

**FINANCIAL ASSISTANCE
FUNDING OPPORTUNITY ANNOUNCEMENT**



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

**Computational Materials Sciences
Funding Opportunity Number: DE-FOA-0001528
Announcement Type: Initial
CFDA Number: 81.049**

Issue Date:	02/09/2016
Letter of Intent Due Date:	03/07/2016 at 5 PM Eastern Time (A Letter of Intent is required)
Pre-Application Due Date:	Not Applicable
Application Due Date:	04/25/2016 at 5 PM Eastern Time

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UPDATES AND REMINDERS

REGULATIONS

This FOA and any awards made under it are controlled by 2 CFR 200, the Uniform Administrative Requirements, Cost Principles, and Audit Requirements for Federal Awards, as modified by 2 CFR 910, the Department of Energy Financial Assistance Rules, and 10 CFR 605, the Office of Science Financial Assistance Program.

DATA MANAGEMENT PLAN

The Office of Science has published a new Statement on Digital Data Management, published at <http://science.energy.gov/funding-opportunities/digital-data-management/>, which governs applications submitted under this FOA, and is detailed in Part IV of this FOA.

ACKNOWLEDGMENT OF FEDERAL SUPPORT

The Office of Science published guidance about how its support should be acknowledged at <http://science.energy.gov/funding-opportunities/acknowledgements/>.

REPORTING

The Office of Science has implemented the federal-wide Research Performance Progress Report (RPPR) through the Portfolio Analysis and Management System (PAMS). The common RPPR format is described at <http://www.nsf.gov/bfa/dias/policy/rppr/>. Progress Reports are generally due 90 days before the end of each budget period. The Principal Investigator (PI) will receive an automated email from PAMS (<PAMS.Autoreply@science.doe.gov>) thirty days prior to the progress report due date. Some information will be prepopulated. Additional details and changes will be contained in the Reporting Requirements Checklist attached to the Assistance Agreement.

RECOMMENDATION

The Office of Science encourages you to register in all systems as soon as possible. You are also encouraged to submit letters of intent, pre-applications, and applications well before the deadline.

Section I – FUNDING OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS FOA SHOULD BE DIRECTED TO:

Technical/Scientific Program Contact:

Dr. James Davenport
301-903-0035
james.davenport@science.doe.gov

STATUTORY AUTHORITY

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

APPLICABLE REGULATIONS

Uniform Administrative Requirements, Cost Principles, and Audit Requirements for Federal Awards, codified at 2 CFR 200
U.S. Department of Energy Financial Assistance Rules, codified at 2 CFR 910
U.S. Department of Energy, Office of Science Financial Assistance Program Rule, codified at 10 CFR 605

SUMMARY

The Office of Basic Energy Sciences (BES) of the U.S. Department of Energy (DOE) announces its interest in receiving applications in Computational Materials Sciences proposing integrated, multidisciplinary teams that will perform research to develop validated community codes and data bases for predictive design of functional materials, excluding structural materials. Computational Materials Sciences Teams could also involve new approaches to enhance the use of large data sets derived from advanced characterization of materials, materials synthesis, processing, and properties assessments and the parallel data that are generated by large scale computational efforts that model materials phenomena. Computational Materials Sciences will support the Materials Genome Initiative for Global Competitiveness (MGI) that was announced by the President in June 2011. The goal of the MGI is to reduce the time from discovery to deployment of new materials by a factor of two and is tied to advancement of American manufacturing capability. This funding opportunity continues the BES commitment to the MGI and the development of open source codes that can take full advantage of today's petascale and future exascale leadership computing facilities.

In FY 2015, the first Computational Materials Sciences awards were made. Additional information on these awards can be found at the website listed in the references below. Projects selected in 2016 will support research for functional materials topics and types of software not supported in 2015. See the Summary Criteria section for more information on excluded research areas for this funding opportunity.

SUPPLEMENTARY INFORMATION

BACKGROUND

Recent major strides in materials synthesis, processing, and characterization, combined with concurrent advances in computational science – enabled by improvements in high performance computing capabilities – have opened an unprecedented opportunity to design new materials with targeted properties. The opportunity is to leap beyond simple extensions of current theory and models of materials towards a paradigm shift in which specialized computational codes and software, coupled with innovative availability and use of experimental and theoretical data, enable the ability to design, discover, and develop new materials, and in turn, create new advanced, innovative technologies. Given the importance of materials to virtually all technologies, computational materials science is a critical area in which the United States needs to be competitive.

If successful, this paradigm shift of integration would significantly accelerate the design of revolutionary materials to meet the Nation's energy goals and enhance economic competitiveness. Development of fundamentally new design principles could enable stand-alone research codes and software packages to address multiple length and time scales for prediction of the total functionality of materials over a lifetime of use. Recent scientific workshops and National Research Council studies have identified enticing scientific challenges that would advance these goals. Examples include dynamics and strongly correlated matter, conversion of solar energy to electricity, design of new catalysts for a wide range of industrial uses, and electron transport in materials for improved electronics. Success will require extensive research and development with the goal of creating and experimentally validating, robust community codes that will enable functional materials innovation. Utilization of today's petascale leadership class computers and planning for algorithms and software codes that can be implemented for exascale computing are critical aspects of the required software.

Research and development to create the computational codes will require a fully integrated, multi-investigator team approach, combining the skills of experts in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication. The range of the research will include development of new *ab initio* theory, advanced materials modeling, mining the data from both experimental and theoretical databases, performing advanced *in situ/in operando* characterization to generate the specific parameters needed for computational models, and well controlled synthesis to confirm the predictions of the codes. Many of the underlying phenomena require understanding the material dynamics at ultrafast time scales and with near atomic resolution - requiring effective use of the unique world leading tools and instruments at DOE's user facilities, from ultrafast free electron lasers to aberration corrected electron microscopes to the best tools for controlled synthesis.

An ideal end product would be open source, robust, validated, user friendly software (and the associated experimental and computational data) that captures the essential physics and chemistry of relevant systems and can be used by the broader research community and by industry to dramatically accelerate the design of new functional materials. As appropriate,

multiple software approaches can be incorporated, for example, software that uses the most advanced supercomputers coupled with derivative software for more general, routine use on computer clusters.

In FY 2015, the first Computational Materials Sciences awards were made. Additional information on these awards can be found at the website listed in the references below. Projects selected in 2016 will support research for functional materials topics and types of software not supported in 2015. See the Summary Criteria section for more information on excluded research areas for this funding opportunity.

SUMMARY CRITERIA

To be considered, an application must address the Eligibility requirements in Section III and the Review Criteria in Section V. In particular, an application should:

- Focus on functional materials research. Suitable classes of functional materials include, for example, semiconductors, transition metal oxides, magnetic or superconducting materials, metal-halide perovskites, and heterogeneous catalysts. Explicitly excluded are proposals on structural, thermoelectric, and energy storage materials; structural properties; and synthesis of 2-d layered materials, assemblies of nanoparticles, isolated molecules, liquids (including ionic liquids), and homogeneous catalysts.
- Focus on research leading to open source software. Suitable types of software will emphasize strong correlations, excited states, transport, electronic or optical properties. Explicitly excluded are proposals that emphasize density functional methods as currently implemented or semi-empirical approaches, dynamical mean field theory, and classical and first principles molecular dynamics.
- Describe a plan to deliver experimentally validated research codes and the associated experimentally and theoretically derived data for the design of functional materials to academia, National Laboratories, and industry. Software developed under this FOA should have broad applicability. Applicants must describe how the software will be distributed as open source in an Open Source Software Distribution Plan.
- Provide a detailed plan for the full utilization of today's petascale and tomorrow's exascale leadership computing facilities.
- Use integrated, multi-investigator teams combining expertise in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication.
- Articulate a clear management plan which insures a coherent team approach and provides for the maintenance and long-term accessibility of software and data.
- Include a Data Management Plan.
- Provide mechanisms for community input to software and database development and validation.

References:

Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science (<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#CMSC>)

From Quanta to the Continuum: Opportunities for Mesoscale Science

<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#OFMS>

Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science

http://science.energy.gov/~media/bes/besac/pdf/Reports/CFME_rpt_print.pdf

FY 2015 Awards:

<http://science.energy.gov/bes/funding-opportunities/closed-foas/computational-materials-sciences-awards/>

MGI Strategic Plan

https://www.whitehouse.gov/sites/default/files/microsites/ostp/NSTC/mgi_strategic_plan_-_dec_2014.pdf

Collaboration

Collaborative applications will not be accepted under this FOA.

Section II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT

DOE anticipates awarding grants under this FOA.

A DOE field work authorization or other appropriate instrument will be awarded to a successful DOE/NNSA National Laboratory contractor. Participation by non-DOE/NNSA Federal agencies and their Federally Funded Research and Development Center (FFRDC) contractors will be funded under an interagency agreement (see Section III. A. ELIGIBLE APPLICANTS). A grant will be awarded to any other successful domestic entity including, but not limited to, universities, nonprofit organizations, and for-profit organizations.

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

B. ESTIMATED FUNDING

DOE expects to make multiple Computational Materials Sciences awards for a period of up to four years for each award. Total funding, estimated at a maximum of \$4,000,000 annually across all awards with the potential for additional annual funding in future fiscal years, is expected to be available to support the awards from this FOA and DOE National Laboratory Program Announcement LAB 16-1528, subject to appropriation of funds by Congress. DOE is under no obligation to pay for any costs associated with preparation or submission of applications. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this FOA.

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

C. MAXIMUM AND MINIMUM AWARD SIZE

(See B. Estimated Funding section above.)

DOE anticipates that individual award sizes will range from \$1,500,000 per year to \$2,500,000 per year. The individual award size will depend on the merit review, the number of meritorious applications, and the availability of appropriated funds.

DOE does not expect to receive applications that fall outside of the maximum and minimum amounts stated above.

Ceiling

\$2,500,000 per year

Floor

\$1,500,000 per year

D. EXPECTED NUMBER OF AWARDS

(See B. Estimated Funding Section above.)

The number of awards will depend on the number of meritorious applications and the availability of appropriated funds. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this FOA.

E. ANTICIPATED AWARD SIZE

(See B. Estimated Funding Section above.)

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

F. PERIOD OF PERFORMANCE

(See B. Estimated Funding section above.)

Awards are expected to be made for a period of up to four years.

Continuation funding (funding for the second budget year and subsequent budget years) is contingent on: (1) availability of funds appropriated by Congress and future year budget authority; (2) substantial progress towards meeting the objectives of the approved application; (3) submittal and approval of required reports; and (4) compliance with the terms and conditions of the award. Additionally, funding for the final two budget years is contingent upon satisfactory completion of an extensive progress review during the second year of each project, which may include an external peer review. BES will use the mid-term review to assess the productivity and impact of each project and progress toward meeting the stated four-year scientific research goals.

G. TYPE OF APPLICATION

DOE will only accept new applications under this FOA.

H. VALUE/FUNDING FOR DOE/NNSA NATIONAL LABORATORY CONTRACTORS AND NON-DOE/NNSA FFRDC CONTRACTORS

For grant awards, the value of, and funding for, a DOE/NNSA National Laboratory contractor, a non-DOE/NNSA FFRDC contractor, or another Federal agency's portion of the work will not be included in the award to the successful applicant. DOE will fund a DOE/NNSA National Laboratory contractor through the DOE field work authorization system or other appropriate process and will fund non-DOE/NNSA FFRDC contractors and other Federal agencies through an interagency agreement in accordance with the Economy Act, 31 U.S.C. 1535, or other statutory authority.

I. RESPONSIBILITY

The successful prime applicant/awardee (lead organization) will be the responsible authority regarding the settlement and satisfaction of all contractual and administrative issues, including but not limited to, disputes and claims arising out of any agreement between the applicant and any team member, and/or subawardee.

If an award is made to a DOE/NNSA National Laboratory, all Disputes and Claims will be resolved in accordance with the terms and conditions of the DOE/NNSA National Laboratory's M&O contract, as applicable, in consultation between DOE and the prime awardee.

If an award is made to another Federal agency or its FFRDC contractor, all Disputes and Claims will be resolved in accordance with the terms and conditions of the interagency agreement in consultation between DOE and the prime awardee.

Section III – ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS

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

Institutions that received prime awards made under FOA DE-FOA-0001276 (Computational Materials Sciences, FY2015) are not eligible to submit applications as prime applicants under this Funding Opportunity Announcement (DE-FOA-1528) and its companion Laboratory Announcement (LAB 16-1528). Current prime awardees may participate as subawardees other prime applicant institutions.

Institutions participating as subawardees in awards made under FOA DE-FOA-0001276 (Computational Materials Sciences, FY2015) are eligible to submit applications as prime applicants under this Funding Opportunity Announcement (DE-FOA-0001528) and its companion Laboratory Announcement (LAB 16-1528).

DOE National Laboratories and other Federal agencies are not eligible to receive financial assistance awards under this FOA, but they may be considered as part of an unincorporated consortium as described below. A parallel, companion announcement (LAB 16-1528) is available for applications led by DOE laboratories, including DOE/NNSA Federally Funded Research and Development Center (FFRDC) Contractors.

Applicants that are not domestic organizations should be advised that:

- Individual applicants are unlikely to possess the skills, abilities, and resources to successfully accomplish the objectives of this FOA. Individual applicants are encouraged to address this concern in their applications and to demonstrate how they will accomplish the objectives of this FOA.
- Non-domestic applicants are advised that successful applications from non-domestic applicants include a detailed demonstration of how the applicant possesses skills, resources, and abilities that do not exist among potential domestic applicants.

UNINCORPORATED CONSORTIA

Unincorporated consortia (team arrangements), which may include domestic and foreign entities, must designate one member of the consortium to serve as the prime recipient/consortium representative (lead organization). The prime recipient/consortium representative must be incorporated (or otherwise formed) under the laws of a State or territory of the United States.

Upon request, unincorporated consortia must provide the DOE contracting officer with a collaboration agreement, commonly referred to as the articles of collaboration, which sets out the rights and responsibilities of each consortium member. This agreement binds the individual consortium members together and should discuss, among other things, the consortium's:

- Management structure;
- Method of making payments to consortium members;

- Means of ensuring and overseeing members' efforts on the project;
- Provisions for members' cost sharing contributions; and
- Provisions for ownership and rights in intellectual property developed previously or under the agreement.

Note that a consortium is applied for in one application and results in one award with subawards to consortia members. Collaborations are applied for separately with identical applications and result in multiple awards to the collaborating institutions.

B. COST SHARING

Cost sharing is not required.

C. ELIGIBLE INDIVIDUALS

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

D. OTHER ELIGIBILITY REQUIREMENTS

Letter of Intent (LOI)

To be considered eligible for an award under this FOA, potential prime applicants (lead organizations) are *required* to submit a LOI in accordance with the instructions provided in Section IV.B.1 of this FOA below. Applications received from an applicant who has not submitted the required LOI will be deemed non-responsive and will be rejected without further review.

The lead organization on an application must be the same as on the required LOI. **If an application is received for which the lead organization has changed since submission of the LOI, then the application will be deemed non-responsive and will be rejected without further review.** The Lead Principal Investigator (PI) or Project Director should not be changed unless unavoidable and only minor edits should be made, if necessary, to the title. If necessary, the applicant may make changes to other senior/key personnel and other participating institutions, although DOE discourages extensive changes.

The Lead Organization and Limitation on Number of Applications

An entity may not submit more than **one** application as the lead organization. If more than one application is received from an entity, DOE will consider only the application that matches a qualified LOI (as described below in Section IV.B.1). The remaining applications will be deemed non-responsive and rejected without further review. However, there is no limitation on the number of applications in which an entity may participate as a team member or subawardee.

The Project Director and Limitation on Number of Applications

The Project Director is the Lead Principal Investigator and must be employed or have an agreement in place to be hired by the lead organization. **An individual may not be named as the Project Director on more than one application.** If the proposed Project Director will not be employed by the lead organization, the application will be deemed non-responsive and will be rejected without further review. Further, if more than one application is received from an applicant identifying the same individual as the Project Director, DOE will consider only the application (if any) that matches a qualified LOI (as described in Section IV.B.1). The remaining applications will be deemed non-responsive and rejected without further review. However, there is no restriction on the number of applications in which an individual may participate as a Principal Investigator (This is not the Lead Principal Investigator/Project Director).

Team Arrangements

Entities proposing as a team must designate a lead organization. LOIs and applications must be submitted on behalf of the team members by the lead organization and DOE will enter into a prime award relationship with the designated lead organization. Only one LOI and one application are to be submitted for each team. The designated lead organization, i.e., the prime applicant, must perform a greater percentage of the effort than any other partner organization or subawardee. The percentage of effort will be determined by reviewing the total budget for each participating organization as a percentage of proposed total project costs. **If an application is received in which the prime applicant is not performing a greater percentage of the effort than each of the other institutional partners, team members, or subawardees, as determined by the budget, the application will be deemed non-responsive and rejected without further review.**

Eligible/Ineligible Entities

If an application is received that includes an ineligible entity, or an employee of an ineligible entity performing activities as a team member and/or subawardee, the application will be deemed non-responsive and rejected without further review. Note, however, that otherwise ineligible entities are not precluded from serving as vendors of materials, supplies, equipment, and providing scientific and technical advisory services to a proposed Team, if they are acting purely in that role. Scientific and technical advisory services allow for the provision of scientific and technical expertise without actually performing research activities; examples of such services include serving as members of advisory committees and technical peer review panels or participation in scientific workshops or conferences.

Performance of Work in the United States

DOE requires all work performed by the prime recipient under funding agreements resulting from this FOA to be performed in the United States except as discussed below: – i.e., a prime recipient must expend its total project costs in the United States.

This requirement does not apply to travel or to equipment, materials and supply purchases. Like all proposed costs, proposed travel, equipment, and material and supply costs will be evaluated to determine whether they are necessary and appropriate for the conduct of the effort. Furthermore, it is the sense of Congress that, to the greatest extent practicable, all equipment and products purchased with funds made available under awards resulting from this FOA should be American-made.

Work funded as a subaward from the prime recipient may be performed outside of the United States.

DATA MANAGEMENT PLAN

A Data Management Plan as described in Section IV C. “Application Contents and Forms” - Appendix 6, is required. Applications that do not have a Data Management Plan will be deemed nonresponsive and will be not reviewed.

OPEN SOURCE SOFTWARE DISTRIBUTION PLAN

An Open Source Software Distribution Plan as described in Section IV C. “Application Contents and Forms” - Appendix 7, is required. Applications that do not have an Open Source Software Distribution Plan will be deemed nonresponsive and will be not reviewed.

RESEARCH FOCUS

Applications must address predictive design of functional materials, excluding structural, thermoelectric, and energy storage materials; structural properties; and synthesis of 2-d layered materials, assemblies of nanoparticles, isolated molecules, liquids (including ionic liquids), and homogeneous catalysts. Applications related to these topics will not be reviewed.

Applications must propose research that leads to open source software, excluding density functional methods as currently implemented or semi-empirical approaches, dynamical mean field theory, and classical and first principles molecular dynamics. Applications related to these topics will not be reviewed.

Section IV – APPLICATION AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST APPLICATION PACKAGE

Application forms and instructions are available at [grants.gov](http://www.grants.gov). To access these materials, go to <http://www.grants.gov>, select “Apply for Grants”, and then select “Download Application Package.” Enter the CFDA number (81.049) and/or the funding opportunity number (DE-FOA-0001528) shown on the cover of this FOA and then follow the prompts to download the application package.

Applications submitted through www.FedConnect.net will not be accepted.

B. LETTER OF INTENT AND PRE-APPLICATION

1. Letter of Intent

LETTER OF INTENT DUE DATE

March 7, 2016 at 5 PM Eastern Time

A Letter of Intent is required and must be submitted at March 7, 2016 at 5 PM Eastern Time. **Any application received for which there is not an associated LOI will be deemed non-responsive and will be rejected without further review.** In addition, the lead organization on the application must be the same as on the LOI. If an application is received for which the lead organization has changed since submission of the LOI, then the application will be deemed non-responsive and will be rejected without further review. The Lead PI or Project Director should not be changed unless unavoidable and only minor edits should be made, if necessary, to the title. If necessary, the applicant may make changes to other senior/key personnel and other participating institutions, although DOE discourages extensive changes.

The LOI is to help in planning the review and the selection of potential reviewers for the application. For this purpose, the LOI must include the following:

- Letter of Intent Title (this is the Project Name)
- Lead Principal Investigator Name, Job Title (this is the Project Director)
- Lead Organization
- Lead Principal Investigator Phone Number and Email Address
- Funding Opportunity Announcement Number: DE-FOA-0001528

This cover page must be signed by an official of the lead organization who has the authority to commit institutional support for the application and by the proposed Project Director. For DOE National Laboratory applicants, the institutional official should be the Laboratory Director. For other applicants, this official should be someone who has authority over research activities for the entire institution, such as the Vice President for Research, Chief Technology Officer, or the equivalent. **All applicants must provide both of these signatures on the LOI.** Applicants that fail to provide both signatures on the LOI will be required to provide a corrected LOI with both signatures on or before March 19, 2016 in order for their full

application associated with the LOI to be considered for award.

The cover page must be followed by a clear and concise description of the goals, objectives, and technical approaches of the proposed research. The description of the proposed research may not exceed two pages when printed on 8.5 X 11 inch paper, with a minimum text font size no smaller than Times New Roman 12 point and margins no smaller than one inch on all sides. The required header information and any figures and references, if included, must fit within the two-page limit.

In addition, the LOI must include the following two Tables, which will not count toward the two-page limit for the LOI:

Table 1: Senior/key personnel on the application and institutional affiliations

Senior/Key Personnel			Institution
Last Name	First Name	Title	Institution Name

Table 2: Collaborators for senior/key personnel on the application

Collaborator			Institution
Last Name	First Name	Title	Institution Name

** Table 2 must include co-authors over the past 48 months, graduate and postdoctoral advisors of the senior/key personnel, graduate students and postdoctoral associates that have been supervised by the senior/key personnel during the past 60 months, and any other current close associations of the senior/key personnel. Table 2 should exclude all personnel at any of the institutions listed in Table 1.

- Table 1 and Table 2 will not count in the LOI page limitation.

The Lead Organization and Limitation on Number of Letters of Intent

An entity may not submit more than one LOI as the lead organization. If more than one qualified LOI is received from a lead organization, DOE will consider the first qualified LOI received based on the DOE Office of Science Portfolio Analysis and Management Systems (PAMS) date and time stamp. The remaining LOIs will be deemed non-responsive and the applicant will not be allowed to submit full applications tied to those LOIs. However, there is no limitation on the number of LOIs in which an entity may participate as a team member or subawardee.

The Project Director/Lead Principal Investigator and Limitation on Letters of Intent

The Project Director is the Lead Principal Investigator and must be employed or have an agreement in place to be hired by the lead organization in the event an award is made. An individual may not be named as the Project Director on more than one LOI. If more than one qualified LOI is received from an applicant identifying the same individual as the Project Director, DOE will consider the first qualified LOI received based on the PAMS date and time stamp. The remaining LOIs will be deemed non-responsive and the applicant will not be allowed to submit full applications tied to those LOIs.

All LOIs received by DOE will be acknowledged by an automated email to the Project Director. Any individual named as the Project Director on a LOI that is found to be non-responsive to the LOI requirements will be notified by March 21, 2016 and will be ineligible to submit a full application associated with that LOI. LOIs deemed responsive will receive no additional notification.

The LOI must be submitted electronically through the DOE Office of Science Portfolio Analysis and Management System (PAMS) website <https://pamspublic.science.energy.gov/>. It is important that the LOI be a single file with extension .pdf, .docx, or .doc. The filename should not exceed 50 characters. 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 letter of intent. **All PIs and those submitting LOIs on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays.**

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

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

Create PAMS Account:

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

- Click the “No, I have never had an account” link and then the “Create Account” button.
- You will be prompted to enter your name and email address, create a username and password, and select a security question and answer. Once you have done this, click the “Save and Continue” button.
- On the next page, enter the required information (at least one phone number and your mailing address) and any optional information you wish to provide (e.g., FAX number, website, mailstop code, additional email addresses or phone numbers, Division/Department). Click the “Create Account” button.
- Read the user agreement and click the “Accept” button to indicate that you understand your responsibilities and agree to comply with the rules of behavior for PAMS.

PAMS will take you to the “Having Trouble Logging In?” page. (If you have been an Office of Science merit reviewer or if you have previously submitted an application, you may already be

linked to an institution in PAMS. If this happens, you will be taken to the PAMS home page.

Register to Your Institution:

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

Submit Your Letter of Intent:

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

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

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this Funding Opportunity Announcement should reference **DE-FOA-0001528**.

2. Pre-application

A pre-application is not required or invited.

C. CONTENT AND APPLICATION FORMS

APPLICATION PREPARATION

You must download the application package, application forms and instructions, from Grants.gov at <http://www.grants.gov/>. (Additional instructions are provided in [Section IV, Part C](#) of this FOA.)

You are required to use the compatible version of Adobe Reader software to complete a [Grants.gov](#) Adobe application package. To ensure you have the [Grants.gov](#) compatible version of Adobe Reader, visit the download software page at http://www.grants.gov/help/download_software.jsp.

You must complete the mandatory forms and any applicable optional forms (e.g., Disclosure of Lobbying Activities (SF-LLL)) in accordance with the instructions on the forms and the additional instructions below.

Files that are attached to the forms must be in Adobe Portable Document Format (PDF) unless otherwise specified in this announcement. Attached PDF files must be plain files consisting of text, numbers, and images without editable fields, signatures, passwords, redactions, or other advanced features available in some PDF-compatible software. Do not use PDF portfolios or binders.

Please note: you may only use the following UTF-8 characters when naming your application attachments: A-Z, a-z, 0-9, underscore (_), hyphen (-), space, period. You must limit the file name to 50 or fewer characters. Attachments that do not follow this rule may cause the entire application to be rejected or cause issues during processing.

LETTERS

Letters of recommendation are discouraged and will not be reviewed by the DOE.

1. SF-424 (R&R)

Complete this form first to populate data in other forms. Complete all the required fields in accordance with the pop-up instructions on the form. The list of certifications and assurances referenced in Field 17 is available on the DOE Financial Assistance Forms Page at <http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms> under Certifications and Assurances.

DUNS AND EIN NUMBERS (FIELDS 5 AND 6)

The DUNS and EIN number fields on the SF-424 (R&R) form are used in PAMS to confirm the identity of the individual or organization submitting an application.

- Enter each number as a nine-digit number.
- Do not use hyphens or dashes.
- The Office of Science does not use the twelve-digit EIN format required by some other agencies.

TYPE OF APPLICATION (FIELD 8)

A **new** application is one in which DOE support for the proposed research is being requested for the first time. A **renewal** application requests additional funding for a period of time following a current award. If the application requests a significant change in the scope of work, please consult with the Program contact identified in this FOA to determine if the application should be considered new or a renewal.

The Office of Science does not make use of the Continuation or Revision options.

Applications for supplemental support of an existing award should be marked as “New.”

Please answer “yes” to the question “Is this application being submitted to other agencies?” if substantially similar, identical, or closely related research objectives are being submitted to another Federal agency. Indicate the agency or agencies to which the similar objectives have been submitted.

PUBLIC POLICY REQUIREMENTS

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

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

2. Research and Related Other Project Information

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

PROJECT SUMMARY/ABSTRACT (FIELD 7 ON THE FORM)

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

A Really Great Idea

A. Smith, Lead Institution (Principal Investigator)

A. Brown, Institution 2 (Co-Investigator)

A. Jones, Institution 3 (Co-Investigator)

Text of abstract

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

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

DOE COVER PAGE

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

The application narrative should begin with a cover page that will not count toward the project narrative page limitation. The cover page must include the following items:

- The project title
- Applicant/Institution:
- Street Address/City/State/Zip:
- Postal Address:
- Lead PI name, telephone number, email:
- Administrative Point of Contact name, telephone number, email:
- Funding Opportunity FOA Number: DE-FOA-0001528
- DOE/Office of Science Program Office: Basic Energy Sciences
- DOE/Office of Science Program Office Technical Contact: James Davenport
- PAMS Letter of Intent Tracking Number:

The lead applicant/awardee/recipient/organization must be the same as on the required LOI. **If an application is received for which the lead organization has changed since submission of the LOI, then the application will be deemed non-responsive and will be rejected without further review.** The Project Director should not be changed unless unavoidable and only minor edits should be made, if necessary, to the title. If necessary, the applicant may make changes to the other senior/key personnel and other participating institutions, although DOE discourages extensive changes.

On separate pages, as a supplement to the cover page, include the following personnel and summary budget information for all senior/key personnel and all partner institutions:

Table 1: Senior/key personnel on the application and institutional affiliations

Senior/Key Personnel			Institution
Last Name	First Name	Title	Institution Name

** Applicants are strongly encouraged to follow the exact format of the sample table above since the tabular information will be compiled across all applications. This includes the following elements:

- Include grid lines around each cell.
- Do not merge name or institution cells, even if individuals share the same institution.
- Do not change the order of the columns.
- Do not include any additional information (e.g. “PI”, “Co-PI”, or footnote symbols) under “Last Name” and “First Name”.
- Do not include departmental affiliations under Institutions.
- If an individual has a joint appointment, separate the institutions with a “/” (i.e. “Univ of X / National Lab Y”).

Table 2: Summary budget information for all partner institutions

Institution Name	Year 1 Budget	Year 2 Budget	Year 3 Budget	Year 4 Budget	Total Budget
Total Budget					

** Provide the total costs of the budget request in each year for each institution and totals for all rows and columns.

PROJECT NARRATIVE (FIELD 8 ON THE FORM)

The project narrative **must not exceed 30 pages** of technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard 8.5” by 11” paper with 1 inch margins (top, bottom, left, and right). Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph. The font must not be smaller than Times New Roman 12 point. **Only the first 30 pages of the Project Narrative will be reviewed or considered.** This page limit does not apply to the Cover Page, any Table of Contents (optional, but if included should be limited to one page), Budget Page(s), Budget Justification, biographical material, publications and references, and appendices, each of which may have its own page limit. Headers/footers containing page numbers and project titles/logos may be inserted within the required one inch margins

Do not include any Internet addresses (URLs) that provide supplementary or additional information that constitutes a part of the application. Merit reviewers are not required to access

Internet sites; however, Internet publications in a list of references will be treated identically to print publications. See Part VIII.D for instructions on how to mark proprietary application information. To attach a Project Narrative, click “Add Attachment.”

The contents of the Project Narrative are specified in order to ensure that the merit reviewers have the necessary information to conduct proper evaluations. Merit review criteria can be found in Section V. A.2 of this FOA. All Project Narratives must include the following sections:

I. Introduction and Background. This section should place the proposed project in the context of the scientific field in which it would operate by including the following:

- Briefly sketch the background leading to the application, critically evaluate existing knowledge, and specifically identify the scientific gaps for functional materials that the project is intended to fill;
- Describe the role the proposed computational materials research could play in advancing the scientific field;
- Clearly state the four-year scientific research, software development, and data goals;
- Provide an account of any preliminary studies that may be pertinent to the proposed research or any currently available software that will be incorporated;
- State concisely the importance of the research described in the application and its potential scientific impact;
- Include any information that will help to establish the experience and competence of the investigators to pursue the proposed research, including experience in development and management of community software and data resources;
- Discuss the relevant experience of the lead organization, Project Director, and other senior/key personnel in research by teams of investigators.

II. Proposed Research. Applicants must provide detailed information regarding the proposed research. This section should demonstrate the close integration of the proposed research activities aimed at meeting the four year scientific goals and how these will result in capabilities for design and discovery of functional materials. This section, which may be organized in subtasks, must clearly describe the proposed research by including the following:

- Describe a balanced and comprehensive program of basic research that, as needed, supports experimental, theoretical, and computational efforts and the development of new capabilities and approaches in these areas; include a clear statement of the open science questions to be addressed, a detailed research plan, an assessment of the potential scientific impact of the research, and a description of how the research plan will attain the 4-year scientific goals;
- Describe the scientific basis for the software to be developed and how it will be further developed;
- Describe the plan and process that will be used to generate, validate, and utilize computational and experimental data;
- Describe how the software will be experimentally validated and the role of the experimental component of the proposed research;

- Describe how the proposed research will include development of software that will exploit the capabilities of today's petascale and tomorrow's exascale leadership computing facilities;

Describe how the proposed research embodies the scientific approaches detailed in the following reports: *Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science*

(<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#CMSC>), *From Quanta to the Continuum: Opportunities for Mesoscale Science*

(<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#OFMS>) and *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science*

http://science.energy.gov/~media/bes/besac/pdf/Reports/CFME_rpt_print.pdf

- Describe the role and intellectual contribution of the Project Director, each co-Principal Investigator, and each other senior/key person in the application;
- Briefly outline the resources available including access to existing research space, instrumentation, computational capabilities, and other facilities both within the partner institutions and external to the team (Appendix 4 should include detailed information about facilities, equipment, and capabilities available for the research);
- Describe plans for development and utilization of unique facilities, capabilities or approaches to address the scientific goals;
- Relationship to other activities supported by BES or other federal agencies: As appropriate, briefly describe (less than one page) how the proposed research aligns with the core research activities and priorities within BES (<http://science.energy.gov/bes/mse/>, <http://science.energy.gov/bes/csgeb/>); is clearly distinguishable from activities within the BES Energy Frontier Research Centers (<http://science.energy.gov/bes/efrc/>) and the Energy Innovations Hubs (<http://science.energy.gov/bes/research/doe-energy-innovation-hubs/>); and relates to other existing and planned research programs at the participating institutions.

III. Management Plan. This section must provide a clear, substantive overview of the vision, management, and organization of the proposed Team by including the following:

- Describe the strategy and plan for project operations, the means of achieving an integrated research and development team, and plans for leadership and guidance for the scientific and technical direction of the project;
- Describe how the potential community that will use the software and associated data will be engaged to provide input to the research team;
- Describe how codes and data will be developed, maintained and shared; how will users gain access?
- Define an organizational structure that delineates the roles and responsibilities of senior/key personnel and describes the means of providing internal and external oversight and guidance for scientific and technical direction of the research and software development program, including but not limited to an **advisory committee (required)**, executive committees, program committees, or their equivalent; Advisory committee members need not be named unless project is awarded.

- Define proposed management processes for evaluation of research progress, decision making across the team, handling of intellectual property; and intra-team communication;
- Describe the availability of the Project Director, co-principal investigators, and other senior/key personnel, including discussion of their potential involvement in other major projects;
- Include a brief (less than one page) overview of environmental, safety, health, and quality assurance (ES&H and QA) practices and oversight at each participating institution, including any required permits, licenses, and approvals that must be obtained.

IV. Project Performance Site(s). Identify and describe the site(s) where the work will be performed. For research proposed by a team, work sites at all partner institutions should be briefly described. Appendix 4 should include detailed information about facilities, equipment, and capabilities available for the research. Costs for new construction (including new buildings or additions to existing buildings) will not be allowed in the award.

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the project director/principal investigator (PD/PI) and each senior/key person listed in Section A on the R&R Budget form.

- Provide the biographical sketch information as an appendix to your project narrative.
- Do not attach a separate file.
- The biographical sketch appendix will not count in the project narrative page limitation.
- The biographical information (curriculum vitae) for each person should not exceed 2 pages when printed on 8.5” by 11” paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 12 point and must include:

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

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

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

Synergistic Activities: List no more than 5 professional and scholarly activities related to the effort proposed.

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

- **Collaborators and Co-editors:** List in alphabetical order all persons, including their current organizational affiliation, who are, or who have been, collaborators or co-authors with you on

a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of this application. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the Principal Investigator interacted on a regular basis while the research was being done. Also, list any individuals who are currently, or have been, co-editors with you on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of this application. If there are no collaborators or co-editors to report, state "None."

- **Graduate and Postdoctoral Advisors and Advisees:** List the names and current organizational affiliations of your graduate advisor(s) and principal postdoctoral sponsor(s). Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates.
- **Advisory Committees:** List all advisory committees on which the PI serves, including the name of the institution and department.

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

Director Statement of Employment: Documentation must be submitted evidencing that the proposed Project Director is an employee or will become an employee of the prime applicant upon award. The statement of employment is limited to one page and must be signed by both the Project Director and an authorized representative of the prime applicant. This document is not included in the three page limit for each biographical sketch.

Individual Commitment Statement: For the Lead Principal Investigator/Project Director, each Principal Investigator, and each additional senior/key person, provide a signed statement that reflects their commitment to this project, including their individual level of time commitment, for a minimum period of four years. Multiple personnel representing the same institution may sign the same letter of commitment, as applicable. Each letter of commitment is limited to one page (this page is not included in the three page limit for each biographical sketch).

Provide the Biographical Sketches as an appendix to your project narrative.

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

APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support (both Federal and non-Federal) for the Project Director/Principal Investigator(s) (PD/PI) and senior/key persons, including subawardees, for ongoing projects and pending applications.

List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid.

For every activity, list the following items:

- The sponsor of the activity or the source of funding

- The award or other identifying number
- The title of the award or activity
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The person-months of effort per year being dedicated to the award or activity

Provide the Current and Pending Support as an appendix to your project narrative. Concurrent submission of an application to other organizations for simultaneous consideration will not prejudice its review.

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

APPENDIX 3: BIBLIOGRAPHY & REFERENCES CITED

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

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

APPENDIX 4: FACILITIES, EQUIPMENT & OTHER RESOURCES

This information is used to assess the capability of the organizational resources, including subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). List major items of equipment already available for this project and, if appropriate, identify location and pertinent capabilities. 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. For proposed investigations requiring access to experimental user facilities maintained by institutions other than the applicant, please provide a document from the facility manager confirming that the researchers will have access to the facility. Please provide the Facility and Other Resource information as an appendix to your project narrative.

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

APPENDIX 5: ADDITIONAL FUNDING

Discuss any additional funding and contributions-in-kind for the proposed project, including, but not limited to, optional cost sharing. If there is no additional funding, contributions-in-kind, or cost sharing, state “None.”

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

APPENDIX 6: DATA MANAGEMENT PLAN

Provide a Data Management Plan (DMP) that addresses the following requirements:

1. DMPs should describe whether and how data generated in the course of the proposed research will be shared and preserved. If the plan is not to share and/or preserve certain data, then the plan must explain the basis of the decision (for example, cost/benefit considerations, other parameters of feasibility, scientific appropriateness, or limitations discussed in #4). At a minimum, DMPs must describe how data sharing and preservation will enable validation of results, or how results could be validated if data are not shared or preserved.
2. DMPs should provide a plan for making all research data displayed in publications resulting from the proposed research open, machine-readable, and digitally accessible to the public at the time of publication. This includes data that are displayed in charts, figures, images, etc. In addition, the underlying digital research data used to generate the displayed data should be made as accessible as possible to the public in accordance with the principles stated in the Office of Science Statement on Digital Data Management (<http://science.energy.gov/funding-opportunities/digital-data-management/>). This requirement could be met by including the data as supplementary information to the published article, or through other means. The published article should indicate how these data can be accessed.
3. DMPs should consult and reference available information about data management resources to be used in the course of the proposed research. In particular, DMPs that explicitly or implicitly commit data management resources at a facility beyond what is conventionally made available to approved users should be accompanied by written approval from that facility. In determining the resources available for data management at Office of Science User Facilities, researchers should consult the published description of data management resources and practices at that facility and reference it in the DMP. Information about other Office of Science facilities can be found in the additional guidance from the sponsoring program.
4. DMPs must protect confidentiality, personal privacy, Personally Identifiable Information, and U.S. national, homeland, and economic security; recognize proprietary interests, business confidential information, and intellectual property rights; avoid significant negative impact on innovation, and U.S. competitiveness; and otherwise be consistent with all applicable laws, and regulations. There is no requirement to share proprietary data.

DMPs will be reviewed as part of the overall Office of Science research proposal merit review process. Applicants are encouraged to consult the Office of Science website for further information and suggestions for how to structure a DMP: <http://science.energy.gov/funding-opportunities/digital-data-management/>

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

APPENDIX 7: OPEN SOURCE SOFTWARE DISTRIBUTION PLAN

Applicants are required to submit an Open Source Software Distribution Plan as part of their proposal. This plan describes how software produced under this FOA will be distributed. Submission of an Open Source Software Distribution Plan is required; failure to submit a complete Plan may result in a determination of non-compliance for your Application. For a DOE National Laboratory or a FFRDC, the data rights clause, including rights and requirements pertaining to computer software, in its M&O Contract shall apply and shall take precedence over any requirement set forth in this Appendix.

The plan must include the following elements:

1. A complete description of any existing software that will be modified or incorporated into software produced under this FOA, including a description of the license rights. The license rights must allow the modified or incorporated software to be distributed as open source.
2. A discussion of the open source license that the Applicant plans to use for the software it plans to produce under the FOA, and how that choice furthers the goals of this FOA. The discussion should also discuss whether the proposed license is approved by the Open Source Initiative (OSI) <http://www.opensource.org>. Use of an OSI approved license is preferred.
3. A method for depositing the software in a source code repository or otherwise making the code widely available.
4. A method for sharing and disseminating the software and other information to team members or others when multiple parties will contribute to the development of the software or the FOA requires that the software or other information be shared or disseminated to others.

The Open Source Software Distribution Plan will be reviewed as part of the research proposal merit review process.

- Do not attach a separate file; and
- This appendix will not count in the Project Narrative page limitation.

APPENDIX 8: STATEMENT OF CONFLICT OF INTEREST

At the time of submission, the applicant shall include information identifying potential, apparent, or actual organizational and individual conflicts of interest and proposed mitigation. This shall include the applicant, their team members, and senior/key personnel named in the application. Negative responses are also required. Prior to award, DOE reserves the right to require the submission of a Conflict of Interest Management Plan describing the applicants approach to managing conflicts of interest.

- Do not attach a separate file; and
- This appendix will not count in the Project Narrative page limitation.

APPENDIX 9: ORGANIZATIONAL LETTERS OF COMMITMENT

A single organizational letter of commitment is required from each organization participating as a team member. Each organizational letter of commitment is limited to one page and must be current, signed, and dated by a person authorized to commit the participating organization to a legally binding agreement for this project.

- Do not attach a separate file; and
- This appendix will not count in the Project Narrative page limitation.

APPENDIX 10: LIST OF COLLABORATORS AND POSSIBLE CONFLICTS OF INTEREST

In tabular form following the example below, provide a list of collaborators for all senior/key personnel, including co-authors over the past 48 months, graduate and postdoctoral advisors of the senior/key personnel, graduate students and postdoctoral associates that have been supervised by the senior/key personnel during the past 60 months, and any other current close associations of the senior/key personnel. The table should exclude all personnel at any of the institutions participating in this application.

Collaborator			Institution
Last Name	First Name	Title	Institution Name

** Applicants are strongly encouraged to follow the exact format of the sample table because the tabular information will be compiled across all applications. This includes the following elements:

- Include grid lines around each cell.
 - Do not merge name or institution cells, even if individuals share the same institution.
 - Do not change the order of the columns.
 - Do not include any additional information (e.g. “PI”, “Co-PI”, or footnote symbols) under “Last Name” and “First Name”.
 - Do not include departmental affiliations under Institutions.
 - If an individual has a joint appointment, separate the institutions with a “/” (i.e. “Univ of X / National Lab Y”).
- Do not attach a separate file; and
 - This appendix will not count in the Project Narrative page limitation.

APPENDIX 11: OTHER ATTACHMENT

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

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.
- **Do not attach any of the requested appendices described above as files for fields 9, 10, 11, and 12.**
- **Follow the above instructions to include the information as appendices to the project narrative file.**
- **These appendices will not count toward the project narrative’s page limitation.**
- **Do not attach any files to fields 9, 10, 11, or 12.**

3. Research And Related Budget

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

Budget Fields

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

<p>Section D Travel</p>	<p>For purposes of this section only, travel to Canada or to Mexico is considered domestic travel. In the budget justification, list each trip's destination, dates, estimated costs including transportation and subsistence, number of staff traveling, the purpose of the travel, and how it relates to the project. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). To qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results. Domestic travel is to be justified separately from foreign travel.</p>
<p>Section E Participant/Trainee Support Costs</p>	<p>If applicable, submit training support costs. Educational projects that intend to support trainees (precollege, college, graduate and post graduate) must list each trainee cost that includes stipend levels and amounts, cost of tuition for each trainee, cost of any travel (provide the same information as needed under the regular travel category), and costs for any related training expenses. Participant costs are those costs associated with conferences, workshops, symposia or institutes and breakout items should indicate the number of participants, cost for each participant, purpose of the conference, dates and places of meetings and any related administrative expenses. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).</p>
<p>Section F Other Direct Costs</p>	<ul style="list-style-type: none"> • 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. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). • 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. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). • 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. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). • 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

	<p>information may be requested. In the budget justification, include the established computer service rates at the proposing organization if applicable. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).</p> <ul style="list-style-type: none"> • Subawards/Consortium/Contractual Costs: Enter total costs for all subawards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details. • Equipment or Facility Rental/User Fees: Enter total funds requested for Equipment or Facility Rental/User Fees. In the budget justification, identify each rental/user fee and justify. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). • Alterations and Renovations: Enter total funds requested for Alterations and Renovations. In the budget justification, itemize by category and justify the costs of alterations and renovations, including repairs, painting, removal or installation of partitions, shielding, or air conditioning. Where applicable, provide the square footage and costs. • Other: Add text to describe any other Direct Costs not requested above. Enter costs associated with “Other” item(s). Use the budget justification to further itemize and justify.
Section G Direct Costs	This represents Total Direct Costs (Sections A through F)
Section 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. Include the cognizant Federal agency and contact information if using a negotiated rate agreement.
Section I Total Direct and Indirect Costs	This is the total of Sections G and H

BUDGET JUSTIFICATION (FIELD K ON THE FORM)

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

4. R&R Subaward Budget Attachment(s) Form

Budgets for Subawardees, other than DOE FFRDC Contractors: You must provide a separate R&R budget for each subawardee. Download the R&R Budget Attachment from the

R&R SUBAWARD BUDGET ATTACHMENT(S) FORM and e-mail it to each subawardee that is required to submit a separate budget. After the subawardee has e-mailed its completed budget back to you, attach it to one of the blocks provided on the form. Use up to 10 letters of the subawardee's name (plus.pdf) as the file name (e.g., ucla.pdf or energyres.pdf). Filenames should not exceed 50 characters.

If the project involves more subawardees than there are places in the SUBAWARD BUDGET ATTACHMENT(S) FORM, the additional subaward budgets may be saved as PDF files and appended to the Budget Justification attached to Field K.

Ensure that any files received from subawardees are the PDF files extracted from the SUBAWARD BUDGET ATTACHMENT(S) FORM. Errors will be created if a subawardee sends a prime applicant a budget form that was not extracted from the application package.

If a subaward is being proposed for a DOE/NNSA National Laboratory Contractor, then the applicant must also submit the appropriate Field Work Proposal and should also include the Cognizant Federal Contracting Officer authorization as described in "Budget for DOE/NNSA National Laboratory Contractor" below. If a subaward is being proposed for a non-DOE/NNSA FFRDC contractor, the required authorization by the Cognizant Contracting Officer for the Federal sponsoring agency, as required in Section III.D., Other Eligibility Requirements, must be submitted. Use up to 10 letters of the non-DOE/NNSA FFRDC contractor name as the file name and attach to the R&R Other Project Information form in Field 12.

Budget for DOE/NNSA National Laboratory Contractor, if applicable: If a DOE/NNSA National Laboratory contractor is to perform any portion of the work, as the lead organization or as a team member, the DOE/NNSA National Laboratory must provide a DOE Field Work Proposal in accordance with the requirements in DOE Order 412.1A, Work Authorization System. This order and a sample of the DOE Field Work Proposal (FWP) form are available at <https://www.directives.doe.gov/directives-documents/400-series/0412.1-BOrder-a-admchg1>.

For purposes of satisfying this requirement, applicants are required to submit the DOE FWP face and budget pages (pages 1 and 2 of the sample form) with the application as part of the Budget for DOE/NNSA National Laboratory Contractor file. Furthermore, the information requested in blocks 1. through 15. and 17. through 19. of the sample FWP must be furnished with the application. The remainder of the information requested in blocks 16., 20., and 21. of the sample form will be required to be submitted through the DOE Work Authorization System by the successful applicant after selection.

In addition, include the required cognizant Federal Contracting Officer approval authorizing the participation of the DOE/NNSA National Laboratory as described in Section III.D. This information is required in addition to the budgetary information requested herein (R&R Budget, R&R Subaward Budget, and Budget Justification, as applicable). Use up to 10 letters of the DOE/NNSA National Laboratory name as the file name and attach to the R&R Other Project Information form in Field 12.

5. Project/Performance Site Location(s)

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

Note that the Project/Performance Site Congressional District is entered in the format of the 2 digit state code followed by a dash and a 3 digit Congressional district code, for example VA-001. Hover over this field for additional instructions.

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

6. Summary of Required Forms/Files

Your application must include the following items:

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

D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS

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

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

E. SUBMISSION DATES AND TIMES

1. Letter of Intent Due Date

March 7, 2016 at 5 PM Eastern Time

You are encouraged to submit your Letter of Intent well before the deadline.

2. Pre-application Due Date

None

3. Application Due Date

April 25, 2016 at 5 PM Eastern Time.

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

4. Late Submissions

Delays in submitting letters of intent, pre-applications, and applications may be unavoidable. DOE has accepted late submissions when applicants have been unable to make timely submissions because of widespread technological disruptions or significant natural disasters. DOE has made accommodations for incapacitating or life-threatening illnesses and for deaths of immediate family members. Other circumstances may or may not justify late submissions. Unacceptable justifications include the following:

- Failure to begin submission process early enough.
- Failure to provide sufficient time to complete the process.
- Failure to understand the submission process.
- Failure to understand the deadlines for submissions.
- Failure to satisfy prerequisite registrations.
- Unavailability of administrative personnel.
- An upper respiratory infection (a “cold”) the week of the deadline.

You are responsible for beginning the submission process in sufficient time to accommodate reasonably foreseeable incidents, contingencies, and disruptions.

Applicants must contact the Program Office/Manager listed in this Funding Opportunity Announcement to discuss the option of a late submission.

Requests for late submission are only rarely approved.

F. INTERGOVERNMENTAL REVIEW

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

G. FUNDING RESTRICTIONS

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

Costs for new construction (including new buildings or additions to existing buildings) will not be allowed.

Cost Principles: Costs must be allowable, allocable and reasonable in accordance with the applicable Federal cost principles referenced in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation).

Pre-award Costs: Recipients may charge to an award resulting from this FOA pre-award costs that were incurred within the ninety (90) calendar day period immediately preceding the effective date of the award, if the costs are allowable in accordance with the applicable Federal cost principles referenced in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation). Recipients must obtain the prior approval of the contracting officer for any pre-award costs that are for periods greater than this 90 day calendar period.

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

H. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS

1. Systems to Register In

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

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

Applicants must register with the System for Award Management (SAM) at <http://www.sam.gov/>. If you had an active registration in the Central Contractor Registry (CCR), you should have an active registration in SAM. More information about SAM registration for applicants is found at [https://www.sam.gov/sam/transcript/Quick Guide for Grants Registrations v1.7.pdf](https://www.sam.gov/sam/transcript/Quick%20Guide%20for%20Grants%20Registrations%20v1.7.pdf).

Applicants must provide a Taxpayer Identification Number (TIN) to complete their registration in SAM.gov. An applicant's TIN is an Employer Identification Number (EIN) assigned by the Internal Revenue Service (IRS). In limited circumstances, a Social Security Number (SSN) assigned by the Social Security Administration (SSA) may be used as a TIN. You may obtain an EIN from the IRS at [http://www.irs.gov/Businesses/Small-Businesses-%26-Self-Employed/Apply-for-an-Employer-Identification-Number-\(EIN\)-Online](http://www.irs.gov/Businesses/Small-Businesses-%26-Self-Employed/Apply-for-an-Employer-Identification-Number-(EIN)-Online).

DOE discourages the use of a SSN as a TIN. You are encouraged to obtain a TIN from the Internal Revenue Service (IRS) using the website listed above.

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

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

2. Registering in Grants.gov

Applicants must register with grants.gov.

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

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

For individuals, please follow the procedures detailed below:

<http://www.grants.gov/web/grants/applicants/individual-registration.html>

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

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

FIRST-TIME REGISTRATION PROCESS IN GRANTS.GOV

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

the process. **IMPORTANT:** During the SAM registration process, you will be asked to designate an E-Business Point of Contact (EBIZ POC). The EBIZ POC must obtain a special password called "Marketing Partner Identification Number" (MPIN). When you have completed the process, you should call the Grants.gov Helpdesk at 1-800-518-4726 to verify that you have completed the final step (i.e., Grants.gov registration).

3. Application Receipt Notices

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

Number 1 - Grants.gov Submission Receipt Number

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

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

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

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

3. Where to Submit an Application

Applications must be submitted through grants.gov to be considered for award.

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

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

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

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

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

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

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

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

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

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

1. CREATE PAMS ACCOUNT:

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

- Click the “No, I have never had an account” link and then the “Create Account” button.
- You will be prompted to enter your name and email address, create a username and password, and select a security question and answer. Once you have done this, click the “Save and Continue” button.
- On the next page, enter the required information (at least one phone number and your mailing address) and any optional information you wish to provide (e.g., FAX number, website, mailstop code, additional email addresses or phone numbers, Division/Department). Click the “Create Account” button.
- Read the user agreement and click the “Accept” button to indicate that you understand your responsibilities and agree to comply with the rules of behavior for PAMS.
- PAMS will take you to the “Having Trouble Logging In?” page. (If you have been an Office of Science merit reviewer or if you have previously submitted an application, you may already be linked to an institution in PAMS. If this happens, you will be taken to the PAMS home page.)

2. REGISTER TO YOUR INSTITUTION:

- Click the link labeled “Option 2: I know my institution and I am here to register to the institution.” (Note: If you previously created a PAMS account but did not register to an institution at that time, you must click the Institutions tab and click the “Register to Institution” link.)
- PAMS will take you to the “Register to Institution” page.
- Type a word or phrase from your institution name in the field labeled, “Institution Name like,” choose the radio button next to the item that best describes your role in the system, and click the “Search” button. A “like” search in PAMS returns results that contain the word or phrase you enter; you do not need to enter the exact name of the institution, but you should enter a word or phrase contained within the institution name. (If your institution has a frequently used acronym, such as ANL for Argonne National Laboratory or UCLA for the Regents of the University of California, Los Angeles, you may find it easiest to search for the

acronym under “Institution Name like.” Many institutions with acronyms are listed in PAMS with their acronyms in parentheses after their names.)

- Find your institution in the list that is returned by the search and click the “Actions” link in the Options column next to the institution name to obtain a dropdown list. Select “Add me to this institution” from the dropdown. PAMS will take you to the “Institutions – List” page.
- If you do not see your institution in the initial search results, you can search again by clicking the “Cancel” button, clicking the Option 2 link, and repeating the search.
- If, after searching, you think your institution is not currently in the database, click the “Cannot Find My Institution” button and enter the requested institution information into PAMS. Click the “Create Institution” button. PAMS will add the institution to the system, associate your profile with the new institution, and return you to the “Institutions – List” page when you are finished.

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this Funding Opportunity Announcement should reference DE-FOA-000XXXX.

5. Viewing Submitted Applications

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

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

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

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

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

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

1. Log in to PAMS at <https://pamspublic.science.energy.gov/>.
2. Click the “Proposals” tab and click “Access Previously Submitted Grants.gov Proposal.”
3. Enter the following information:
 - Proposal ID: Enter the ten-digit PAMS proposal ID, including the leading zeros (e.g., 00002xxxxx). Do not use the grants.gov proposal number. Use the PAMS number previously sent to you in the email with subject line, “Receipt of Proposal ...”.
 - Email (as entered in grants.gov application): Enter your email address as it appears on the SF424(R&R) Cover Page.
 - Choose Role: Select the radio button in front of the role corresponding to the SF-424 (R&R) cover page. If your name appears in block 19 of the SF-424 (R&R) cover page as the authorizing representative, select “SRO/BO/AO (Sponsored Research Officer/Business Officer/Administrative Officer).” If your name appears in block 14 of the SF424 R&R cover page as the PI, select “Principal Investigator (PI).” If your name appears in block 5 of the SF424 R&R as the point of contact, select “Other (POC).”
4. Click the “Save and Continue” button. You will be taken to your “My Proposals” page. The grants.gov proposal will now appear in your list of proposals. Click the “Actions/Views” link in the options column next to this proposal to obtain a dropdown list. Select “Proposal” from the dropdown to see the proposal. Note that the steps above will work only for proposals submitted to the DOE Office of Science since May 2012.

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

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

- the SF424 R&R cover page as the PI, select “Principal Investigator (PI).” If your name appears in block 5 of the SF424 R&R as the point of contact, select “Other (POC).”
8. Click the “Save and Continue” button. You will be taken to your “My Proposals” page. The grants.gov proposal will now appear in your list of proposals. Click the “Actions/Views” link in the options column next to this proposal to obtain a dropdown list. Select “Proposal” from the dropdown to see the proposal.

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

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this Funding Opportunity Announcement should reference **DE-FOA-0001528**.

Section V - APPLICATION REVIEW INFORMATION

A. CRITERIA

1. Initial Review Criteria

Prior to a comprehensive merit evaluation, DOE will perform an initial review in accordance with 10 CFR 605.10(b) to determine that (1) the applicant is eligible for the award; (2) the information required by the FOA has been submitted; (3) all mandatory requirements are satisfied; (4) the proposed project is responsive to the objectives of the funding opportunity announcement, and (5) the proposed project is not duplicative of programmatic work. Applications that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

Be advised that proposals focused on structural, thermoelectric, and energy storage materials; structural properties; and synthesis of 2-d layered materials, assemblies of nanoparticles, isolated molecules, liquids (including ionic liquids), and homogeneous catalysts will be considered non-responsive. Research that emphasizes density functional methods as currently implemented or semi-empirical approaches, dynamical mean field theory, and classical and first principles molecular dynamics will be considered non-responsive.

2. Merit Review Criteria

The application will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria, the first five of which will be weighted more heavily than the final two. The first five criteria are of equal value with each other. The final two criteria are of equal value with each other. The questions after each are intended to guide the reviewers; reviewers will not be required to provide written responses to each of these questions.

- Scientific and/or Technical Merit of the Project;
- Appropriateness of the Proposed Method or Approach;
- Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
- Reasonableness and Appropriateness of the Proposed Budget.
- Strength of the Management Plan
- Synergy Among the PIs, including Cohesion and Integration of the Research and Software Development Activities
- Development and Utilization of Unique Facilities, Capabilities or Approaches

SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROPOSED RESEARCH

- Does the application present a balanced and comprehensive program of basic research that, as needed, supports experimental, theoretical, and computational efforts and development of new capabilities for predictive design of functional materials?
- Does the proposed research embody the scientific approaches detailed in the following reports: *Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science*

(<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#CMSC>), *From Quanta to the Continuum: Opportunities for Mesoscale Science* (<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#OFMS>) and *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science* http://science.energy.gov/~media/bes/besac/pdf/Reports/CFME_rpt_print.pdf

- Does the application contain clearly defined four-year scientific research, data, and software goals?
- Will the research develop software that takes advantage of current and future DOE leadership class computing resources?
- Do the scientific, software, and data goals of the project have sufficient programmatic focus?
- Is the proposed research program likely to meet the stated four-year scientific research, software, and data goals?
- Is the Data Management Plan suitable for the proposed research; to what extent does it make the data available and useful to the scientific community?
- Will the proposed research likely result in useful software and data that will accelerate the design, discovery, and development of new functional materials?

APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

- Are the strategy and the plan for the development and operation of the project including the need for an approach involving several senior/key personnel, the means for achieving an integrated Team, and plans for leadership and guidance for the scientific and technical direction, appropriate?
- Does the application present integrated research that embodies the “team science” approach in which the research challenges to be addressed are those that are likely to be overcome only by a centrally managed, multi-disciplinary team?
- Are the proposed scientific methods or approaches detailed in the proposal appropriate to achieve the stated scientific goals?
- Are the plans (if any) for external collaborations and partnerships reasonable and appropriate?
- Are the roles and intellectual contributions of the Project Director, Principal Investigator(s), and all other senior/key personnel adequately described and appropriate?
- Is the proposed approach for making a community code and the associated experimental and computational data available to general users from the research community, including the Open Source Software Distribution Plan, likely to be effective? Is there a plan to get input from the community that will use the data and software?

COMPETENCY OF APPLICANT’S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES

- Do the applicant’s senior/key personnel have a proven record of research in the disciplines needed for success in this project?
- Do the lead organization, the Director, and the other senior/key personnel have proven records of success in project, program, and personnel management of diverse teams of scientific and technical professionals for projects of comparable complexity and magnitude?

- Is the plan for recruiting any additional scientific and technical personnel including new senior staff, students and postdocs reasonable and appropriate?
- Is the proposed access to existing research space, instrumentation and facilities at the partner institutions likely to meet the needs of the proposed team?
- Is there adequate access to experimental and computational capabilities as needed to ensure successful completion of the proposed research, including access to research capabilities and resources outside of the Team?
- Will the Project Director and senior/key personnel be sufficiently available given their role particularly taking into account their potential involvement in other major projects?
- Does the team have expertise and capabilities required to support the development and maintenance of community research codes and data?

REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET

- Are the requested operating budget and the distribution of the funds among research tasks/themes, software development and partners reasonable for the program?
- Are the equipment needs adequately identified, and costs for needed new instrumentation or upgrades realistically estimated?
- Are the budgeted costs for preparing space for existing and new equipment and instrumentation appropriate and reasonable?
- Are all subawards, travel, student costs and other ancillary expenses adequately estimated and justified?

STRENGTH OF THE MANAGEMENT PLAN

- Is there a clear lead organization and a Project Director with qualifications to manage a large team?
- Does the applicant present a comprehensive management plan? What is the likelihood that the applicant can overcome key scientific challenges and shift research directions in response to promising developments? Has the application presented a clearly defined mechanism to evaluate success/failure and to reconfigure research thrusts as needed?
- If needed, is there a well-defined plan to the use of state-of-the-art technology and frequent virtual meetings to enable meaningful, efficient long distance collaboration?
- Does the applicant present an organizational structure that delineates the roles and responsibilities of senior/key personnel and describes the means of providing external oversight and guidance for scientific and technical direction of the research program?
- Is the role of an advisory committee (required) and any executive committee, program committee, or their equivalent adequately described and appropriate?
- Are environment, safety, health and quality assurance (ESH & QA) issues responsibly anticipated and addressed? Does the applicant have a work planning and control process which considers them?

SYNERGY AMONG THE PIS, INCLUDING COHESION AND INTEGRATION OF THE RESEARCH AND SOFTWARE DEVELOPMENT ACTIVITIES

- Does the application describe a well-integrated team based approach to addressing the scientific and software development goals?

- Is the proposed team of researchers likely to work together in a cohesive and integrated manner? Have they demonstrated their ability to do so in the past?
- Have the applicants defined scientific problems that are likely to be addressed only through close collaboration among the researchers on the application?
- Are the elements of the proposed research appropriately integrated, coordinated, and synergistic?

DEVELOPMENT AND UTILIZATION OF UNIQUE FACILITIES, CAPABILITIES OR APPROACHES

- Does the research plan include full utilization of current (petascale) and future (exascale) leadership class computing resources?
- Does the proposed research rely on the use of unique facilities at the applicants' home institutions or at US or international user facilities?
- Have the applicants proposed the development of unique facilities, capabilities, or approaches to achieve the stated scientific goals?

B. REVIEW AND SELECTION PROCESS

1. Merit Review

Applications that pass the initial review will be subjected to a formal merit review and will be evaluated based on the criteria codified at 10 CFR 605.10(d) in accordance with the guidance provided in the “Office of Science Merit Review System for Financial Assistance,” which is available at: <http://science.energy.gov/grants/policy-and-guidance/merit-review-system/>.

2. Selection

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

- Scientific and technical merit of the proposed activity as determined by merit review
- Availability of funds
- Relevance of the proposed activity to Basic Energy Science (BES) priorities
- Ensuring an appropriate balance of BES activities
- Previous performance
- Delineation of the scope of the proposed research from other research activities in which the principal investigators are involved, particularly those supported by DOE and by other federal agencies
- Diversity of research activities that will address the scientific grand challenges and use-inspired basic research as articulated in the Basic Energy Sciences Advisory Committee (BESAC) and BES workshop reports
- Relationship of the proposed project to other research and development programs in DOE, including but not limited to the Energy Frontier Research Centers, Energy Innovation Hubs, and the core research activities within the BES Materials Sciences and Engineering or Chemical Sciences, Geosciences, and Biosciences Divisions
- Potential for developing synergies between the proposed project and other ongoing BES research activities

3. Review of Risk

Pursuant to 2 CFR 200.205, DOE will conduct an additional review of the risk posed by applications submitted under this FOA. Such review of risk will include:

- Technical merit of the application,
- Reports and findings from audits performed under 2 CFR 200 or OMB Circular A-133, and
- Systems maintained under 2 CFR 180, including the SAM “Exclusions” and “Do Not Pay” systems.

DOE may make use of other publicly available information and the history of an applicant’s performance under DOE or other Federal agency awards.

Applicants with no prior performance of DOE awards may be asked to provide information about their financial stability and or their ability to comply with the management standards of 2 CFR 200.

4. Discussions and Award

The Government may enter into discussions with a selected applicant for any reason deemed necessary, including but not limited to the following: (1) the budget is not appropriate or reasonable for the requirement; (2) only a portion of the application is selected for award; (3) the Government needs additional information to determine that the recipient is capable of complying with the requirements in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation); and/or (4) special terms and conditions are required. Failure to resolve satisfactorily the issues identified by the Government will preclude award to the applicant.

C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES

It is anticipated that the award selection will be completed by September 30, 2016. It is expected that awards will be made in Fiscal Year 2016.

DOE is interested in seeing projects supported under this FOA begin work by September 30, 2016.

Section VI - AWARD ADMINISTRATION INFORMATION

A. AWARD NOTICES

1. Notice of Selection

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

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

2. Notice of Award

An Assistance Agreement issued by the contracting officer is the authorizing award document. It normally includes, either as an attachment or by reference, the following items: (1) Special Terms and Conditions; (2) Applicable program regulations, if any; (3) Application as approved by DOE; (4) 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation); (5) National Policy Assurances To Be Incorporated As Award Terms; (6) Budget Summary; and (7) Federal Assistance Reporting Checklist, which identifies the reporting requirements.

For grants and cooperative agreements made to universities, non-profits and other entities subject to Title 2 CFR, awards made under this funding opportunity should include the government-wide Research Terms and Conditions. A new version of the Terms and Conditions based on the changes to 2 CFR 200 is not yet available. Once the Terms and Conditions become available, they will be located at <http://www.nsf.gov/bfa/dias/policy/rtc/index.jsp>. If an award is made under this funding opportunity before the Terms and Conditions are posted, alternative Terms and Conditions may be included in the award.

B. ADMINISTRATIVE AND NATIONAL POLICY REQUIREMENTS

1. Administrative Requirements

The administrative requirements for DOE grants and cooperative agreements are contained in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation).

For grants and cooperative agreements made to universities, non-profits and other entities subject to Title 2 CFR, awards made under this funding opportunity should include the government-wide Research Terms and Conditions. A new version of the Terms and Conditions based on the changes to 2 CFR 200 is not yet available. Once the Terms and Conditions become available, they will be located at <http://www.nsf.gov/bfa/dias/policy/rtc/index.jsp>. If an award is made under this funding opportunity before the Terms and Conditions are posted, alternative Terms and Conditions may be included in the award.

NONDISCLOSURE AND CONFIDENTIALITY AGREEMENTS REPRESENTATIONS (JUNE 2015)

In submitting an application in response to this FOA the Applicant represents that:

(1) It **does not and will not** require its employees or contractors to sign internal nondisclosure or confidentiality agreements or statements prohibiting or otherwise restricting its employees or contractors from lawfully reporting waste, fraud, or abuse to a designated investigative or law enforcement representative of a Federal department or agency authorized to receive such information.

(2) It **does not and will not** use any Federal funds to implement or enforce any nondisclosure and/or confidentiality policy, form, or agreement it uses unless it contains the following provisions:

a. *“These provisions are consistent with and do not supersede, conflict with, or otherwise alter the employee obligations, rights, or liabilities created by existing statute or Executive order relating to (1) classified information, (2) communications to Congress, (3) the reporting to an Inspector General of a violation of any law, rule, or regulation, or mismanagement, a gross waste of funds, an abuse of authority, or a substantial and specific danger to public health or safety, or (4) any other whistleblower protection. The definitions, requirements, obligations, rights, sanctions, and liabilities created by controlling Executive orders and statutory provisions are incorporated into this agreement and are controlling.”*

b. The limitation above shall not contravene requirements applicable to Standard Form 312, Form 4414, or any other form issued by a Federal department or agency governing the nondisclosure of classified information.

c. Notwithstanding provision listed in paragraph (a), a nondisclosure or confidentiality policy form or agreement that is to be executed by a person connected with the conduct of an intelligence or intelligence-related activity, other than an employee or officer of the United States Government, may contain provisions appropriate to the particular activity for which such document is to be used. Such form or agreement shall, at a minimum, require that the person will not disclose any classified information received in the course of such activity unless specifically authorized to do so by the United States Government. Such nondisclosure or confidentiality forms shall also make it clear that they do not bar disclosures to Congress, or to an authorized official of an executive agency or the Department of Justice, that are essential to reporting a substantial violation of law.

REGISTRATION REQUIREMENTS

Additional administrative requirements for DOE grants and cooperative agreements are contained in 2 CFR 25 (See: <http://www.ecfr.gov>). Prime awardees must keep their data at the System for Award Management (SAM) current at <http://www.sam.gov>. SAM is the government-wide system that replaced the Central Contractor Registry (CCR). If you had an active registration in the CCR, you have an active registration in SAM. Subawardees at all tiers must obtain DUNS numbers and provide the DUNS to the prime awardee before the subaward can be issued.

SUBAWARD AND EXECUTIVE REPORTING

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

PROHIBITION ON LOBBYING ACTIVITY

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

2. Terms and Conditions

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

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

<http://energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards>

3. National Policy Assurances

The National Policy Assurances To Be Incorporated As Award Terms are located at <http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms> under Award Terms.

4. Statement of Substantial Involvement

Only grants may be awarded under this FOA.

5. Additional Conditions

CONFERENCE SPENDING (FEBRUARY 2015)

The recipient shall not expend any funds on a conference not directly and programmatically related to the purpose for which the grant or cooperative agreement was awarded that would defray the cost to the United States Government of a conference held by any Executive branch department, agency, board, commission, or office for which the cost to the United States Government would otherwise exceed \$20,000, thereby circumventing the required notification

by the head of any such Executive Branch department, agency, board, commission, or office to the Inspector General (or senior ethics official for any entity without an Inspector General), of the date, location, and number of employees attending such conference.

CORPORATE FELONY CONVICTION AND FEDERAL TAX LIABILITY REPRESENTATIONS (MARCH 2014)

In submitting an application in response to this FOA the Applicant represents that:

- It is **not** a corporation that has been convicted of a felony criminal violation under any Federal law within the preceding 24 months,
- It is **not** a corporation that has any unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or have lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability.

For purposes of these representations the following definitions apply:

- A Corporation includes any entity that has filed articles of incorporation in any of the 50 states, the District of Columbia, or the various territories of the United States [but not foreign corporations]. It includes both for-profit and non-profit organizations.

PUBLICATIONS

The recipient is expected to publish or otherwise make publicly available the results of the work conducted under any award resulting from this Funding Opportunity Announcement.

Publications and other methods of public communication describing any work based on or developed under an award resulting from this Funding Opportunity Announcement must contain an acknowledgment of DOE Office of Science support. The format for such acknowledgments is provided at <http://science.energy.gov/funding-opportunities/acknowledgements/>. The author's copy of any peer-reviewed manuscript accepted for funding must be announced to DOE's Office of Scientific and Technical Information and made publicly available in accordance with the instructions contained in the Reporting Requirements Checklist incorporated in all Assistance Agreements.

C. REPORTING

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

Section VII - QUESTIONS/AGENCY CONTACTS

A. QUESTIONS

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

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this Funding Opportunity Announcement should reference **DE-FOA-0001528**.

Please contact the PAMS help desk for technological issues with the PAMS system.

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

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

B. AGENCY CONTACTS

Grants.gov Customer Support	800-518-4726 (toll-free) support@grants.gov
PAMS Customer Support	855-818-1846 (toll-free) 301-903-9610 sc.pams-helpdesk@science.doe.gov
Program Manager Scientific Contact	James Davenport; 301-903-0035; james.davenport@science.doe.gov

Section VIII - OTHER INFORMATION

A. MODIFICATIONS

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

B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE

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

C. COMMITMENT OF PUBLIC FUNDS

(a) A DOE financial assistance award is valid only if it is in writing and is signed, either in writing or electronically, by a DOE Contracting Officer.

(b) Recipients are free to accept or reject the award. A request to draw down DOE funds constitutes the Recipient's acceptance of the terms and conditions of this Award.

D. PROPRIETARY APPLICATION INFORMATION

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

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

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

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

E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL

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

F. INTELLECTUAL PROPERTY DEVELOPED UNDER THIS PROGRAM

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

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

G. NOTICE OF RIGHT TO REQUEST PATENT WAIVER

Applicants may request a waiver of all or any part of the rights of the United States in inventions conceived or first actually reduced to practice in performance of an agreement as a result of this FOA, in advance of or within 30 days after the effective date of the award. Even if such advance waiver is not requested or the request is denied, the recipient will have a continuing right under the award to request a waiver of the rights of the United States in identified inventions, i.e., individual inventions conceived or first actually reduced to practice in performance of the award. Any patent waiver that may be granted is subject to certain terms and conditions in 10 CFR 784. For more information, see <http://energy.gov/gc/services/technology-transfer-and-procurement/office-assistant-general-counsel-technology-transf-1>

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

H. NOTICE REGARDING ELIGIBLE/INELIGIBLE ACTIVITIES

Eligible activities under this program include those which describe and promote the understanding of scientific and technical aspects of specific energy technologies, but not those

which encourage or support political activities such as the collection and dissemination of information related to potential, planned or pending legislation.

I. AVAILABILITY OF FUNDS

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