

Program Announcement To DOE National Laboratories

LAB 12-751: **Amendment**

Office of Science Early Career Research Program

This Announcement was amended 9/4/2012. On page 2, in the PAMS preproposal submission instructions, the phrase, “View Funding Opportunity Announcements” was replaced with “View DOE National Laboratory Announcements”. No other changes were made.

GENERAL INQUIRES ABOUT THIS PROGRAM ANNOUNCEMENT SHOULD BE DIRECTED TO:

Administrative Contact: Questions about program rules should be sent to early.career@science.doe.gov.

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 Announcement.

PREPROPOSALS ARE REQUIRED.

Preproposals are **REQUIRED** and must be submitted by September 6, 2012, 5:00 P.M. Eastern Time. The preproposal should be created as a Portable Document Format (pdf) file and submitted electronically through the DOE Office of Science Portfolio Analysis and Management System (PAMS) website <https://pamspublic.science.energy.gov/>.

To access PAMS, please use either Internet Explorer or Firefox. Currently, PAMS does not support the Chrome or Safari browsers, but an upgrade in the future will make it possible to use them.

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 preproposal. Registering to PAMS is a two-step process. First, click “Create New PAMS Account” on the website <https://pamspublic.science.energy.gov/> and follow the instructions for creating an account. You will be prompted to create a username and password and to enter your contact information.

Second, once you create an individual account, you must associate yourself with (“register to”) your institution. Follow the onscreen instructions to do this.

All PIs and those submitting on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays.

Once you have created your account and associated yourself with your institution in PAMS, you can submit the preproposal. To submit the preproposal, log in to PAMS. Select ~~“View Funding Opportunity Announcements”~~ **“View DOE National Laboratory Announcements”** and find the current announcement in the list. Click on “Actions/Views” for this announcement, select “Submit Preproposal” from the dropdown menu, and follow the instructions from there.

- Note that you must select one and only one Principal Investigator (PI) per preproposal; click on “Select PI” on the far right side of the screen and then select the appropriate PI from the list of all registered users from your institution returned by PAMS. If you are submitting a preproposal for a PI whose name does not appear on the list, he or she has not yet registered in PAMS. In this case, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, choose “Invite PI” at the top left of the “Select PI” screen. You can enter an optional personal message to the PI in the “Comments” box that PAMS presents, and it will be included in the email sent by PAMS to the PI.
- When submitting the preproposal, you will be asked to select a program manager. Select the program manager associated with the detailed program description contained in this announcement to which the proposed research idea is responsive.
- To upload the preproposal as an attachment into PAMS, select “Attach File” at the far right side of the screen. Search for your file and then select “Attach” to upload the file. You may enter an optional description of the file you are attaching. Using the dropdown at the bottom of the screen, save the preproposal and then submit it to DOE.
- Upon submission, the PI will receive an email from the PAMS system acknowledging receipt of the preproposal.

Each laboratory is responsible for ensuring that the research ideas submitted in its preproposals fit within the scope of Office of Science-funded programs at the national laboratory.

Preproposals will be reviewed for responsiveness of the proposed work to the research topics identified in this DOE national laboratory announcement. DOE will send a response by email to each applicant encouraging or discouraging the submission of a formal proposal by Thursday, October 4, 2012. Applicants who have not received a response regarding the status of their preproposal by this date are responsible for contacting the program to confirm this status. **Only those applicants that receive notification from DOE encouraging a formal proposal may submit full proposals.** No other formal proposals will be considered.

The preproposal attachment should include, at the top of the first page, the following information:

Title of Preproposal
Principal Investigator Name, Job Title
Institution
PI Phone Number, PI Email Address
Year Doctorate Awarded: XXXX
DOE National Laboratory Announcement Number: LAB 12-751

This information should be followed by a clear and concise description of the objectives and technical approach of the proposed research. The preproposal 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 preproposal per Principal Investigator is allowed.

Those preproposals that are encouraged will be used to help the Office of Science begin planning for the formal proposal peer review process. The intent of the Office of Science in discouraging submission of certain full proposals is to save the time and effort of applicants in preparing and submitting formal proposals not responsive to this funding announcement.

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

Collaborators and Co-editors: 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 November 2012. 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 November 2012. If there are no collaborators or co-editors to report, state "None."

Graduate and Postdoctoral Advisors and Advisees: 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.

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, please contact the Office of Science PAMS Support Center. The PAMS Support Center can be reached Monday-Friday 7:00 AM-6:00 PM Eastern Time. Telephone: (301) 903-5313, Email: scsc@science.doe.gov. All submission and inquiries about this announcement must reference Announcement **LAB 12-751**.

Preproposals submitted outside PAMS will not be considered.

PROPOSAL DUE DATE: Formal proposals submitted in response to this Program Announcement must be submitted into the DOE Office of Science Portfolio Analysis and Management System (PAMS) by November 26, 2012, 5:00 P.M. Eastern Time, to permit timely consideration of awards. **The Principal Investigator (PI) and anyone submitting on behalf of the PI must register for an account in PAMS before it will be possible to submit a proposal.** To register, click “Create New PAMS Account” on the website <https://pamspublic.science.energy.gov/> and follow the instructions for creating an account and registering to an institution.

You are encouraged to transmit your proposal well before the deadline. Only those proposers that receive notification from DOE encouraging a formal proposal may submit full proposals. PROPOSALS RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.

SUMMARY:

The Office of Science of the Department of Energy hereby invites proposals 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 disciplines 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 and Biosystems Design for Bioenergy Production by Novel Platform Organisms
- (b) Environmental System Science
- (c) Uncertainty Characterization for Integrated Earth System Modeling

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)
- (l) 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) BES Nanoscale Science Research Centers and Electron-Beam Microcharacterization Centers Research
- (w) BES Accelerator and Detector Research
- (x) BES X-ray and 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 High Energy Physics Research
- (b) Theoretical High Energy Physics Research
- (c) Advanced Technology 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 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 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 understanding 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

Program Manager: Sandy Landsberg, 301-903-8507, sandy.landsberg@science.doe.gov

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:

1. 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 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, 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

Program Manager: Sonia R. Sachs, 301-903-0060, sonia.sachs@science.doe.gov

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 three key research challenges for exascale platforms, namely:

1. Programming models, language constructs, compilers and runtime systems that address the challenges of programming applications which are characterized by computations on irregular data structures and with unstructured and dynamic communication patterns;
2. Software solutions that dynamically capture data movement patterns in applications and enable the adaptive selection of optimal data movement strategies, leveraging heterogeneous processors and novel hardware architectures;
3. Scientific data management, including data provenance representation and capture; data integration/fusion; data interoperability; and scientific workflow systems that support data analysis and visualization for petabyte to exabyte data sets.

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. Topics which are out of scope for this program include hardware architecture, and performance modeling and assessment tools, software development tools and methods (e.g., debuggers, integrated development environments, etc.), interoperability at the application level, 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, and research which is only applicable to hand-held, portable, desktop, cluster or cloud computing.

II. Biological and Environmental Research (BER)

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

The mission of the Biological and Environmental Research (BER) program is to support fundamental research focused on three scientific drivers: exploring the frontiers of 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.

Biological Systems Science

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

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

(a) Systems Biology and Biosystems Design for Bioenergy Production by Novel Platform Organisms

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

Research aimed at developing systems biology knowledge and genetic tools for the functional modification of an expanded suite of microbes and plants for sustainable bioenergy production. Relevant organisms include bioenergy relevant microbes (i.e. those capable of deconstruction of cellulosic plant material, photosynthetic capture of CO₂, or synthesis of next generation biofuel compounds) or non-food plants that can serve as dedicated biomass feedstocks. Proposals should focus on understanding metabolic and regulatory networks governing functional properties, underlying biological design principles, and systems scale biodesign strategies for improvement of bioenergy relevant properties. Proposals are not encouraged for food plants or organisms of primarily biomedical relevance. Research on well established model organisms will need to justify how the research contributes to an expanded set of novel platform organisms for bioenergy research.

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 two areas:

(b) Environmental System Science

Program Manager: Mike Kuperberg, 301-903-3511, michael.kuperberg@science.doe.gov

Research that combines measurements, experiments, and modeling that provide improved quantitative and predictive understanding of the coupled biological, chemical and physical interactions of the belowground carbon cycle processes that in turn influence the directions of terrestrial ecology and global climate change. The goal should be to provide a refined understanding of critical belowground processes (e.g., soil carbon turnover, root dynamics, rhizo deposition, mycorrhizal interactions) in non-managed terrestrial ecosystems which mediate carbon cycling and feedbacks in a changing climate. Research should be posed in the context of representing terrestrial carbon cycle processes in Earth system models.

(c) Uncertainty Characterization for Integrated Earth System Modeling

Program Manager: Dorothy Koch, 301-903-0105, Dorothy.koch@science.doe.gov

Development of methodologies that characterize uncertainties in integrated global earth system models, by examining the components that contribute significantly to climate system and projection uncertainties. It is expected that proposed research will include novel approaches that examine nonlinear relationships between different component level uncertainties due to, e.g., data limitations associated with initial and boundary conditions, simplifications of parameterizations and submodel codes, resolution, correlated error analyses across system components, numerical methods, and validation.

BER EXCLUSIONS: Proposals for BER research should specifically identify which of the three topics listed above, (a) Systems Biology and Biosystems Design for Bioenergy Production by Novel Platform Organisms, (b) Environmental System Science, (c) Uncertainty Characterization for Integrated Earth System Modeling, is the focus of the proposed research and how the proposed research will address the stated aims. Proposals that address other BER-related topics or that do not make specific reference to the stated aims of these three topics **will not** be accepted.

III. Basic Energy Sciences (BES)

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

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

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 2011 Research Descriptions:

http://science.energy.gov/~media/bes/pdf/reports/files/bes_fy2011_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/csgeb/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

Program Manager: Michael Sennett, 301-903-6051, Michael.Sennett@science.doe.gov

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 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; and the study and control of surface and interfacial chemistry including electrochemistry.

Recent BES Basic Research Needs (and other) workshops and reports, have articulated those areas of the materials sciences which 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 make progress towards that goal by emphasizing research on the chemistry-based discovery, design and synthesis of new materials and/or morphologies that have the potential to enable next generation energy technologies, including energy conversion (thermal, solar, mechanical, chemical), energy storage and transport (electrical, mechanical, thermal), and carbon capture.

The program **will not** support projects aimed at *optimization* of material properties for specific applications, device fabrication, nanoparticle synthesis as a primary goal, or materials focused on hydrogen storage technologies.

(b) Biomolecular Materials

Program Manager: Michael Markowitz, 301-903-6779, mike.markowitz@science.doe.gov

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 for a broad range of non-biological conditions; bio-inspired 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 will seek to advance the ability for materials to self-repair, regulate, clean, sequester impurities, and tolerate abuse. Bio-inspired materials discovery—linking physical and chemical synthesis with the synthesis strategies of biology—will continue to be a focus to create new materials *in vitro* with altered morphologies and desired materials properties, including both inorganic materials and polymers. The activity will also expand research on dynamically adaptive, self-repairing materials and functional structures that take inspiration from biological membranes, pores, gates, and motors. Enhanced integration of theory and experiment leading to new design ideas and opportunities for discovery is sought.

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

(c) Synthesis and Processing Science

Program Manager: Bonnie Gersten, 301-903-0002, bonnie.gersten@science.doe.gov

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 researching 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 activities to accelerate progress in understanding synthesis and discovery of new materials will be emphasized, while research in ion beam assisted growth techniques, and synthesis of individual nanowires and particles will be reduced.

Synthesis and Processing **does not** fund research on device fabrication or optimization of material properties.

(d) Experimental Condensed Matter Physics

Program Manager: Andrew Schwartz, 301-903-3535, andrew.schwartz@science.doe.gov

This program supports experimental research aimed at gaining 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 under extreme conditions such as low temperature and high magnetic field. 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, and new topological states of matter, and has begun to explore whether ultracold atom research can provide insight into open questions about correlated electron behavior in hard condensed matter systems. The program does not support research in electrochemistry, thermoelectric materials, photovoltaic materials, or mechanical properties of materials. It also does not support projects aimed at materials optimization or device development.

(e) Theoretical Condensed Matter Physics

Program Manager: James Davenport, 301-903-0035, james.davenport@science.doe.gov

This activity supports Theoretical Condensed Matter Physics with an emphasis on electron correlation, electron and phonon transport, fundamental research in materials related to energy technologies, and theory relevant to the interpretation of experimental results at BES user facilities. Suitable topics include strongly correlated electron systems, quantum phase transitions, magnetism, superconductivity, optical response, 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.

(f) Physical Behavior of Materials

Program Manager: Refik Kortan, 301-903-3308, refik.kortan@science.doe.gov

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

In the near term, four central topics define the current program: electronic and magnetic behavior of materials; corrosion and electrochemistry science; nano-scale phenomena; and multiscale modeling of materials behaviors. Major efforts in these areas will continue. Increased investment in plasmonics, metamaterials and organic electronic materials will be considered. In addition, focus in theory and modeling at universities and national laboratories, taking advantage of the vast advances in computing speed and power, will be emphasized.

The long term goals of this program to understand the macroscopic behavior of materials it is important to understand the relationship between a material's properties and its response to external stimuli. This can be achieved by determining structure over multiple length scales, with emphasis at the atomic level, and by understanding the response of the nanometer and larger features of the material to those external stimuli. Studies of the physical response of a single nanometer-scale feature needs to be related to the macroscopic behavior of the material. This can often be done with modeling, but further advances are necessary to fully couple the length scales from atomic to macroscopic. Currently, atomistic simulation methods can be used to study systems containing hundreds of thousands of atoms, but these systems are still orders of magnitude too small to describe macroscopic behavior. Continuum methods, typically using finite element methods, fail to adequately describe many important properties because they use phenomenology that has little connection to the real processes that govern physical interactions. Modeling at an intermediate length scale, the mesoscale, where many defects can be included and from which predictive models at the continuum scale can be developed is required for advances in materials science. At this intermediate length-scale it is necessary to model the collective phenomena that include well over a billion atoms. Developing and applying novel techniques to these problems will be emphasized in coordination with the investment in theory and modeling. This program also seeks to foster theory, modeling, and simulation activities that address the following key topics in organic electronic materials: charge and energy transfer; electronic structure calculation; exciton dynamics and transport; and spin dynamics.

(g) Mechanical Behavior and Radiation Effects

Program Manager: 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.

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.

(h) X-ray Scattering

Program Manager: Lane Wilson, 301-903-5877, lane.wilson@science.doe.gov

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 2013 Early Career 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.

(i) Neutron Scattering

Program Manager: Pappannan Thiyagarajan (Thiyaga), 301-903-9706, p.thiyagarajan@science.doe.gov

This activity supports basic research on the fundamental interactions of neutrons with matter to achieve an understanding of the atomic, electronic, and magnetic structures and excitations of materials and their relationship to materials properties. Major emphasis is on the application of neutron scattering and spectroscopy for materials research, primarily at BES-supported user facilities. 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 in-depth understanding of the structure and dynamics. Also supported are innovative focusing optics for time-of-flight instruments, application of polarized neutrons for materials characterization and materials behavior at extreme conditions such as temperature, pressure, magnetic fields and combinations thereof.

Research on soft condensed matter and that at the intersection of hard and soft condensed matter sciences will be high priority as polymers, biomaterials and hybrid nanocomposites are ubiquitous in various advanced applications. *In situ* research can measure properties dynamically, during synthesis and use of materials in appropriate environments and operational conditions, yielding direct data for comparison to predictions. Proposals that take advantage of the *in situ* capabilities and unique aspects of neutron scattering that can lead to the discovery of advanced materials for electrodes and electrolytes for the next generation energy storage systems, fuel cell membranes, carbon dioxide sequestration and radiation resistant self healing materials are encouraged. The goal is to facilitate stronger interaction between the neutron scattering experiments and theory coupled with high performance computation to ensure that the experimental and computational data on structure and dynamics of functional materials are available for the prediction of materials properties and materials design.

Based on programmatic priorities in the 2013 Early Career Program this program will not support research on superconductivity, magnetism and organic photovoltaics.

(j) Electron and Scanning Probe Microscopies

Program Manager: Jane Zhu, 301-903-3811, jane.zhu@science.doe.gov

This activity supports basic research in condensed matter physics and materials science 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 will build upon the tremendous advancements in electron and scanning probe microscopy capabilities in the last decade and use scattering, imaging and spectroscopy methods to understand functionality and fundamental processes at the atomic or nanometer scale. Characterization of semiconducting, superconducting, magnetic, and ferroelectric materials benefits greatly from these abilities and from other research supported in this program. Concurrently, new frontiers in fundamental understanding of materials are being opened with the creation of novel characterization techniques.

Development of advanced electron and scanning probe microscopy techniques will be continued in order to meet our energy and basic science challenges. Significant improvements in resolution and sensitivity will provide an array of opportunities for groundbreaking science. These include the possibilities of understanding and controlling nanoscale inhomogeneity, new phenomena emerging at nanoscale, atomic-scale tomography, probing magnetism at the atomic scale with spin excitation spectroscopy, imaging spin density and spin waves, imaging functionality at the atomic scale, combination of multiple probes, and *in situ* analysis capabilities (under perturbing parameters such as temperature, irradiation, stress, magnetic 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. Significant advances will be made in the fundamental understanding of the mechanisms by which electrons, individual atoms, surface/interfaces and defects influence the properties and behavior of materials.

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

Program Manager: Jeffrey Krause, 301-903-5827, jeff.krause@science.doe.gov

This program supports experimental and theoretical research aimed at understanding the structural and dynamical properties of atoms, molecules and nanostructures. The research emphasizes fundamental interactions of these systems with photons and electrons to characterize and control their behavior. The goal is to develop accurate quantum mechanical descriptions of dynamical processes such as chemical bond breaking and forming, interactions in strong fields, 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 ultrafast light-matter interactions. 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 atomic and molecular inner-shell photoionization. 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 **does not** support research in quantum information science, ultracold quantum gases, condensates, or plasmas.

(I) Gas Phase Chemical Physics (GPCP)

Program Manager: Wade Sisk, 301-903-5692, wade.sisk@science.doe.gov

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

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

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

(m) Computation and Theoretical Chemistry

Program Manager: Mark Pederson, 301-903-9956, mark.pederson@science.doe.gov

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 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.

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

Program Manager: Gregory J. Fiechtner, 301-903-5809,

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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 photon-driven 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, including the development of a structural basis for gas/surface interactions, while 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, emphasizing studies of the molecular origins of condensed phase behavior and the nature and effects of non-covalent interactions, and including topics such as 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 tools with advances in spatial and temporal 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 goal is to support new experimental and computational tools and techniques in order to discover and measure previously inaccessible chemical and physical phenomena. 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 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, and (3) studies for understanding surface and subsurface adsorption at the molecular level to control chemical reactivity and selectivity.

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

(o) Catalysis Science

Program Manager: Raul Miranda, 301-903-8014, raul.miranda@science.doe.gov

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 be a particular concern. 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 CO₂ will not be considered.

Examples of research funded in this category can be found in Catalysis Science Program Meeting Reports at the link ‘Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings’, <http://www.science.energy.gov/bes/csgb/principal-investigators-meetings/> (search for “catalysis” in the book title. 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 (http://www.science.energy.gov/~media/bes/pdf/reports/files/cat_rpt.pdf.) The content is current except for the noted exclusion of solar photochemical conversion of water or CO₂ from this activity.

(p) Separations and Analysis

Program Manager: Larry Rahn, 301-903-2508, larry.rahn@science.doe.gov

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 nano- and 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.

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

(q) Heavy Element Chemistry (HEC)

Program Manager: Philip A. Wilk, 301-903-4537, philip.wilk@science.doe.gov

This activity supports basic research in 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 wastefoms, 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.

* http://science.energy.gov/~media/bes/pdf/reports/files/anes_rpt.pdf

Abstracts from the 2011 Separations and Heavy Element Chemistry Research Meeting:
http://science.energy.gov/~media/bes/csgb/pdf/docs/2011_separations_and_hec.pdf

Recent abstracts of Heavy Element Chemistry research projects are included in *Basic Energy Sciences FY 2011 Research Summaries*:
http://science.energy.gov/~media/bes/pdf/reports/files/bes_fy2011_research_summaries.pdf

(r) Geosciences Research

Program Manager: Nicholas Woodward, 301-903-4061, nick.woodward@science.doe.gov

This activity supports basic experimental and theoretical research in geochemistry and geophysics. Geochemical research emphasizes fundamental understanding of geochemical processes and reaction rates 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 new approaches to understand 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 (geochemistry focus) using x-ray sources, neutron sources, mass spectrometry and scanning microscopies, and large-scale imaging (geophysics focus) of physical properties. 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. Improved energy resources exploitation and energy waste storage options will require high-resolution measurements, monitoring and verification at a new level of sophistication. The Geosciences activity focuses on developing the improved fundamental technical understanding that will be needed to provide these improvements. The Geosciences research activity focuses on physical sciences research and leaves geo-biological dynamics and soil science to other programs. Targeted projects to exploit a single resource or waste type are also most appropriately addressed to the appropriate DOE applied program.

(s) Solar Photochemistry

Program Manager: Mark Spitler, 301-903-4568, mark.spitler@science.doe.gov

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, CO₂ in its reduction to fuels and H₂O in its oxidation or reduction via transformative catalytic cycles. This spans the range from dark catalytic reactions to those driven by the energy of an absorbed photon and in both homogeneous and heterogeneous environments. The major scientific challenge for photoelectrochemical energy conversion for fuel generation is that small band gap semiconductors capable of absorbing solar photons are susceptible to oxidative degradation, whereas wide band gap semiconductors, which are resistant to oxidative degradation in aqueous media, absorb too little of the solar spectrum. Also of emphasis are new hybrid systems that feature molecular catalysis at solid surfaces and new nanoscale structures for the photochemical generation of fuels.

Research areas concerned with separation of charge that might result in electricity include 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 which have a long term impact upon the understanding of radiolytic degradation of nuclear tank waste, the reactivity of solid surfaces in reactor coolant systems, and the chemistry of reagents used in separations processes in nuclear cycles.

Solar Photochemistry does not fund research on device development or optimization. Not of interest during FY 2013 are proposals that involve the assembly of dye sensitized solar cells with TiO₂.

(t) Photosynthetic Systems

Program Manager: 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 photo-protection.

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

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

(u) Physical Biosciences

Program Manager: Robert Stack, 301-903-5652, robert.stack@science.doe.gov

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 bio-inspired 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 or optimization of devices/processes; 4) development or optimization of microbial strains or plant varieties for biofuel/biomass production; 5) cell wall breakdown or deconstruction. Projects should ideally be hypothesis-driven; projects that develop or rely primarily on high-throughput screening approaches **will not** be supported nor will theory/modeling projects that lack experimental verification.

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

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

Program Manager: Mihal Gross, 301-903-6827, mihal.gross@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 proposals 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.

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 Berkeley 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. Instrumentation and technique development efforts are supported in areas including 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.

(w) BES Accelerator and Detector Research

Program Manager: Eliane Lessner, 301-903-9365, eliane.lessner@science.doe.gov

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.

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 seeding 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.

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. Improved detectors are especially important in the study of multi-length-scale systems such as protein- membrane interactions as well as nucleation and crystallization in nanophase materials. This program strongly interacts with BES programmatic research that uses synchrotron radiation and neutron sources.

(x) BES X-ray and Neutron Scattering Instrumentation and Technique Development

Program Manager: Peter Lee, 301-903-8484, peter.lee@science.doe.gov

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 and neutron scattering facilities. This program **will not** support proposals 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 facilities.

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 in materials science, physical, chemical, and biological sciences, medical and pharmaceutical sciences, geological sciences, environmental sciences, and metrology. 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.

Neutrons are a unique and effective tool for probing the structure of matter, particularly the positions, as well as the fluctuations in the positions of atoms (phonons), and the structure (position and direction) of atomic magnetic moments in solids and the excitations in their magnetic structure (spin waves). Such studies increase the understanding of phenomena such as melting, magnetic order, and superconductivity. At the three BES neutron facilities, measurements of structure and dynamics can cover length scales of 0.01 to 10 nm and time scales of 10 fs to 1 μ s.

In order to fully exploit the wide range of capabilities of these light sources and 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, different wavelength ranges and time structures, and novel approaches to data visualization and analysis.

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 which support our share of the project. In addition, the FES program supports research in high-energy-density 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 competitiveness 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, mark.foster@science.doe.gov

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/workshop-reports/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, john.mandrekas@science.doe.gov

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. Strong synergies and connections with other program elements exist, from the crosscutting plasma science of magnetic reconnection and plasma turbulence to the experimental validation of theoretical models and codes enabled by collaborations with the experimental plasma science and plasma diagnostics development programs.

(c) High-Energy-Density Plasma Science and Inertial Fusion Energy Science

Program Manager: Sean Finnegan, 301-903-4920, sean.finnegan@science.doe.gov

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, nirmol.podder@science.doe.gov

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 but not limited to: (1) astrophysical, solar, and space plasmas, (2) plasmas in biological and environmental science, (3) plasma modification, synthesis and processing of materials, (4) dusty, non-neutral and antimatter plasmas, (5) advanced plasma diagnostics, and (6) advanced methods for plasma modeling and simulation.

(e) Materials Science and Enabling Technologies for Fusion

Program Manager: Peter Pappano, 301-903-4883, peter.pappano@science.doe.gov

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, but is not limited to, the following research topics: development of tungsten as a plasma facing material, plasma material interactions, fabrication, joining and cooling of plasma facing materials, development of both solid and liquid blanket concepts that can breed tritium and provide necessary heat transfer capabilities, and development of ferritic steels and oxide-dispersion strengthened steels as first wall structural materials.

V. High Energy Physics (HEP)

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

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

The HEP program focuses on three scientific frontiers:

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

In addition, technology related research and development programs include:

- *Accelerator Science and Technology Research and Development*, advancing the basic science of particle beams in order to design, build, and operate the accelerator facilities essential for making new discoveries; and
- *Particle Detector Research and Development*, advancing the basic science of particle detection in order to design, build, and operate the detector facilities essential for making new discoveries.

Together, these interrelated and complementary discovery frontiers offer the opportunity to answer some of the most basic questions about the world around us. 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.

(a) Experimental High Energy Physics Research

Program Manager: James Stone, 301-903-3367, james.stone@science.doe.gov

The experimental HEP research area supports experiments that utilize both high energy accelerator beams and natural particle sources to study the properties of fundamental particles and their interactions, to explore the basic nature of space and time, and to detect new phenomena through sensitive measurements that probe the Standard Model of particle physics.

Topics studied may include, but are not limited to: fundamental particles and their interactions using proton-(anti) proton collisions at the highest possible energies; high intensity lepton-lepton collisions; studies of the properties of neutrinos produced by accelerators, nuclear reactors and natural sources; studies of rare processes using high intensity proton beams on fixed targets; studies of particle physics using naturally occurring phenomena; measurements on the nature of dark energy; and detection of the particles constituting dark matter.

Studies of gravitational physics, classical astrophysics, and heavy ion physics are not included in this research area.

(b) Theoretical High Energy Physics Research

Program Manager: Simona Rolli, 301-903-0504, simona.rolli@science.doe.gov

The theoretical HEP research area provides the vision and mathematical framework for understanding and extending the knowledge of particles, forces, space-time, and the universe.

Topics studied in the HEP theoretical research area include, but are not limited to: construction and exploration of phenomenological and theoretical studies that support the experimental HEP research area, both in understanding the data and in finding new directions for experimental exploration; developing novel analytical and numerical computational techniques for these studies; and finding theoretical frameworks for understanding fundamental particles and forces at the deepest level possible.

(c) Advanced Technology Research and Development in High Energy Physics

Program Manager: L.K. Len, 301-903-3233, lk.len@science.doe.gov

The advanced technology R&D research area develops the next generation of particle accelerators, detectors, and related computing technologies for the advancement of high energy physics and other sciences by supporting world leading research in the physics of particle beams and fundamental advances in particle detection. This research area primarily supports long range exploratory research aimed at developing innovative concepts.

Topics studied in the accelerator science and technology program include, but are not limited to: analytic and computational techniques for modeling particle beams; novel acceleration concepts; muon colliders and neutrino factories; high brightness beam sources; superconducting materials and conductor development; innovative magnet design and development of high-field superconducting magnets; and cutting edge beam diagnostic techniques.

Topics studied in the particle detector R&D program include, but are not limited to: low mass, high channel density charged particle tracking detectors; high resolution, fast readout calorimeters and particle identification detectors; and advanced electronics and data acquisition systems. In addition, this subprogram develops next generation computational tools and techniques to complement the experimental and theoretical physics research programs.

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* (<http://science.energy.gov/np/nsac/>), 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.

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

Research, development and fabrication of equipment directed toward research in any NP subprogram may be proposed but applications including such projects requiring detailed review of scope, budget and schedule beyond the procedures for this FOA may be rejected. Under this Funding Opportunity Announcement, NP does not support investigations into the development of nuclear reactors for purposes outside the scope of the NP subprograms described below.

(a) Medium Energy Nuclear Physics

Program Manager: Frank E (Ted) Barnes, 301-903-3212, ted.barnes@science.doe.gov

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 it 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, cyrus.baktash@science.doe.gov

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, george.fai@science.doe.gov**

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, ted.barnes@science.doe.gov**

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), models of the properties of nuclei and nuclear matter, nuclear astrophysics, and studies of novel approaches to particle acceleration.

(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 for the next generation rare isotope beam accelerator facility, the Facility for 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, dennis.phillips@science.doe.gov

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, gulshan.rai@science.doe.gov

The Nuclear Physics program supports an annual 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 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 which are aligned with the primary mission of other DOE programs or other funding Agencies. Early Career Award applications will be considered that demonstrate strong partnerships with the intended application stakeholder(s) and which 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 cost-effective 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. Key programmatic factors shall include an evaluation of the innovative nuclear science advances and its relevance to the application, cost effectiveness, performance, and impact of science & technology transfer.

ADDITIONAL INFORMATION:

DOE anticipates awarding laboratory work authorization awards under this Program Announcement. DOE will accept new laboratory technical proposals through the Portfolio Analysis and Management System, PAMS (<https://pamspublic.science.energy.gov/>), under this Announcement. **Note the following change in procedures from previous years:** DOE is only accepting laboratory technical proposals submitted into PAMS for this announcement. Do not submit or attach a DOE Field Work Proposal (FWP) at this time. Do not use Searchable FWP to respond to this announcement.

The program office will request submission of Field Work Proposals later from only those who are selected for funding.

All PIs and those submitting on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays. You may establish a PAMS account at <https://pamspublic.science.energy.gov/>.

For help with PAMS, please contact the Office of Science PAMS Support Center. The PAMS Support Center can be reached Monday-Friday 7:00 AM-6:00 PM Eastern Time. Telephone: (301) 903-5313, Email: scsc@science.doe.gov. All submission and inquiries about this Program Announcement must reference Program Announcement **LAB 12-751**.

Everything other than the budget and the budget justification should be combined into a single Portable Document Format (PDF) file. Submit the budget, budget justification, and proposal pdf into PAMS. Each DOE national laboratory has already appointed and registered at least one administrative business officer into PAMS. If you need contact information for your Administrative business officer, please contact early.career@science.doe.gov or the PAMS Support Center.

PROGRAM FUNDING: It is anticipated that up to \$10M will be available for laboratory work authorization awards in FY 2013. This amount is approximate and subject to availability of funds. It is anticipated that 15-35 awards will be made in Fiscal Year 2013. The number of awards is subject to availability of funds. The typical award size is expected to be \$2,500,000 over five years. The minimum award size is \$500,000 per year over five years. DOE national laboratories are encouraged to propose research expenditures as close to this funding minimum as possible. The size of a national laboratory award is commensurate with the requirement to

charge twelve-month annual salaries (compared with professors, who are partially paid by academic institutions). Thus, a minimum of 50% and up to 100% of the principal investigator's salary should be proposed.

ELIGIBLE INVESTIGATORS: The Principal Investigator must be a full-time, permanent, non-postdoctoral national laboratory employee as of the deadline for the proposal. 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 proposal (for the present competition, those who received doctorates no earlier than 2002 are eligible). Each Principal Investigator may only submit one Office of Science Early Career Research Program proposal per annual competition. Additionally, a Principal Investigator may not participate in more than three Office of Science Early Career Research Program competitions.

The act of submitting a proposal implies that the national laboratory has checked, confirmed, and certifies that the Principal Investigator is eligible. No additional certifying documentation is required.

Proposals must be submitted through a DOE national laboratory. A companion funding opportunity announcement (DE-FOA-0000751) describes the Early Career Research Program opportunity for tenure-track untenured assistant professors and tenure-track untenured associate professors at U.S. academic institutions. 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.

There can be no co-Principal Investigators.

There is no limit on the number of preproposals from a DOE national laboratory in a given year. Each laboratory is responsible for ensuring that the research ideas submitted in its preproposals fit within the scope of Office-of-Science-funded programs at the national laboratory.

Only those Principal Investigators that receive notification from DOE encouraging a formal proposal may submit full proposals.

Each formal proposal must be accompanied by a letter from the national laboratory director to the technical point of contact confirming that the proposed research idea fits within the scope of Office-of-Science-funded programs at the national laboratory.

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.

Principal Investigators who received awards in FY 2010, FY2011, or FY2012 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.

If an investigator is a current recipient of one of the following awards and is selected for an award under this announcement, the institution must forgo any remaining years of funding for the current award when the new award begins. The previous awards covered by this condition are (1) Office of Advanced Scientific Computing Research Early Career Principal Investigator Program; (2) Office of Fusion Energy Sciences Plasma Physics Junior Faculty Award Program; (3) Office of High Energy Physics Outstanding Junior Investigator Program; (4) Office of Nuclear Physics Outstanding Junior Investigator Program; and (5) DOE Presidential Early Career Award for Scientists and Engineers (PECASE).

Eligibility exemptions will not be granted.

Letters of recommendation are not allowed.

AWARD ADMINISTRATION INFORMATION

Annual progress reports from the award investigators will be required and will be due 90 days before the end of each budget year.

Execution of the annual funding is solely at the discretion of the principal investigator in accordance with the DOE-approved budget.

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 proposal. If the scope of work has not changed, the award can be transferred. If the scope of work has changed, the new proposal will be subject to merit review as described below. Transfer awards will be for the remaining award period only, and the requested budget cannot exceed the remaining budget for the original award. If a laboratory employee transfers to a university, the requested budget should be as close to \$150,000 per year as possible for each remaining year. While a transfer proposal 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.

The award period is five years, conditional on adequate annual progress and appropriation of funds. At the end of this period, the DOE national laboratory employing the principal investigator has the primary responsibility to address funding transition issues that arise when the award ends.

AWARD NOTICES: DOE will notify proposers selected for award. This notice of selection is not an authorization to begin performance. Organizations whose proposals have not been selected will be advised as promptly as possible. This notice will explain why the proposal was not selected.

The instructions and format described below should be followed. You must reference Program Announcement LAB 12-751 on all submissions and inquiries about this program.

OFFICE OF SCIENCE
GUIDE FOR PREPARATION OF SCIENTIFIC/TECHNICAL PROPOSALS
TO BE SUBMITTED BY NATIONAL LABORATORIES

The following guidelines for content and format are intended to facilitate an understanding of the requirements necessary for SC to conduct a merit review of a proposal. Please follow the guidelines carefully, as deviations could be cause for declination of a proposal without merit review.

1. Review Criteria: Prior to a comprehensive merit evaluation, DOE staff will perform an initial evaluation of each proposal to ensure that the information required is provided, that the proposed effort is technically sound and feasible, and that the effort is consistent with program funding priorities. For proposals that pass the initial evaluation, DOE shall review and evaluate them based on the criteria set forth below.

Proposals will be subjected to scientific merit review (peer review) and will be evaluated against the following evaluation criteria which are listed in descending order of importance:

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.
4. Reasonableness and appropriateness of the proposed budget.

The following announcement-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 proposal 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 announcement and the programmatic needs of the DOE Office of Science. 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 a proposal constitutes agreement that this is acceptable to the investigator and the submitting institution.

The following questions will be posed to reviewers for each of the review criteria 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 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.

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

The selection official will consider the merit review recommendation, program policy factors, and the amount of funds available.

DOE is striving to make awards within seven months. The time interval begins on the date proposals are due or the date the proposal is received. **Awards will be made in Fiscal Year 2013.**

2. Summary of Proposal Contents and Information about PAMS

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

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 two and only two sentences and must use the following format:

Dear <Principal Investigator Name>:

If your proposal entitled, "<Proposal 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>

Each proposal will contain the following sections:

- Budget, entered into PAMS as structured data using the PAMS budget form
- Budget justification, entered into PAMS as a separate pdf
- Proposal, combined into a single pdf containing the following information:
 - Proposal Cover Page
 - Project Summary/Abstract (no more than one page)
 - Project Narrative (**No more than 15 pages long**)
 - Appendix 1: Biographical Sketch
 - Appendix 2: Current and Pending Support
 - Appendix 3: Bibliography and References Cited
 - Appendix 4: Facilities and Other Resources
 - Appendix 5: Equipment
 - Appendix 6: Other Attachment (optional)

Full laboratory technical proposals must be submitted into the DOE Office of Science Portfolio Analysis and Management System (PAMS). **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 preproposal.** To register, click “Create New PAMS Account” on the website <https://pamspublic.science.energy.gov/> and follow the instructions for creating an account. You will be prompted to create a username and password and to enter your contact information. Registering to PAMS is a two-step process; once you create an individual account, you must associate yourself with (“register to”) your institution. Follow the onscreen instructions to do this.

To access PAMS, please use either Internet Explorer or Firefox. Currently, PAMS does not support the Chrome or Safari browsers, but an upgrade in the future will make it possible to use them.

To submit the proposal, log in to PAMS. Select “View DOE National Laboratory Announcements” and find the current announcement in the list. Click on “Actions/Views” for this announcement, select “Submit Proposal” from the dropdown, and follow the instructions from there. Note that you must select one and only one Principal Investigator (PI) per proposal; to do so, click on “Select PI” on the far right side of the screen and then select the PI from the list of all registered users from your institution returned by PAMS. If the PI for whom you are submitting does not appear on the list, 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, choose “Invite PI” at the top left of the “Select PI” screen. You can enter an optional personal message to the PI in the “Comments” box that PAMS presents, and it will be included in the email PAMS sends to the PI.

The cover page, budget, and attachments sections of the DOE national laboratory proposal are required by PAMS. Complete the sections in PAMS one at a time, starting with the cover page and following the instructions for each section. Save each section using the dropdown at the bottom of the screen. Once you have saved all of the sections, the “Submit to DOE” option will appear in the dropdown. If you save the proposal and navigate away from it, you may return later to edit the proposal by selecting “View My Proposals” or “My Proposals.” You must enter a budget for each annual budget period. In the “attachments” section of the lab proposal, the budget justification and the proposal narrative are required and must be submitted as separate files. You must bundle everything other than the budget and budget justification into one single pdf to be attached under “Proposal Attachment.” Do not attach anything under “Other Attachments.”

To upload an attachment into PAMS, select “Attach File” at the far right side of the screen. Search for your file and then select “Attach” to upload the file. You may enter an optional description of the file you are attaching.

Upon submission, the PI will receive an email from the PAMS system acknowledging receipt of the proposal.

Please only submit a PAMS lab technical proposal in response to this announcement; do not submit a DOE Field Work Proposal (FWP) at this time. The program office will request FWPs later from those who are selected for funding under this announcement.

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

Each DOE national laboratory has already appointed and registered at least one administrative business officer into PAMS. If you need contact information for your Administrative business officer, please contact early.career@science.doe.gov or the PAMS Support Center.

3. Detailed Contents of the Proposal

Budget and Budget Explanation

The size of a national laboratory award is commensurate with the requirement to charge twelve-month annual salaries (compared with professors, who are partially paid by academic institutions). Thus, a minimum of 50% and up to 100% of the principal investigator's salary should be proposed.

The budget must be submitted into PAMS using the PAMS budget form. Research proposed under this announcement should have five annual budget periods. Please enter the following budget period start and end dates into PAMS for proposals submitted to this announcement:

- Budget Period 1: 7/1/2013 – 6/30/2014
- Budget Period 2: 7/1/2014 – 6/30/2015

- Budget Period 3: 7/1/2015 – 6/30/2016
- Budget Period 4: 7/1/2016 – 6/30/2017
- Budget Period 5: 7/1/2017 – 6/30/2018

PAMS will calculate the cumulative budget totals for you.

A written justification of each budget item is to follow the budget pages. The budget justification should be placed in a separate, single pdf document and attached on the appropriate screen in PAMS.

Further instructions regarding the budget and justification are given below and in the PAMS software.

Proposal

Proposals must have 1-inch margins at the top, bottom, and on each side. Type sizes must be at least 11 point. Line spacing is at the discretion of the researcher, but there must be no more than 6 lines per vertical inch of text. Pages should be standard 8 1/2" x 11" (or metric A4, i.e., 210 mm x 297 mm).

Proposal Cover Page

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

DOE National Laboratory:
Street Address/City/State/Zip:
Principal Investigator (PI):
Position Title of PI:
Business Mailing Address of PI:
Telephone Number of PI:
Email of PI:
Program Announcement Number: LAB 12-751
DOE/Office of Science Program Office (ASCR, BER, BES, FES, HEP, or NP):
Topic Area*:
Topic Area Program Manager:
Year Doctorate Awarded:
Number of Times Previously Applied[†]:
PAMS Preproposal Number:
PECASE Eligible (Yes or No)?**

* The topic area can be found in the summary section of this Program Announcement. For example, the topic area might be Environmental System Science or Magnetic Fusion Energy Science Theory and Simulation. Please select from the list in the summary section.

[†] Indicate how many times the PI has previously submitted a full proposal in the Office of Science Early Career Research Program. The program has been offered in three previous years,

FY 2010, FY 2011, and FY 2012. Participation in the competition is defined as submission of a full, formal proposal. 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 the agencies each year to nominate candidates for the Presidential Early Career Awards for Scientists and Engineers (PECASE). A Principal Investigator is PECASE-eligible if he or she is a U.S. citizen, U.S. national, or permanent resident and if she or he has not received a PECASE previously through any agency. Investigators from the top proposals in the Office of Science Early Career Research Award competition may be nominated for PECASE.

Project Summary/Abstract (no more than one page)

The project summary/abstract must contain a summary of the proposed activity suitable for public dissemination. It should be a single page that identifies the national laboratory, the principal investigator, the project title, the objectives of the project, a description of the project, including methods to be employed, and the potential impact of the project (i.e., benefits, outcomes). The document should be written to appeal to a general audience and not just scientific experts in the specialty of the proposed research. This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must not exceed one page when printed using standard 8.5” by 11” paper with 1” margins (top, bottom, left and right) with font not smaller than 11 point.

Project Narrative (No more than 15 pages long)

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 method to be used. It should also include a timeline for the major activities of the proposed project.

The body of the Project Narrative **must not exceed 15 pages** when printed using standard 8.5” by 11” paper with 1 inch margins (top, bottom, left, and right). The font must not be smaller than 11 point. Do not include any Internet addresses (URLs) that provide information necessary to review the proposal, because the information contained in these sites will not be reviewed. Each proposal should be in a single PDF file.

Appendix 1: Biographical Sketch

Provide a biographical sketch for the Principal Investigator (PI). 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. This information is required for

the Principal Investigator submitting the proposal. Provide the biographical sketch information as an appendix to your project narrative. **This appendix will not count in the project narrative page limitation.** The biographical sketch is limited to a maximum of three pages when printed on 8.5” by 11” paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include:

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

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

Publications. Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications. 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 no more than 5 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 the Principal Investigator on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of the proposal. 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, include those individuals who are currently or have been co-editors with the Principal Investigator of a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of the proposal. If there are no collaborators or co-editors to report, state “None.”

Graduate and Postdoctoral Advisors and Advisees: 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.

Appendix 2: Current and Pending Support

Provide a list of all current and pending support (both Federal and non-Federal) for the Principal Investigator (PI) for ongoing projects and pending proposals. 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. If the PI has submitted a similar research proposal 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 proposal. Concurrent submission of a proposal to other organizations for simultaneous consideration will not prejudice its review. **This appendix will not count in the project narrative page limitation.**

Appendix 3: Bibliography and References Cited

Give full bibliographic entries for each publication cited in the narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. Include only bibliographic citations. Principal investigators should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal. 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. **This appendix will not count in the project narrative page limitation.**

Appendix 4: Facilities and Other Resources

This information is used to assess the capability of the organizational 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. **This appendix will not count in the project narrative page limitation.**

Appendix 5: Equipment

List major items of equipment already available for this project and, if appropriate, identify location and pertinent capabilities. **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 an appendix, but do not use the appendix to circumvent the page limitations of the proposal. Reviewers are not required to consider information in an appendix, and reviewers may not have time to read extensive appendix materials with the same care they would use with the proposal 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. **This appendix will not count in the project narrative page limitation.** Each optional letter of collaboration may contain two and only two sentences and must use the following format:

Dear <Principal Investigator Name>:

If your proposal entitled, “<Proposal 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>

4. Detailed Instructions for the Budget

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 proposals without subcontracts with the exception of those that propose small subcontracts for essential supporting work such as sample analysis. Subcontracts that pay salary for scientific collaborators outside the proposing institution are discouraged.

Budgets are required for the entire project period. A budget form should be completed for each budget period of the award, and a cumulative budget form for the entire project period will be populated by PAMS. A detailed budget justification narrative should be included after the budget pages. The justification should cover labor, domestic and foreign travel, equipment, materials and supplies, and anything else that will be covered with project funds.

To edit a section on the budget, click the edit icon () for each section on the page. Remember to save all budget periods before moving on to the next section.

A. Senior/Key Person (Required)

For each Senior/Key Person, enter the appropriate information. List personnel, salary funds, and the number of months that person will be allocated to the project. Also include a written narrative in the budget justification that fully justifies the need for requested personnel.

B. Other Personnel

List personnel, salary funds, and the number of months that person will be allocated to the project. Also include a written narrative in the budget justification that fully justifies the need for requested personnel.

C. Equipment Description

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 each item of equipment separately and justify each in the budget justification section. Allowable items ordinarily will be limited to research equipment and apparatus not already available for the conduct of the work. General-purpose office equipment, such as a personal computer, is not eligible for support unless primarily or exclusively used in the actual conduct of scientific research.

D. 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 whether travel cost estimates are based upon quotes from travel agencies; upon past experience of similar number of trips to similar travel destinations; or something else (describe). 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.

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. In the budget justification, indicate whether trainee cost estimates are based upon past experience of support of similar number of trainees on similar projects; past experience of support of similar number of participants attending similar conferences/workshops/symposia; or something else (describe).

F. Other Direct Costs:

Enter Other Direct Costs information for each item listed.

- **Materials and Supplies:** Enter total funds requested for materials 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. In the budget justification, indicate whether cost estimates are based upon past experience of purchase of similar or like items; quotes/catalog prices of similar or like items; or something else (describe).
- **Publication Costs:** 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. In the budget justification, indicate whether cost estimates are based upon past experience of purchase of similar or like items; vendor quotes of similar publication services; or something else (describe).
- **Consultant Services:** 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. In the budget justification, indicate whether

consultant cost estimate is based upon previous experience/quotes for similar or like services; or something else (describe).

- ADP/Computer Services: Enter total funds requested for 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. In the budget justification, indicate whether cost estimates are based upon quotes/past experience of purchase of similar computer services; established computer service rates at the proposing institution; or something else (describe).
- 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. In the budget justification, indicate whether cost estimates are based upon past experience with similar or like items; vendor quotes of similar items; or something else (describe).
- 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.

G. Direct Costs

This represents Total Direct Costs (Sections A thru F) and will be calculated by PAMS.

H. Other Indirect Costs

Enter the Indirect Cost information for each field. Only four general categories of indirect costs are allowed/requested on this form, so please consolidate if needed.

I. Total Direct and Indirect Costs

This amount will be calculated by PAMS (Sections G + H)