materials synthesis or materials focused on hydrogen storage technologies. In addition, projects that mainly focus on tribology, fluid dynamics or engineering scale-up and development will not be supported.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Science and Engineering (MSE) Division funded programs at the laboratory of the applicant.

#### (d) Experimental Condensed Matter Physics Technical Contact: Andrew Schwartz, 301-903-3535, <u>andrew.schwartz@science.doe.gov</u>

This program supports research in Experimental Condensed Matter Physics that will advance our fundamental understanding of the relationships between intrinsic electronic structure, particularly strong electron correlation effects, and the properties of complex materials such as superconductors, magnetic materials, and two-dimensional electron gases. A particular emphasis is placed on investigating the physics of low-dimensional systems (particularly 1D and 2D) as

well as studies of electronic structure at low (mK) temperature and high magnetic field ( $\leq 100$ T). The program will continue to invest in research to understand the mechanisms of unconventional superconductivity through studies of the electronic properties of these materials. Recently, the program has increased support for studies of spin physics, nanomagnetism, new topological states of matter, and ultracold atom research where the results provide insight into open questions about correlated electron behavior in the condensed phase. The Early Career Research Program does not support research on conventional superconductivity, electrochemistry, thermoelectric materials, photovoltaic materials, or mechanical properties of materials. It also does not support projects aimed at materials optimization or device development.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

#### (e) Theoretical Condensed Matter Physics Technical Contact: James Davenport, 301-903-0035, james.davenport@science.doe.gov

This program supports research in the area of 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, semiconductors, thermoelectric materials, and neutron and photon scattering. Properties of nanoscale and mesoscale systems are of interest. Novel, physics based computational techniques are supported along with techniques relevant to the discovery and design of new materials. Suitable topics include quantum Monte Carlo, improvements to density functional theory, extensions of dynamical mean field theory, density matrix renormalization group and self-consistent GW calculations. The Early Career Research Program does not support research on conventional superconductivity.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

#### (f) Physical Behavior of Materials Technical Contact: Refik Kortan, 301-903-3308, <u>refik.kortan@science.doe.gov</u>

This program supports research to understand the Physical Behavior of materials and is focused on developing an understanding of the relationship between a material's properties and its response to external stimuli such as temperature, electromagnetic fields, chemical environments, and the proximity effects of surfaces and interfaces. The program emphasizes the impact of the external stimuli on the materials structure, including microstructure and defects, and how these impact thermal, electrical, magnetic, optical, and electrochemical properties. Included within the activity are research projects designed to establish the role of defects on the previously listed material properties, research on phase equilibria and kinetics of reactions in materials in harsh environments (not including environments found in nuclear reactors), and research on diffusion and transport phenomena. The program will continue to support research on plasmonics, metamaterials and organic electronic materials. This program also supports theory, modeling, and simulation activities, especially in combination with experimental research, that address the influence of external stimuli on: charge and energy transfer, electronic structure, exciton dynamics and transport, and spin dynamics. Research is supported that will advance our understanding of materials properties over multiple length scales by developing predictive models for the influence of the nanoscale, mesoscale and macroscale structure on the material's response to external stimuli.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

#### (g) Mechanical Behavior and Radiation Effects Technical Contact: John Vetrano, 301-903-5976, john.vetrano@science.doe.gov

This activity supports hypothesis-driven 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 fundamental studies of deformation of ultra-fine scale materials, radiation resistance of structural materials, and intelligent microstructural design for increased strength, formability, and fracture resistance in energy relevant materials. The goals are to develop the scientific underpinning for predictive models for the design of materials having superior mechanical properties and radiation resistance. Proposals emphasizing mechanics of materials, rather than materials science, will not be considered responsive.

Research opportunities that can be realized by the application of mechanics fundamentals to the general areas of self-assembly, physical behavior, and behavior under extreme environments (primarily environments that are experienced in current or future fission reactors) of structural materials will be emphasized. With the emerging importance of nanoscale structures with high surface-to-volume ratios, it is appropriate to take advantage of the new, unprecedented capabilities to fabricate and test tailored structures down to the nanoscale, taking advantage of more powerful parallel computational platforms and new experimental tools. High-strain rate deformation **will not** be explored in this program at this time.

Radiation is increasingly being used as a tool and a probe to gain a greater understanding of fundamental atomistic behavior of materials. Incoming fluxes can be uniquely tuned to generate a materials response that can be detected *in situ* over moderate length and time scales. Materials also sustain damage after long times in high-radiation environments typical of current and projected nuclear energy reactors and in geological waste storage. As nuclear energy is projected to play a larger role in U.S. energy production, these are issues that need to be addressed at a fundamental level. High-dose studies **will not** be explored in this program at this time.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Science and Engineering (MSE) Division funded programs at the laboratory of the applicant.

#### (h) X-ray Scattering Technical Contact: Lane Wilson, 301-903-5877, <u>lane.wilson@science.doe.gov</u>

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 directed at the study of ultrafast physical phenomena in materials, is an integral part of the portfolio. Based on programmatic priorities, this activity **will not** support ultra-fast source development in the FY 2014 Early Career Research Program, but will focus on the application of ultra-fast probe interactions with materials and the resulting connection to materials dynamics.

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

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Science and Engineering (MSE) Division funded programs at the laboratory of the applicant.

#### (i) Neutron Scattering Technical Contact: P. Thiyagarajan (Thiyaga), 301-903-9706, <u>p.thiyagarajan@science.doe.gov</u>

This activity supports basic research on the fundamental interactions of neutrons with matter to achieve an understanding of the atomic, electronic, and magnetic structures and excitations of materials and their relationship to macroscopic properties. Major emphasis is on the advancement of techniques and application of neutron scattering, spectroscopy and imaging for materials research, primarily at BES-supported user facilities. The goal is to foster strong interaction between the neutron scattering experiments, theory and high performance computation to accelerate fundamental understanding needed for predictive design of advance materials for future energy needs.

New investments in the FY 2014 Early Career Research Program will focus on the science at mesoscale where materials macroscopic properties are manifested. Characterizing and controlling the patterns and evolution of mesoscale heterogeneity are key to optimizing and exploiting a wide range of materials performance and functionality. *In situ* research can measure structure and properties dynamically during synthesis and use of materials in appropriate environments and operational conditions, yielding direct data for comparison to predictions. The

program will develop 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. A continuing theme of this program is the integration of material synthesis, neutron scattering experiments, and computational modeling as this is vital to obtain controlled samples for careful neutron scattering measurements and modeling for an in-depth understanding of the relationship between the structure and dynamics and the macroscopic properties.

Based on programmatic priorities, applications in the areas of superconductivity, magnetism and organic photovoltaics will NOT be accepted under this topic in the 2014 Early Career Research Program.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Science and Engineering (MSE) Division funded programs at the laboratory of the applicant.

#### (j) Electron and Scanning Probe Microscopies Technical Contact: Jane Zhu, 301-903-3811, jane.zhu@science.doe.gov

This activity supports basic research in materials sciences using electron and scanning probe microscopy and spectroscopy techniques. The research includes experiments and theory to understand the atomic, electronic, and magnetic structures and properties of materials. This activity also supports the development of new instrumentation and techniques, including ultrafast 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.

This program builds upon the tremendous advancements in electron and scanning probe microscopy capabilities in the recent decades and use scattering, imaging and spectroscopy methods to understand functionality and fundamental processes from atomistic to mesoscopic scales. Significant improvements in resolution and sensitivity will provide an array of opportunities for groundbreaking science. These include the possibilities of understanding and controlling nano or meso-scale inhomogeneity, new phenomena emerging at nanoscale, probing magnetism at the atomic scale with spin excitation spectroscopy, imaging spin density and spin waves, imaging functionality at the atomic scale, understanding phase transitions and transport properties on multiple length-scales, understanding the interplay between charge, orbital, spin and lattice in complex materials, combination of multiple probes, and *in situ* analysis capabilities (under perturbing parameters such as temperature, irradiation, stress, magnetic & electric field, and chemical environment). New methods and approaches addressing the scientific challenges will lead to the development of unique new analysis tools and breakthroughs in materials. The combined new experimental and theoretical capabilities will enable the fundamental understanding of atomic origins of materials properties.

Based on programmatic priorities this activity does not support projects aimed at technique development without science goals. Examples of research funded in this category can be found in the Electron and Scanning Microscopies Principal Investigators' Meetings' Reports at <a href="http://science.energy.gov/bes/mse/principal-investigators-meetings/">http://science.energy.gov/bes/mse/principal-investigators-meetings/</a>.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

# (k) Atomic, Molecular, and Optical Sciences (AMOS) Technical Contact: Jeffrey Krause, 301-903-5827, jeff.krause@science.doe.gov

This program supports basic experimental and theoretical research aimed at understanding the structural and dynamical properties of atomic and molecular systems. 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, and electron correlation. 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 quantum control of 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 the interaction of ultrafast light with matter. Key targets for greater investment include attosecond science, electron-driven processes, and quantum control of molecular systems.

The program emphasizes ultrafast, strong-field, short-wavelength science, and correlated dynamics in atoms and molecules. Examples are 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), 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 inner-shell photoionization of atoms and molecules. Coherent control of nonlinear optical processes and tailoring of quantum mechanical wave functions with lasers will continue to be of interest, particularly in molecular systems. Experimental and theoretical tools 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 **is not** accepting applications in the areas of quantum information science, nanoscience, bioscience, ultracold quantum gases, condensates, or plasmas

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

#### (1) Gas Phase Chemical Physics (GPCP) Technical Contact: Wade Sisk, 301-903-5692, <u>wade.sisk@science.doe.gov</u>

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

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

#### (m) Computation and Theoretical Chemistry Technical Contact: Mark Pederson, 301-903-9956, <u>mark.pederson@science.doe.gov</u>

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 especially in relation to providing groundwork for computational design of molecular- to meso- scale materials and processes. Part of the focus is on next-generation simulation of processes that are so complex that efficient computational implementation must be accomplished in concert with development of theories and algorithms. Efforts should be tightly integrated with the research and goals of BES, especially the chemical physics programs, and should provide fundamental

solutions that enhance or enable conversion to clean, sustainable, renewable, novel or highly efficient energy use. Efforts should include application to real molecular- and nano- scale systems. This may include the development or improvement of reusable computational tools that enhance analysis of measurements at the DOE facilities or efforts aimed at enhancing accuracy, precision, and applicability or scalability of all variants of quantum-mechanical simulation methods. This includes the development of spatial and temporal multi-scale/multistage methodologies that allow for time-dependent simulations of resonant, non-resonant and dissipative processes as well as rare events. Development of capabilities for simulation: of light-matter interactions, conversion of light to chemical energy or electricity, and the ability to model and control externally driven electronic and spin-dependent processes in real environments are encouraged. These phenomena may be modeled using a variety of time-independent and time-dependent simulation approaches. Examples include:

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

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

Methods and/or investigations that do not require consideration of electronic rearrangements or coupling of electronic and vibrational degrees of freedom to external stimuli are not supported by this program.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

#### (n) Condensed Phase and Interfacial Molecular Science (CPIMS) Technical Contact: Gregory Fiechtner, 301-903-5809, gregory.fiechtner@science.doe.gov

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 well-characterized metal and metal-oxide surfaces and clusters lead to the development of theories on the molecular origins of surface-mediated catalysis and heterogeneous chemistry; 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.

Some examples of support received by Early Career Research Program applicants include (1) studies of free-radical reactions at interfaces of aqueous aerosols, (2) studies that combine molecular electronics with ultrafast microscopy to pursue an understanding of electron transport in single molecules and at ultrafast time scales, (3) studies for understanding surface and subsurface adsorption at the molecular level to control chemical reactivity and selectivity, (4) studies that visualize interfacial electronic phenomena occurring on femtosecond timescales and submicron length scales, and (5) studies that employ high resolution photoelectron imaging to gain an understanding of the mechanisms and molecular requirements for efficient exciton multiplication through singlet fission.

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.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

#### (o) Catalysis Science Technical Contact: Raul Miranda, 301-903-8014, <u>raul.miranda@science.doe.gov</u>

This activity develops the fundamental scientific principles enabling rational catalyst design and chemical transformation control for energy-related catalytic processes. Research includes the identification of the elementary steps of catalytic reaction mechanisms and their kinetics; construction of catalytic sites at the atomic level; synthesis of ligands, metal clusters, and bio-

inspired reaction centers designed to tune molecular-level catalytic activity and selectivity; the study of structure-reactivity relationships of inorganic, organic, or hybrid catalytic materials in solution or supported on solids; the dynamics of catalyst structure relevant to catalyst stability; the experimental determination of potential energy landscapes for catalytic reactions; the development of novel spectroscopic techniques and structural probes for *in situ* characterization of catalytic processes; and the development of theory, modeling, and simulation of catalytic pathways.

A wealth of experimental information has been accumulated relating catalytic structure, activity, selectivity, and reaction mechanisms. However, for phenomenological catalysis to evolve into predictive catalysis, the principles connecting kinetic phenomena must be more clearly and thoroughly identified. Better understanding of catalysis will result from synthesis of catalyst structures that are identifiable and controllable under working conditions; fast and ultrafast characterization of intermediate and transition states; and hybrid quantum/classical mechanics and microkinetics analysis of complex reactions. The convergence of heterogeneous, homogeneous, and bio-inspired catalysis is emerging and being used to derive new catalysts. For example, designed secondary and tertiary structures add structural flexibility and chemical specificity that affect catalytic properties of inorganic catalysts. Much of the current research focuses on understanding and controlling the synthesis and characterization of novel inorganic, organic, and hybrid catalysts. However, proposals to study solely the synthesis of catalysts or reaction intermediates, or solely the characterization methods without clearly providing innovative advances to full catalytic cycles for reactions relevant to energy will not be considered.

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, carbohydrates and other multifunctional molecules will receive attention. Non-noble metal catalysts to effectively replace classical precious metals and provide innovative reaction pathways for energy-relevant reactions will be welcome; low-temperature, single-pot, solution phase catalysis will also be covered. However, enzyme-catalyzed reactions and other catalytic reactions that pertain to biological life cycles or to the synthesis of drug precursors will not be considered. With novel catalysts and catalytic reactions, emphasis will be placed on the use of theory to provide a fundamental framework or even predict catalytic performance, and the use of spectroscopy and microscopy to probe and understand catalytic systems under realistic working conditions. Emphasis will also be placed on the investigation of catalytic mechanisms, pathways, and bond rearrangements under electrochemical and photoelectrochemical conversion of complex molecules into chemicals and fuels. However, the solar photochemical or electrochemical oxidation of water or reduction of CO<sub>2</sub> will not be considered.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

Examples of research funded in catalysis can be found in Catalysis Science Program Meeting Reports at the link 'Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings', <u>http://www.science.energy.gov/bes/csgb/principal-investigators-</u>

<u>meetings</u>/ (search for "catalysis" in the book title) and in the BES Research Summaries (<u>http://www.science.energy.gov/bes/news-and-resources/program-summaries</u>/). A 2007 BESAC-sponsored workshop, Basic Research Needs: Catalysis for Energy, outlining the current challenges and needs in this field can also be found on the 'Basic Research Needs Reports' web page link (<u>http://www.science.energy.gov/~/media/bes/pdf/reports/files/cat\_rpt.pdf</u>.) The report content is current except for the noted exclusion of solar photochemical conversion of water or  $CO_2$  from this activity.

#### (p) Separations and Analysis Technical Contact: Larry Rahn, 301-903-2508, <u>larry.rahn@science.doe.gov</u>

The overall goal of this activity is to obtain a predictive understanding, at molecular and nanoscale dimensions, of the basic chemical and physical principles involved in separations systems and chemical analysis tools, so that innovative approaches to DOE mission-related problems may be discovered and advanced. A range of multidisciplinary experimental and computational approaches are employed in basic research, inspired by the common fundamental underpinnings associated with a wide range of energy related chemical recognition, separation and analysis problems. These include processing, production and utilization of current and future petroleum, bio, solar, and nuclear fuels, as well as carbon capture, chemical processing with improved efficiency and/or selectivity, and production of strategic energy-relevant materials. The basic research needs in many of these areas are analyzed in workshop reports found at links listed at the beginning of this section, under III. Basic Energy Sciences (BES). Separations research will continue to advance the understanding and control of the atomic and molecular interactions between target species and separations media and the resulting molecular structures, dynamics, kinetics and transport properties resulting in the desired meso- and macroscopic functionality. This fundamental research is motivated by a desire to advance discovery and/or predictive design of future chemical separations-related concepts enabling novel, multifunctional, and/or more efficient capabilities for a broad range of processes. Examples include membrane processes (e.g. separation, reactive separation and fuel cell membranes), complexation, extraction under both standard and supercritical conditions, ionic liquids, selective adsorption and release using materials such as MOFs, ZIFs and COFs, and limited fundamental aspects of chromatography. Analytical research will pursue the elucidation of ionization, chemical interactions, and excitation mechanisms for optical and mass spectrometry that enable temporal and chemical observation and characterization at the nanoand molecular-scale of systems relevant to DOE's energy interests. One focal point of this research is pursuit of the underlying science needed to achieve true chemical imaging, i.e., the ability to selectively image desired 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 scale up or development of narrowly defined processes, devices or sensors, activities directed at lab-on-a-chip development, or research that is directed toward medical applications; as these areas are more appropriately supported through other federally funded programs.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

Research funded in this category in the recent past can be found in Separations and Analysis PI Meeting Reports at <u>http://science.energy.gov/bes/csgb/principal-investigators-meetings</u>. For actinide related separations, see the description below of BES Heavy Element Chemistry.

#### (q) Heavy Element Chemistry (HEC) Technical Contact: Philip Wilk, 301-903-4537, <u>philip.wilk@science.doe.gov</u>

This activity supports basic research on the chemistry of the elements beyond actinium (atomic number greater than 89); typically uranium, neptunium, plutonium, americium, and curium. The unique molecular bonding of these elements is explored using experiment and theory to elucidate electronic and molecular structure as well as reaction thermodynamics. Emphasis is placed on resolving the f-electron challenge; the chemical and physical properties of these elements to determine solution, interfacial and solid-state bonding and reactivity; fundamental transactinide chemical properties; and the fundamental science underpinning the extraction and separation of the actinides.

Resolving the role of the f-electrons is one of the three grand challenges identified in *Basic Research Needs for Advanced Nuclear Energy Systems\**, the report of the Basic Energy Sciences Workshop (July 31 – August 3, 2006) on this topic, and echoed in the report from the Basic Energy Sciences Advisory Committee: *Science for Energy Technology: Strengthening the Link between Basic Research and Industry* (August 2010). Research to meet this challenge is pursued in the HEC program and includes efforts aimed at implementing, for the elements beyond actinium, quantum-mechanical theories that more adequately describe spin-orbit interactions and relativistic effects as well as efforts to expand our ability to predict heavy element chemical behavior under conditions relevant to all stages of fuel reprocessing.

Synthetic research is pursued within the HEC program on molecules that contain heavy elements, with a focus on gaining a fundamental understanding of separations processes and aiding the development of ligands to sequester actinides. Spectroscopic research on the chemical bonding and reactivity of all manner of energy-relevant molecules is also pursued within the HEC program. Better characterization and modeling of the interactions of actinides at liquid-solid and liquid-liquid interfaces is motivated by improving the separations processes that are essential for advanced nuclear fuel.

Based on programmatic priorities, the HEC program does not fund research on: the processes affecting the transport of subsurface contaminants, the form and mobility of contaminants including wasteforms, projects aimed at optimization of materials properties including radiation damage, device fabrication, or biological systems; which are all more appropriately supported through other DOE programs.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

\* http://science.energy.gov/~/media/bes/pdf/reports/files/anes\_rpt.pdf

Program and Abstracts for the 2013 Heavy Element Chemistry and Separations Science Principal Investigators' Meeting:

http://science.energy.gov/~/media/bes/csgb/pdf/docs/HEC\_and\_Sep\_2013\_PI\_Meeting.pdf

#### (r) Geosciences Research Technical Contact: Nicholas Woodward, 301-903-4061, <u>nick.woodward@science.doe.gov</u>

This activity supports basic experimental and theoretical research in geochemistry and geophysics. Geochemical research emphasizes fundamental understanding of geochemical processes and reaction rates, for example focusing on aqueous solution chemistry, mineral-fluid interactions, particulate and nano-particulate transport and geochemistry, and isotopic distributions and migration in natural systems. Geophysical research focuses on developing new approaches to understanding the subsurface physical properties of fluids, rocks, and minerals and develops techniques for determining such properties at a distance; it seeks fundamental understanding of wave propagation physics in complex media and the fluid dynamics of complex fluids through porous and fractured subsurface rock units. The activity seeks new research efforts on imaging of earth processes with attention devoted both to improved small-scale imaging using x-ray sources, neutron sources, mass-spectrometry and scanning microscopies, and large-scale imaging of physical properties through their seismic and electromagnetic responses. Geosciences activities seek to link analytical capabilities with computational capabilities to provide improved understanding of geochemical and geophysical processes occurring at natural time and length scales. The Geosciences research activity focuses on physical sciences research. Studies desiring to focus on geo-biological studies, or soil science, or to target exploitation of a single resource, or to remediate a particular waste/contaminant type won't be considered. Applicants in those cases should consult the appropriate DOE technology program. The Geosciences program held a major workshop in 2007 that is still highly relevant to illustrate our fundamental sciences approach to DOE mission needs:

http://science.energy.gov/~/media/bes/pdf/reports/files/geo\_rpt.pdf

BES Program Summaries for all programs can be found at the following link: <u>http://science.energy.gov/~/media/bes/pdf/reports/files/BES\_FY2012\_research\_summaries.pdf</u> Geosciences summaries begin on page 306.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

#### (s) Solar Photochemistry Technical Contact: Mark Spitler, 301-903-4568, <u>mark.spitler@science.doe.gov</u>

This activity supports fundamental, molecular-level research on solar energy capture and conversion in the condensed phase and at interfaces. These investigations of solar photochemical energy conversion focus on the elementary steps of light absorption, charge separation, and charge transport within a number of chemical systems, including those with significant nanostructured composition. Although the long term mission of this Program is an understanding of the science behind solar-driven production of fuels and electricity, it is recognized that fundamental research in the interaction of light, matter and electrons in these systems is essential to the achievement of Program goals.

Supported research areas include organic and inorganic photochemistry, catalysis and photocatalysis, and photoinduced electron and energy transfer in the condensed phase and across interfaces, photoelectrochemistry, and artificial assemblies for charge separation and transport that mimic natural photosynthetic systems. An enhanced theory and modeling effort is needed for rational design of these artificial solar conversion systems.

Among the challenges for catalytic fuels production, knowledge gained in charge separation and electron transfer needs to be applied in a meaningful way to activation of small molecules including, among others, CO<sub>2</sub> in its reduction to fuels and H<sub>2</sub>O 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 is research on the principles of new hybrid systems that feature molecular catalysis at solid surfaces and of new nanoscale structures for the photochemical generation of fuels. Research areas concerned with separation of charge that might result in electricity include multibandgap, multilayer cascade-type semiconductors, photosensitized nanoparticulate solids, and the study of the mechanism of multiple exciton generation within nanoparticles. There are also challenges in fundamental understanding of photoconversion processes - energy transfer and the generation, separation, and recombination of charge carriers - in organic-based molecular semiconductors, which could lead to a new type of inexpensive and flexible solar cell.

Another regime of chemistry initiated through creation of high energy excited states is highly ionizing radiation, as can be produced through electron pulse radiolysis, to investigate reaction dynamics, structure, and energetics of short-lived transient intermediates in the condensed phase. Among many topics, fundamental research is of interest in areas that 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. Not of interest during FY 2014 are proposals that involve the assembly of dye sensitized solar cells with  $TiO_2$ .

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

#### (t) Photosynthetic Systems Technical Contact: Gail McLean, 301-903-7807, gail.mclean@science.doe.gov

This activity supports basic research on the biological conversion of solar energy to chemically stored forms of energy. Topics of study include but are not limited to light harvesting, exciton transfer, charge separation, transfer of reductant to carbon dioxide, as well as the biochemistry of carbon fixation, metabolism, and storage. Such research will enhance understanding of the weak intermolecular forces governing molecular assembly in photosynthetic systems; the biological machinery for cofactor insertion into photosynthetic proteins and protein subunit assemblies; the structural and mechanistic features of photosynthetic complexes; and the physical and chemical rules that underlie biological mechanisms of repair and photoprotection.

Photosynthetic Systems **does not** fund research in: 1) prokaryotic systems related to human/animal health or disease; 2) development or optimization of devices and/or 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.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division-funded programs at the laboratory of the applicant.

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

#### (u) Physical Biosciences Technical Contact: Robert Stack, 301-903-5652, <u>robert.stack@science.doe.gov</u>

This activity supports basic research that combines the tools of 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 mechanisms by which energy transduction systems are assembled and maintained, the processes that regulate energy-relevant chemical reactions within the cell, the underlying biochemical and biophysical principles determining the architecture of biopolymers and the plant cell wall, and active site protein chemistry that provides a basis for highly selective and efficient bioinspired catalysts.

Future impact is, in general, envisioned through increased use of physical science and computational tools (ultrafast laser spectroscopy, current and future x-ray light sources, and quantum chemistry) to probe spatial and temporal properties of biological systems. For instance, the application of such tools to the study of individual enzymes (and multi-enzyme complexes) will enable the design of improved industrial catalysts and processes (e.g. more cost-effective, highly-efficient, etc) through a more complete understanding of structure and mechanistic principles. One such priority area for the program is achieving a greater understanding of the active site chemistries of multi-electron redox reactions (e.g. CO2 reduction). Another unique aspect of biological systems is their ability to self-assemble and self-repair. These capabilities occur via complex processes that are not well-understood, and enhanced efforts will be devoted to the identification of the underlying chemical/physical principles that govern such behaviors.

Physical Biosciences **does not** fund research in: 1) animal systems; 2) prokaryotic systems related to human/animal health or disease; 3) development and/or optimization of devices and/or processes; 4) development and/or optimization of microbial strains or plant varieties for biofuel/biomass production; 5) cell wall breakdown or deconstruction; 6) transcriptional or translational regulatory mechanisms and/or processes; 7) environmental remediation and/or identification of environmental hazards. 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.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division-funded programs at the laboratory of the applicant.

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

# (v) Nanoscale Science Research Centers and Electron-Beam Microcharacterization Centers Research

#### Technical Contact: George Maracas, 301-903-1264, george.maracas@science.doe.gov

This research area supports work that advances the instruments, techniques, and capabilities of the existing BES Scientific User Facilities and/or contributes to capabilities of future facilities in this area. Research topics that develop and exploit the unique potential of co-located facilities within and across the BES scientific user facilities are encouraged. We do not intend to support applications to establish new, unrelated types of facilities or to develop techniques that do not relate to the missions of the nanoscale science research centers or electron beam microcharacterization facilities.

For DOE national laboratory applicants, the proposed research must fit within the BES Scientific User Facilities (SUF) Division funded programs at the laboratory of the applicant.

Five Nanoscale Science Research Centers (NSRCs) support the synthesis, processing, fabrication, and analysis of materials at the nanoscale: the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory (ORNL), the Molecular Foundry at Lawrence Berkley National Laboratory (LBNL), the Center for Integrated Nanotechnologies at Sandia National Laboratory (SNL)/Los Alamos National Laboratory (LANL), the Center for Nanoscale Materials at Argonne National Laboratory (ANL), and the Center for Functional Nanomaterials at Brookhaven National Laboratory (BNL). These centers are the Department of Energy's premier user facilities for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools for synthesis, fabrication, and analysis, and new computing approaches and capabilities. As such, research is supported across the spectrum of scientific and engineering disciplines to understand and exploit unique and phenomena materials at the nanoscale, including materials for energy conversion, structured materials derived from or inspired by nature, hard and crystalline materials (including the structure of macromolecules), magnetic and soft materials (including polymers and ordered structures in fluids), and nanoscale materials integration. Tools for probing nanoscale materials and phenomena are increasingly multi-modal, to enable characterization of electrical, optical, and/or magnetic properties on the same sample with high resolution over a range of length scales. The ability to characterize functional nanoscale materials in-situ, under operating conditions, is also increasingly important, from, for example, battery electrode charging/discharging, to catalysts at high pressures and temperatures, to biologically-inspired, soft, and/or hybrid materials in liquid environments.

New approaches to probe at the nanoscale, notably leveraging complementary modalities at the electron-beam, x-ray, and neutron facilities are of particular interest. Theory and modeling closely coupled with experiment to advance and accelerate the understanding of nanoscale phenomena, provide insights to inform materials by design, and develop and implement new capabilities leveraging the most advanced computational resources are also encouraged.

In the area of electron-beam microcharacterization the focus is on the development of next generation electron-beam instrumentation and on conducting corresponding research. Electron scattering has key attributes that give such approaches unique advantages and make them complementary to x-ray and neutron beam techniques. These characteristics include strong interactions with matter (allowing the capture of meaningful signals from very small amounts of material, including single atoms under some circumstances) and the ability to readily focus the charged electron beams using electromagnetic lenses. The net result is unsurpassed spatial resolution and the ability to simultaneously get structural, chemical, and other types of information from sub-nanometer regions, allowing study of the fundamental mechanisms of catalysis, energy conversion, corrosion, charge transfer, magnetic behavior, and many other processes. All of these are fundamental to understanding and improving materials for energy applications and the associated physical characteristics and changes that govern performance.

Allowed topics for instrumentation and technique development efforts are limited to scanning, transmission, and scanning transmission electron microscopes, atom probes and related field ion instruments, related surface characterization apparatus and scanning probe microscopes, and ancillary tools such as spectrometers, detectors, and advanced sample preparation equipment. For guidance on the types of projects previously funded, please refer to currently funded **BES Research Summaries** (<u>http://www.science.energy.gov/bes/news-and-resources/program-summaries/</u>).

#### (w) Accelerator and Detector Research Technical Contact: Eliane Lessner, 301-903-9365, <u>eliane.lessner@science.doe.gov</u>

This program supports work that advances the instruments, techniques, and capabilities of the existing and/or future BES Scientific User Facilities. We do not intend to support applications to establish new, unrelated types of facilities or to develop techniques that do not relate to the missions of the light sources and neutron scattering centers.

For DOE national laboratory applicants, the proposed research must fit within the BES Scientific User Facilities (SUF) Division funded programs at the laboratory of the applicant.

In the accelerator and detector research program, the objective is to improve the output and capabilities of light sources and neutron scattering facilities that are the most advanced of their kind in the world. This program supports basic research in accelerator physics and X-ray and neutron detectors. An excellent reference for accelerator physics needs for light sources can be found in *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Volume 618, Issues 1-3*. Research is supported that aims at developing techniques that will strongly benefit the next generation of free electron lasers (FELs), in particular advanced techniques enhancing temporal control of X-ray FELs. Development studies of loss control methods in high-intensity proton sources to neutron spallation facilities are also supported. Examples of research supported by the program can be found in the SUF Principal Investigator's Meeting report at http://science.energy.gov/bes/suf/principal-investigators-meetings/

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. A detailed discussion of opportunities and needs for neutron and photon detector development at the existing and future BES facilities can be found in the Neutron and Photon Detector Workshop report at http://www.science.energy.gov/bes/news-and-resources/reports/workshop-reports/

This program strongly interacts with BES programmatic research that uses synchrotron radiation and neutron sources.

#### (x) X-ray Instrumentation and Technique Development Technical Contact: Peter Lee, 301-903-8484, <u>Peter Lee@science.doe.gov</u>

This program supports work that advances the instruments, techniques, and capabilities of the existing and/or contributes to capabilities of future BES supported light source facilities. This

program **will not** support proposals to establish new, unrelated types of facilities or to develop techniques not applicable to BES x-ray light source facilities.

For DOE national laboratory applicants, the proposed research must fit within the BES Scientific User Facilities (SUF) Division funded programs at the laboratory of the applicant.

The unique properties of the light source facilities include, for storage-ring based synchrotron sources, a continuous spectrum, high flux, and brightness and, for the Linac Coherent Light Source (LCLS), ultra short pulses, high peak power, and high coherence, making them indispensable tools for the exploration of matter. The wide range of emitted photon wavelengths provide incisive probes for advanced research. The three broad categories of experimental measurement techniques performed at the light sources - spectroscopy, scattering, and imaging - probe the fundamental parameters by which we perceive the physical world (energy, momentum, position, and time). By exploiting the short pulse lengths of these light sources, especially the LCLS, each technique can also be performed in a timing fashion.

In order to fully exploit the wide range of capabilities of these x-ray light source facilities, this program will encourage the development of imaginative concepts for new types of scattering instruments as well as innovative uses of existing instruments, especially in the area of advanced optics, novel instrumentation for new experimental capabilities, and novel approaches to data visualization and analysis.

#### (y) Neutron Scattering Instrumentation and Technique Development Technical Contact: James J. Rhyne, 301-903-6827, <u>James.Rhyne@science.doe.gov</u>

This program supports work that advances the instruments, techniques, and capabilities of the existing and/or future BES supported neutron scattering facilities.

Because of their neutral charge and non-destructive characteristics, thermal neutrons are a unique and effective tool for probing the structure and dynamics of matter. Neutron scattering is particularly well-suited for determining the atomic positions of both light and heavy atoms in a solid or fluid and thermal fluctuations in these positions. In addition the neutron scatters from magnetic moments in the material thus providing information on the magnetic structure as well. The neutron energy is well-matched to that of elementary atomic and magnetic excitations (spin waves and phonons) in a material and, via inelastic scattering, can provide data crucial for understanding basic phenomena in a variety of condensed matter systems including superconductors, magnetic systems, and multi-ferroic materials.

In order to fully exploit the wide range of capabilities of the BES neutron scattering facilities, this program will encourage the development of imaginative concepts for new types of scattering instruments as well as innovative uses of existing instruments, including advanced optics, sample environments, and novel approaches to data visualization and analysis.

Note: This program **will not** support proposals to establish new, unrelated types of facilities or to develop techniques not applicable to BES neutron scattering facilities.

For DOE national laboratory applicants, the proposed research must fit within the BES Scientific User Facility (SUF) Division funded programs at the laboratory of the applicant.

# IV. 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 temperature and density 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.

Plasma science is at the center of the research needed to be able to harness the power of the stars on earth. Plasma science has advanced to the point where we are ready to explore the regime of self-sustaining, or burning plasmas. The key activity in this exploration is the U.S. participation in ITER, an experiment to study and demonstrate the sustained burning of fusion fuel. ITER will provide an unparalleled scientific research opportunity and will test the scientific and technical feasibility of magnetic fusion power. Currently FES scientists and engineers are supporting the design activities, technical R&D, hardware procurement and other construction activities that support our share of the project. In addition, the FES program supports research in high-energydensity laboratory plasma (HEDLP) science.

The National Research Council report *Plasma Science: Advancing Knowledge in the National Interest* has recognized that plasma science has a coherent intellectual framework unified by physical processes that are common to many subfields. Because of the wide range of plasma densities and temperatures encountered in fusion applications, it is valuable to support plasma science across many of its subfields in order to advance the fusion energy mission. Accordingly, the FES program has four strategic goals:

- Advance the fundamental science of magnetically confined plasmas to develop the predictive capability needed for a sustainable fusion energy source;
- 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;
- Support the development of the scientific understanding required to design and deploy the materials needed to support a burning plasma environment; 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.

To address these strategic goals, research on the specific topics below is supported by the Fusion Energy Sciences program:

#### (a) Magnetic Fusion Energy Science Experimental Research Program Manager: Mark Foster, 858-455-3360, <u>mark.foster@science.doe.gov</u>

This Experimental Research program seeks to utilize unique magnetic fusion research facilities to develop the physics knowledge needed to advance the FES energy mission and fulfill the FES's role as federal steward for basic plasma science. The effort requires operation of a set of diversified experimental facilities, ranging from smaller-scale university experiments to large national facilities that involve extensive collaborations. The extensive plasma diagnostic systems operating on these facilities provide the experimental data required to study fusion science, basic plasma physics, and fusion energy production and to validate theoretical understanding and computer models, leading ultimately to a predictive understanding of plasma properties, including their dynamics and interactions with surrounding materials. Operation of major fusion facilities will be focused on science issues relevant to ITER design and operation, burning plasma physics, magnetic confinement, and other high priority plasma physics issues. The research needs of the magnetic fusion energy sciences component of this program were detailed in the report of a community-wide Research Needs Workshop (ReNeW) Research Needs for Magnetic Fusion Energy Sciences (http://science.energy.gov/~/media/fes/pdf/workshopreports/Res needs mag fusion report june 2009.pdf). This report describes the scientific research required during the ITER era to develop the knowledge needed for a practical fusion power source. Research in this area also involves small-scale facilities that explore emerging concepts for plasma confinement and stability, address critical issues that may affect the tokamak concept (e.g. plasma disruptions, impulsive heat loads, and operational maintenance and complexity), and investigate topics common to all fusion power plant concepts (e.g. interactions between plasma and material surfaces, and material science issues associated with the high fluxes of heat, charged-particles, and neutrons in a fusion power plant). The program also supports development of ITER-relevant diagnostic systems, advanced diagnostic capabilities to enable close coupling of experiments and theory/computations, and sensors or actuators required for active control of plasma properties to optimize device operation and plasma performance. Scientists from the U.S. also participate in leading experiments on fusion facilities abroad and conduct comparative studies to supplement the scientific understanding they can obtain from domestic facilities.

# (b) Magnetic Fusion Energy Science Theory and Simulation Program Manager: John Mandrekas, 301-903-0552, <u>john.mandrekas@science.doe.gov</u>

The Plasma Theory and Modeling 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, with a strong focus on the prediction, avoidance, control and mitigation of deleterious or performance-limiting macroinstabilities; the understanding and controlling of the multiscale, collisional, and turbulent physical mechanisms responsible for the loss of heat, momentum, and particles from the confining region; the interaction of externally launched radiofrequency waves designed to heat and drive current with the background plasma and surrounding structures; the nonlinear interaction between background plasma, various instabilities, and energetic particle populations, including the alpha

particles generated by the fusion reactions, and its impact on the confinement of these particles and the overall plasma performance; and the effect of multiscale and multiphysics processes at the plasma edge on the plasma performance and on the interaction and interface of the hot plasma boundary with the material walls. The efforts supported by this program provide the foundations for integrated simulations of fusion systems and range from analytical work to the development and application of advanced simulation codes capable of exploiting the potential of next generation high performance computers.

## (c) High-Energy-Density Plasma Science and Inertial Fusion Energy Science Program Manager: Sean Finnegan, 301-903-4920, <u>sean.finnegan@science.doe.gov</u>

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

## (d) General Plasma Science Experiment and Theory Program Manager: Nirmol Podder, 301-903-9536, <u>nirmol.podder@science.doe.gov</u>

The General Plasma Science program is directed toward research that addresses fundamental issues in plasma science and engineering that complements burning plasma science and reaches beyond into many basic and applied physics areas. Dynamic growth in new research areas, fostered by the development of new investigative techniques and tools, continues to present exciting opportunities for fundamental studies in basic plasma science and engineering. At the same time, economic forces are driving the need for improved understanding of the plasma state for the many applications of low temperature plasmas in modern technology. 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. Topics being encouraged include: (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.

## (e) Materials Science and Enabling Technologies for Fusion Program Manager: Peter Pappano, 301-903-4883, <u>peter.pappano@science.doe.gov</u>

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

## V. 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 the nature of matter, energy, and space.

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 three 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;
- 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.

Proposed research should address specific goals in one or more of these frontiers or technology areas, and discuss how the research or technology development supports the broad scientific objectives and mission of the HEP program. Principal investigators should submit their proposal to the HEP subprogram that they consider to be the best "fit" to the preponderance of their research effort.

Proposals should not attempt to bolster the case for facilities not currently approved for funding or not expected to be available during the course of the work.

## (a) Experimental Research at the Energy Frontier in High Energy Physics Program Manager: Abid Patwa, 301-903-0408, <u>abid.patwa@science.doe.gov</u>

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.

## (b) Experimental Research at the Intensity Frontier in High Energy Physics Program Manager: Alan Stone, 301-903-7998, <u>alan.stone@science.doe.gov</u>

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 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 Intensity Frontier experiments are also accepted. Support for LHCb research is <u>not</u> provided under this research area.

## (c) Experimental Research at the Cosmic Frontier in High Energy Physics Program Manager: Kathy Turner, 301-903-1759, <u>kathy.turner@science.doe.gov</u>

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 provides support for scientists to participate in these research areas, including graduate and postdoctoral research training for the next generation of scientists, and equipment and computational efforts to support the 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.

## (d) Theoretical Research in High Energy Physics Program Manager: Simona Rolli, 301-903-0504, <u>simona.rolli@science.doe.gov</u>

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.

# (e) Accelerator Science and Technology Research & Development in High Energy Physics Program Manager: L.K. Len, 301-903-3233, <u>lk.len@science.doe.gov</u>

The accelerator 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.

## (f) Particle Detector Research and Development in High Energy Physics Program Manager: Glen Crawford, 301-903-4829, <u>glen.crawford@science.doe.gov</u>

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.

#### VI. 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? To solve this mystery, the NP

program supports experimental and theoretical research—along with the development and operation of particle accelerators and advanced technologies—to create, detect, and describe the different forms and complexities of nuclear matter that can exist, including those that are no longer commonly found in our universe.

In executing this mission, nuclear physics focuses on three broad yet tightly interrelated areas of inquiry. These areas are described in *The Frontiers of Nuclear Science* (<u>http://science.energy.gov/np/nsac/</u>), a long range plan for nuclear science released in 2007 by the Nuclear Science Advisory Committee (NSAC). The three frontiers are: Quantum Chromodynamics, Nuclei and Nuclear Astrophysics, and Fundamental Symmetries and Neutrinos. Specific questions within these frontiers are addressed by the research activities of subprograms supported by the Office of Nuclear Physics as described below.

In addition, the NP isotope subprogram produces and/or distributes stable and radioactive isotopes that are critical for the Nation and supports research into production techniques for such isotopes.

The NP program supports the development of the tools and capabilities that make fundamental research possible, including accelerator research and development for current and future nuclear physics facilities. It also supports applications of nuclear science and technology to help bridge the gap between basic nuclear physics research and applied science, and an initiative on advanced detector technology research and development.

Research, development and fabrication of equipment directed toward research in any NP subprogram may be proposed, but applications including such extensive projects requiring detailed review of scope, budget and schedule beyond the procedures for this announcement will not be considered. Proposals should not attempt to bolster the case for facilities or major items of equipment not currently approved for funding or not expected to be available during the course of the work. Under this announcement, NP does not support investigations into the development of nuclear reactors for purposes outside the scope of the NP subprograms described below.

Applications are solicited for research in any of the NP subprograms and areas described below.

#### (a) Medium Energy Nuclear Physics Program Manager: Frank E (Ted) Barnes, 301-903-3212, <u>ted.barnes@science.doe.gov</u>

The Medium Energy subprogram of Nuclear Physics focuses primarily on questions having to do with the first frontier of Nuclear Physics, Quantum Chromodynamics (QCD), especially regarding the spectrum of excited mesons and baryons, and the behavior of quarks inside the nucleons (neutrons and protons). Specific questions that are being addressed include: *What does QCD predict for the properties of excited mesons and baryons? 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?* and *What is the internal landscape of the nucleons?* 

This subprogram also supports investigations of some aspects of the second and third frontiers, Nuclei and Nuclear Astrophysics, and Fundamental Symmetries and Neutrinos. Research in these areas addresses questions including: *What is the nature of the nuclear force that binds protons and neutrons into stable nuclei? Why is there now more visible matter than antimatter in the universe?* and *What are the unseen forces that were present at the dawn of the universe, but disappeared from view as the universe evolved?* 

In pursuing these topics the Medium Energy subprogram supports several experimental research programs, notably at the Thomas Jefferson National Accelerator Facility (TJNAF) and the Relativistic Heavy Ion Collider (RHIC). Two major goals of the Medium Energy research program at TJNAF are the discovery of "exotic mesons" which carry gluonic excitations, and the experimental study of the substructure of the nucleons.

## (b) Heavy Ion Nuclear Physics Program Manager: James Sowinski, 301-903-7587, james.sowinski@science.doe.gov

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

## (c) Low Energy Nuclear Physics Program Manager: Cyrus Baktash, 301-903-0258, <u>cyrus.baktash@science.doe.gov</u>

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

*universe but disappeared from view as the universe evolved?* The subprogram seeks to measure, or set a limit on, the neutrino mass and to determine if the neutrino is its own antiparticle. Experiments with cold neutrons also investigate the dominance of matter over antimatter in the universe, as well as other aspects of Fundamental Symmetries and Interactions.

#### (d) Nuclear Theory Program Manager: George Fai, 301-903-8954, <u>george.fai@science.doe.gov</u>

The Nuclear Theory subprogram supports theoretical research at universities and DOE national laboratories with the goal of improving our fundamental understanding of nuclear physics, interpreting the results of experiments, and identifying and exploring important new areas of research. This subprogram addresses all of the field's scientific frontiers described in NSAC's long range plan, as well as the specific questions listed for the experimental subprograms above.

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

## (e) Nuclear Data and Nuclear Theory Computing Program Manager: Frank E (Ted) Barnes, 301-903-3212, <u>ted.barnes@science.doe.gov</u>

This activity supports the National "Nuclear Data" effort, as well as several activities that facilitate the application of high performance computing to Nuclear Theory. The Nuclear Data program collects, evaluates, and disseminates nuclear physics data for basic nuclear research and for applied nuclear technologies through the National Nuclear Data Center (NNDC), which maintains open databases of scientific information gathered over the past 100+ years of nuclear physics research. "Nuclear Theory Computing" includes the NP component of the ASCR program Scientific Discovery through Advanced Computing (SciDAC). SciDAC promotes the use of supercomputers at national laboratories and universities to solve problems of current interest in the sciences. Recent topics in computational nuclear physics investigated under the SciDAC program include the theory of quarks and gluons on a lattice (LQCD), studies of a wide range of applications of models of nuclei and nuclear matter, and the development of theoretical techniques for incorporating lattice QCD results in more traditional many-body nuclear physics calculations.

# (f) Accelerator Research and Development for Current and Future Nuclear Physics Facilities Program Manager: Manouchehr Farkhondeh, 301-903-4398,

manouchehr.farkhondeh@science.doe.gov

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 beams; the development of a possible future electron-ion collider; 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 (FRIB). Also of interest is R&D in accelerator science and technology in support of next generation Nuclear Physics accelerator facilities.

## (g) Isotope Development and Production for Research and Applications Program Manager: Dennis Phillips, 301-903-7866, <u>dennis.phillips@science.doe.gov</u>

The Isotope Development and Production for Research and Applications subprogram supports the production and development of production techniques of radioactive and stable isotopes that are in short supply. The program provides facilities and capabilities for the production and/or distribution of research and commercial stable and radioactive isotopes. The scientific and technical staff associated with general isotope research and production, and a supply of critical isotopes to address the needs of the Nation are also supported. 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 other federal accelerator and reactor facilities throughout the Nation to promote a reliable supply of isotopes domestically. Topics of interest are focused on the development of advanced, cost-effective and efficient technologies for producing, processing, recycling and distributing isotopes in short supply. This includes technologies for production of radioisotopes using reactor and accelerator facilities and new technologies for enriching stable isotopes. Of special interest are innovative approaches to model and predict behavior and yields of targets undergoing irradiation in order to minimize target failures during routine isotope production.

## (h) Applications of Nuclear Science and Technology Technical Contact: Gulshan Rai, 301-903-4702, <u>gulshan.rai@science.doe.gov</u>

The Nuclear Physics program supports a competitive program of targeted initiatives in Applications of Nuclear Science and Technology (ANS&T), the primary goal of which is to pursue forefront nuclear science research and development important to the NP mission, but which is also inherently relevant to applications. One of the goals of this initiative is to help

bridge the gap between basic nuclear physics research and applied science. The ANS&T program is not intended to supplement activities that are within the scope of the NP thematic science subprograms (a)-(d), Major Item of Equipment fabrication projects (MIEs) connected with the NP science subprograms, nor does it consider applications that are aligned with the primary mission of other DOE programs or other funding Agencies. Early Career Research Program applications will be considered that demonstrate strong partnerships with the intended application stakeholder(s) and that can be expected to have a tangible impact on other fields. Evidence of partnership may include proposed cost sharing. Areas of R&D responsive to this subprogram may include (but are not limited to) nuclear physics research relevant to the development of advanced fuel cycles for next generation nuclear power reactors; advanced costeffective accelerator technology and particle detection techniques for medical diagnostics, treatment or improving human health; environmental and water resource management; food and agriculture; and research in developing neutron, gamma, and particle beam sources with applications in contraband material screening and nuclear forensics. Applications may be peer reviewed with participation from the applied sciences community. For this subprogram, the programmatic priorities will include an evaluation of the innovative nuclear science advances and their relevance to the application, the cost effectiveness and performance relative to existing technologies, and the impact of the expected science and technology transfer.

## (i) Advanced Detector Technology Research and Development in Nuclear Physics Technical Contact: Gulshan Rai, 301-903-4702, <u>gulshan.rai@science.doe.gov</u>

Future nuclear physics experiments will require new radiation detection material, measurement techniques and data acquisition architectures. Advances in these areas could allow the development of significantly high channel density, higher timing, position and/or energy resolution, particle identification, data bandwidth, high radiation tolerant devices, higher precision or extremely low noise per detection element. Many experiments will need two or more of these features at approximately the same or lower cost as present generation experiments. This program supports applications for innovative R&D efforts directed at achieving **radically new advancements of detector technologies** needed to perform or conceive future state-of-the-art nuclear physics experiments at NP's present, upgraded or planned accelerator facilities, or at non-accelerator research institutions supported by NP. The emphasis is **on generic detector R&D concepts that are transformative**, rather than incremental advancement of established ideas or fabrication techniques.

Interesting technologies include but are not limited to: new types of low-mass, high-channeldensity radiation hard charged particle tracking detectors or calorimeters; particle identification detectors that have improved resolution, are lower in cost, or can be read out faster than currently available detectors; novel efficient gamma-ray, neutron and charged particle detectors; detector readout systems that eliminate wires or integrate wireless technologies; nanotechnology; novel materials such as composite polymers, ceramics and organics; non-planar 3-dimensional monolithic sensors or data processing circuitry; large scale self-calibrating detectors or novel detection methodologies. Applications will be excluded that are deemed appropriate for consideration by existing detector R&D programs administered at NP User Facilities.

Final engineering or fabrication of detectors for specific experiments will not be funded by this program. Applications to develop detector technology that is targeted at experiments for nearer term enhancements of existing detectors should not be submitted.

# Section II – AWARD INFORMATION

# A. TYPE OF AWARD INSTRUMENT

DOE anticipates awarding grants under this FOA.

# **B. ESTIMATED FUNDING**

It is anticipated that up to \$6,000,000 per year will be available under this FOA, contingent on satisfactory peer review and the availability of appropriated funds. Between 30 and 50 awards are anticipated, and applicants should request project support for five years, with out-year support contingent on the availability of appropriated funds, progress of the research, and programmatic needs. Awards are expected to begin in **FY 2014**.

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

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

Ceiling

None

**Floor** \$750,000 over five years

# **D. EXPECTED NUMBER OF AWARDS**

DOE anticipates making 30-50 awards under this FOA. The number of awards is subject to the availability of FY 2014 funds.

# E. ANTICIPATED AWARD SIZE

While the minimum award size is \$750,000, DOE expects the typical award size will be \$750,000 over five years. Applicants are encouraged to propose research expenditures as close to the funding minimum as possible. Typical budgets will be \$150,000 per year for five years.

# F. PERIOD OF PERFORMANCE

DOE anticipates making awards with a project period of five years.

# G. TYPE OF APPLICATION

DOE will accept new applications under this FOA.

# Section III – ELIGIBILITY INFORMATION

# A. ELIGIBLE APPLICANTS

Only U.S. academic institutions are eligible to apply. Other Federal agencies, 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 are not eligible to apply.

The Principal Investigator must be an **untenured** Assistant Professor on the tenure track or an **untenured** Associate Professor on the tenure track at a U.S. academic institution as of the deadline for the application. No more than ten (10) years can have passed between the year the Principal Investigator's Ph.D. was awarded and the year of the deadline for the application. For the present competition, those who received doctorates no earlier than 2003 are eligible.

There can be no co-Principal Investigators.

Each Principal Investigator may only submit one Office of Science Early Career Research Program application per annual competition. Additionally, a Principal Investigator may not participate in more than three Office of Science Early Career Research Program competitions.

Participation in the competition is defined as submission of a full application.

The act of submitting an application implies that the submitting institution has checked, confirmed, and certifies that the Principal Investigator is eligible. No additional certifying documentation is required.

Applications must be submitted through a U.S. academic institution. A companion announcement (LAB 13-958) describes the Early Career Research Program opportunity for full-time DOE national laboratory employees. An employee with a joint appointment between a university and a DOE national laboratory must apply through the institution that pays his or her salary and provides his or her benefits; the eligibility criteria above must also be met.

Eligibility exemptions will not be granted.

# **B. COST SHARING**

Cost sharing is not required.

# **C. ELIGIBLE INDIVIDUALS**

There is NOT a U.S. citizenship requirement for the Principal Investigator or any project participants.

Principal Investigators of early career awards from other agencies or entities are eligible, but the proposed research must have a scope different from that already funded by the other organization.

Principal Investigators who received awards in FY 2010, FY 2011, FY 2012, or FY 2013 under the Office of Science Early Career Research Program are not eligible.

If a Principal Investigator has multiple doctorates, the discipline of the one they have earned within the ten-year eligibility window should be relevant to the proposed research.

Letters of recommendation are not allowed. Applications that include recommendation letters will be subject to elimination from consideration during DOE's initial review. A department chair letter is not required and should not be included.

Eligible individuals with the skills, knowledge, and resources necessary to carry out the proposed research as a 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-0000958**) 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

A Letter of Intent is not required.

## 2. Pre-application

PRE-APPLICATION DUE DATE September 5, 2013, 5 PM Eastern Time

ENCOURAGE/DISCOURAGE DATE October 3, 2013, 5 PM Eastern Time

A pre-application is required and must be submitted by 09/05/2013 at 5 PM Eastern Time. The pre-application must be submitted electronically through the DOE Office of Science Portfolio Analysis and Management System (PAMS) website https://pamspublic.science.energy.gov/.

Pre-applications will be reviewed for responsiveness of the proposed work to the research topics identified in this FOA. DOE will send a response by email to each applicant encouraging or discouraging the submission of a full application by October 3, 2013. Applicants who have not received a response regarding the status of their pre-application by this date are responsible for contacting the program to confirm this status. **Only those applicants that receive notification from DOE encouraging a full application may submit full applications.** No other full applications will be considered.

The pre-application attachment should include, at the top of the first page, the following information:

Title of Pre-application Principal Investigator Name, Job Title Institution PI Phone Number, PI Email Address Year Doctorate Awarded: XXXX Number of Times Previously Applied<sup>†</sup>: Funding Opportunity Announcement Number: **DE-FOA-0000958** 

<sup>†</sup> Indicate how many times the PI has previously submitted a full application in the Office of Science Early Career Research Program. The program has been offered in four previous years, FY 2010, FY 2011, FY 2012, and FY 2013. Participation in the competition is defined as submission of a full, formal application. A PI who has participated in three past Office of Science Early Career Research Program competitions is not eligible.

This information should be followed by a clear and concise description of the objectives and technical approach of the proposed research. The pre-application may not exceed two pages, with a minimum text font size of 11 point and margins no smaller than one inch on all sides. Figures and references, if included, must fit within the two-page limit.

Only one pre-application per Principal Investigator is allowed.

To help the Office of Science avoid conflicts of interest in identifying potential reviewers, a onepage list of the Principal Investigator's collaborators, co-editors, and graduate/postdoctoral advisors and advisees must be submitted with the pre-application. The one-page list should be the last page in the pre-application file and will not count against the two-page limit for the preapplication. Further guidance on how to prepare this list is included in the next two paragraphs:

<u>Collaborators and Co-editors</u>: List, in alphabetical order, all persons, including their current organizational affiliations, who are, or who have been, collaborators or co-authors with the Principal Investigator on a research project, book or book article, report, abstract, or paper during the 48 months preceding the closing date of this announcement. 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 in the past co-editors with the Principal Investigator on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the closing date of this announcement. If there are no collaborators or co-editors to report, state "None."

<u>Graduate and Postdoctoral Advisors and Advisees</u>: List the names of the Principal Investigator's own graduate advisor(s) and principal postdoctoral sponsor(s) and their current organizational affiliations. Also list the names of the Principal Investigator's graduate students and postdoctoral associates during the past five years and their current organizational affiliations.

Since the Office of Science will never use individuals from your institution as reviewers, you may omit them from the preproposal list to save space. Listing collaborators on your preproposal is to help us identify reviewers and does not affect the decision to encourage or discourage submission of a full proposal.

Those pre-applications that are encouraged are used to help the Office of Science begin planning for the full application peer review process. The intent of the Office of Science in discouraging submission of certain full applications is to save the time and effort of applicants in preparing and submitting full applications not responsive to this funding opportunity announcement.

The Principal Investigator will be automatically notified when the pre-application is encouraged or discouraged. The DOE Office of Science Portfolio Analysis and Management System (PAMS) will send an email to the Principal Investigator from <u>PAMS.Autoreply@science.doe.gov</u>, and the status of the pre-application will be updated at the PAMS website <u>https://pamspublic.science.energy.gov/</u>. Notifications are sent as soon as the decisions to encourage or discourage are finalized.

It is important that the pre-application be a single file with extension .pdf, .docx, or .doc. The pre-application must be submitted electronically through the DOE Office of Science Portfolio Analysis and Management System (PAMS) website <u>https://pamspublic.science.energy.gov/</u>. The Principal Investigator and anyone submitting on behalf of the Principal Investigator must register for an account in PAMS before it will be possible to submit a pre-application. All PIs and those submitting pre-applications on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays.

To access PAMS, you may use the Internet Explorer, Firefox, Google Chrome, or Safari browsers.

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.

#### **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. (Note: If you reviewed for or were listed as PI on a prior submission to the Office of Science but have not previously

created an account, you may already be linked to an institution in PAMS. If this is the case, PAMS will take you to the PAMS home page.)

# **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 need not enter the exact name of the institution, but you should enter a word or phrase contained within the institution name. (Hint: If your institution has an acronym, such as ANL for Argonne National Laboratory or UCLA for the Regents of the University of California, Los Angeles, you may 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.

# **Submit Your Pre-Application:**

- Create your pre-application (called a preproposal in PAMS) outside the system and save it as a file with extension .docx, .doc, or .pdf. Make a note of the location of the file on your computer so you can browse for it later from within PAMS.
- Log into PAMS and click the Proposals tab. Click the "View / Respond to Funding Opportunity Announcements" link and find the current announcement in the list. Click the "Actions/Views" link in the Options column next to this announcement to obtain a dropdown menu. Select "Submit Preproposal" from the dropdown.
- On the Submit Preproposal page, select the institution from which you are submitting this preproposal from the Institution dropdown. If you are associated with only one institution in the system, there will only be one institution in the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per preproposal; to do so, click the "Select PI" button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the "Actions" link

in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose "Select PI."

- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the "Invite PI" link at the top left of the "Select PI" screen. You can enter an optional personal message to the PI in the "Comments" box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the preproposal. Save the preproposal for later work by clicking the "Save" button at the bottom of the screen. It will be stored in "My Preproposals" for later editing.
- Enter a title for your preproposal.
- Select the appropriate technical contact from the Program Manager dropdown.
- To upload the preproposal file into PAMS, click the "Attach File" button at the far right side of the screen. Click the "Browse" (or "Choose File" depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the "Upload" button to upload the file.
- At the bottom of the screen, click the "Submit to DOE" button to save and submit the preproposal to DOE.
- Upon submission, the PI will receive an email from the PAMS system <<u>PAMS.Autoreply@science.doe.gov</u>> acknowledging receipt of the preproposal.

You are encouraged to register for an account in PAMS at least a week in advance of the preproposal submission deadline so that there will be no delays with your submission.

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-0000958**.

Pre-applications submitted outside PAMS will not be considered. Pre-applications should not be submitted through Grants.gov or Fedconnect.

# C. CONTENT AND APPLICATION FORMS

APPLICATION DUE DATE November 19, 2013, 5 PM Eastern Time

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.

## LETTERS

Letters of recommendation are not allowed. Applications that include recommendation letters will be subject to elimination from consideration during DOE's initial review.

A department chair letter is not required and should not be included.

Optional letters of collaboration for unfunded or funded collaborations may be placed in Appendix 6 (Other Attachments). Letters of collaboration should state the intention to participate, but they should not be written as recommendation or endorsement letters, which are not allowed.

Each optional letter of collaboration may contain <u>two and only two</u> sentences and must use the following format:

Dear < Principal Investigator Name>:

If your application entitled, "<Application Name>," is selected for funding under the DOE Office of Science Early Career Research Program, it is my intent to collaborate in this research by <Complete Sentence With a Very Short Description of What the Collaborator Offers to Do or Provide>. Thank you for the opportunity to participate.

Sincerely,

<Collaborator's Name and Signature Block>

# 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 represents and certifies the following:

- 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 must contain a summary of the proposed activity suitable for dissemination to the public. It should be a self-contained document that identifies the name of the applicant, the Principal Investigator (PI), the project title, the objectives of the project, a description of the project, including methods to be employed, the potential impact of the project (i.e., benefits, outcomes). This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must

not exceed 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."

The abstract may be used to prepare publicly accessible reports about DOE-supported research.

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

The following application cover page information may be placed on a plain page. No form is required. This cover page will not count in the project narrative page limitation.

- Institution:
- Street Address/City/State/Zip:
- Principal Investigator (PI):
- Position Title of PI:
- Business Mailing Address of PI:
- Telephone Number of PI:
- Email of PI:
- Funding Opportunity Announcement Number: DE-FOA-0000958
- DOE/Office of Science Program Office (ASCR, BER, BES, FES, HEP, or NP):
- Topic Area\*:
- Topic Area Program Manager:
- Year Doctorate Awarded:
- Is the PI in a Tenure-Track Appointment (Yes or No)?
- Does the PI have tenure (Yes or No)?
- Number of Times Previously Applied<sup>†</sup>:
- PAMS Preproposal Number:
- PECASE Eligible\*\*: (Yes or No)?

\* The topic area can be found in Part I, Supplementary Information, of this funding opportunity announcement. For example, the topic area might be Synthesis and Processing Science or Magnetic Fusion Energy Science Theory and Simulation. Please select from the list in Part I.

<sup>†</sup> Indicate how many times the PI has previously submitted a full application in the Office of Science Early Career Research Program. The program has been offered in four previous years, FY 2010, FY 2011, FY 2012, and FY 2103. Participation in the competition is defined as submission of a full, formal application. A PI who has participated in three past Office of Science Early Career Research Program competitions is not eligible.

\*\* The White House Office of Science and Technology Policy may ask federal agencies each year to nominate candidates for the Presidential Early Career Awards for Scientists and Engineers (PECASE). Investigators from the top applications in the Office of Science Early Career Research Award competition may be nominated for PECASE if they are eligible. A PI is PECASE-eligible if he or she is, as of the closing date of this FOA, a U.S. citizen, U.S. national

or permanent resident and if she or he has not received a PECASE previously through any agency. PECASE eligibility is not required for an award under the current FOA.

PROJECT NARRATIVE (FIELD 8 ON THE FORM)

The project narrative **must not exceed 15 pages** 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. Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph.

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 narrative should provide a clear, concise statement of the specific objectives/aims of the proposed project. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also include a timeline for the major activities of the proposed project.

Do not include any Internet addresses (URLs) that provide supplementary or additional information that constitutes a part of the application. Using Internet sites in an attempt to avoid page limits will fail: The content of those sites will not be reviewed. See Part VIII.D for instructions on how to mark proprietary application information. To attach a Project Narrative, click "Add Attachment."

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the Principal Investigator (PI) as an appendix to your technical narrative. As part of the sketch, provide information that can be used by reviewers to evaluate the PI's potential for leadership within the scientific community. Examples of information of interest are invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society activities, special international or industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences. The biographical information (curriculum vitae) must not exceed 3 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 the following:

**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. An abbreviated style such as the Physical Review Letters (PRL) convention for citations (list only the first author) may be used for publications with more than 10 authors.

**Synergistic Activities**: List professional and scholarly activities related to the effort proposed. Some examples might be invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society membership and/or activities, special international or industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences.

**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.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

## APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support (both Federal and non-Federal) for the Principal Investigator(s) (PI) 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 PI. Do not list start-up funds provided to the PI by the employing academic institution. If the PI has submitted a similar research application to an early career program at another agency or foundation, she or he should provide a few sentences explaining the similarities and/or differences with the current Early Career Research Program application. 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.
- This appendix will not count in the project narrative page limitation.

## 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). 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.
- This appendix will not count in the project narrative page limitation.

## 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.
- This appendix will not count in the project narrative page limitation.

## **APPENDIX 5: EQUIPMENT**

List 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.
- This appendix will not count in the project narrative page limitation.

# APPENDIX 6: OTHER ATTACHMENTS

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, and reviewers may not have time to read extensive appendix materials with the same care they would use with the application proper. Do not include scientific publications. Although the preference of this program is to support PI-led efforts without paid collaborators, if a funded or unfunded collaboration is proposed, an optional letter of collaboration may be included in this appendix. Letters of collaboration should state the intent to participate and nothing else. They should not be written as recommendation or endorsement letters, which are not allowed. Each optional letter of collaboration may contain two and only two sentences and must use the following format:

Dear < Principal Investigator Name>:

If your application entitled, "<Application Name>," is selected for funding under the DOE Office of Science Early Career Research Program, it is my intent to collaborate in this research by <Complete Sentence With a Very Short Description of What the Collaborator Offers to Do or Provide>. Thank you for the opportunity to participate.

## Sincerely,

<Collaborator's Name and Signature Block>

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

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 in the project narrative file. These appendices will not count toward the project narrative's page limitation.

## 3. Research And Related Budget

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

Budget Fields

Section A Senior/Key Person Section B Other Personnel	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 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. Allowable items ordinarily will be limited to research equipment and apparatus not already available for the conduct of the work. General-purpose office equipment is not eligible for support unless primarily or exclusively used in the actual conduct of scientific research.
Section D Travel	For purposes of this section only, travel to Canada or to Mexico is considered domestic travel. In the budget justification, list each trip's 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 Participant/Trainee Support Costs	If applicable, submit training support costs. Educational projects that intend to support trainees (precollege, college, graduate and post graduate) must list each trainee cost that includes stipend levels and 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	• Materials and Supplies: Enter total funds requested for materials
Other Direct Costs	and supplies in the appropriate fields. In the budget justification,
	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).
	• <b>Publication Costs:</b> Enter the total publication funds requested. The
	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).
	• <b>Consultant Services:</b> Enter total funds requested for all consultant
	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>
	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).
	• 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.
	• 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).
	• 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.
	• 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.		
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		
	information if using a negotiated rate agreement.		
Section I	This is the total of Sections G and H		
Total Direct and			
Indirect 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

Under the Early Career Research Program, preference will be given to applications without subawards with the exception of those that propose small subawards for essential supporting work such as sample analysis. Subawards that pay salary for scientific collaborators outside the proposing institution are discouraged.

**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
<b>RESEARCH AND RELATED Other</b> <b>Project Information</b>	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**

A letter of intent is not required.

# 2. Pre-application Due Date

September 5, 2013, 5 PM Eastern Time

# **3. Application Due Date**

November 19, 2013, 5 PM Eastern Time

You are encouraged to transmit your application well before the deadline.

Modifications to the application are not allowed after the application due date.

# 4. Late Submissions

Delays in submitting letters of intent, pre-applications, and applications may be unavoidable. DOE has accepted late submissions when applicants have been unable to make timely submissions because of technological disruptions or significant natural disasters. Other circumstances do not justify late submissions. Unacceptable justifications include but are not limited to the following:

- Failure to begin submission process early enough.
- Failure to provide sufficient time to complete the process.
- Failure to understand the submission process.
- Failure to understand the deadlines for submissions.
- Failure to satisfy prerequisite registrations.
- Unavailability of administrative personnel.

Applicants must email early.career@science.doe.gov to discuss the option of a late submission in the case of unavoidable circumstances.

DOE notes that not all requests for late submission will be approved.

# 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 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.

Support for paid collaborators of the Principal Investigator will be considered only in rare cases where a collaborator (either early career or senior) brings something unique to the project. However, preference will be given to Principal-Investigator-led efforts without paid collaborators for which the budget covers research support staff (e.g., students and postdoctoral fellows), travel, supplies, equipment, and other expenses necessary for the Principal-Investigator-led project.

Preference will be given to applications without subawards with the exception of those that propose small subawards for essential supporting work such as sample analysis. Subawards that pay salary for scientific collaborators outside the proposing institution are discouraged.

# 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 http://www.grants.gov/applicants/get\_registered.jsp). 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/assets/OrganizationRegCheck.pdf</u> to guide you through the process. 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

#### 4. 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.

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-0000958**.

# 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.

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

The following FOA-specific evaluation criteria will also be used during the scientific merit review (peer review):

- 5. Relevance to the mission of the specific program (e.g., ASCR, BER, BES, FES, HEP, or NP) to which the application is submitted.
- 6. Potential for leadership within the scientific community.

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 following questions will be posed to reviewers for each of the review criterion listed above:

#### 1. Scientific and/or Technical Merit of the Project

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

thinking in relevant scientific fields of research? What is the likelihood of achieving influential results?

# 2. Appropriateness of the Proposed Method or Approach

Does the proposed research employ innovative concepts or methods? How logical and feasible are the research approaches? 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?

#### 3. Competency of Applicant's Personnel and Adequacy of Proposed Resources

Does the proposed work take advantage of unique facilities and capabilities? 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?

#### 4. 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?

# **5.** Relevance to the mission of the specific program (e.g., ASCR, BER, BES, FES, HEP, or NP) to which the application is submitted

How does the proposed research contribute to the mission of the program in which the application is being evaluated?

# 6. Potential for leadership within the scientific community

Scientific leadership can be defined very broadly and can include direct research contributions. How has the PI demonstrated the potential for scientific leadership and creative vision? How has the PI been recognized as a leader?

#### For criterion 5, the missions of the program areas are:

Advanced Scientific Computing Research (ASCR): 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.

**Biological and Environment Research (BER):** To support fundamental research focused on three scientific drivers: exploring the frontiers of genome-enabled 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.

**Basic Energy Sciences (BES):** 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.

**Fusion Energy Sciences (FES):** 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 interactions with its surroundings across wide ranges of temperature and density, developing advanced diagnostics to make detailed measurements of its properties and dynamics, and creating theoretical and computational models to resolve the essential physics principles.

**High Energy Physics (HEP):** 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.

**Nuclear Physics (NP):** 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, familiar and unfamiliar, is still largely unknown.

# **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 Official will consider the merit review recommendations, program policy factors, programmatic priorities, and the amount of funding available.

# 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 under this program within 7 months**. The time interval begins on the date applications are due or the date the application is received, if there is no specified due date/deadline. Awards are expected to be made in Fiscal Year 2014.

# Section VI - AWARD ADMINISTRATION INFORMATION

Office of Science Early Career Research Program investigators intending to transfer to a new institution must submit a request for transfer along with a new application. If the scope of work has not changed, the award can be transferred. If the scope of work has changed, the new application will be subject to merit review as described above. Transfer awards will be for the remaining award period only, and the requested budget cannot exceed the remaining budget for the original award. While a transfer application can be submitted any time of the year, it should be submitted at least six months before the transfer to allow time for execution of merit review. To transfer an award to an academic institution, the investigator must move into a tenure-track or tenured position at the academic institution. To transfer an award to a DOE National Laboratory, the investigator must move into a full-time, permanent, non-postdoctoral national laboratory position.

To retain an award at an academic institution, the investigator must remain on the tenure track (e.g., be either tenured or untenured but on the tenure track).

# 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 materials: (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 <a href="http://www.nsf.gov/bfa/dias/policy/rtc/index.jsp">http://www.nsf.gov/bfa/dias/policy/rtc/index.jsp</a>.

#### **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: <u>http://www.ecfr.gov</u>). 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: http://energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards

# **3. National Policy Assurances**

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

# **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.

Annual progress reports from the award investigator will be required.

# 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 <a href="mailto:support@grants.gov">support@grants.gov</a>. DOE cannot answer these questions.

Please only 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-0000958**. 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
Administrative Contact	Questions about program rules should be sent to
	early.career@science.doe.gov.
Program Manager	Questions regarding the specific program areas/technical
Scientific Contact	requirements can be directed to the program managers listed for
	each program 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.