

**DEPARTMENT OF ENERGY  
OFFICE OF SCIENCE  
BASIC ENERGY SCIENCES**



**COMPUTATIONAL MATERIALS SCIENCES**

**FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER:  
DE-FOA-0002040**

**FOA TYPE: INITIAL  
CFDA NUMBER: 81.049**

<b>FOA Issue Date:</b>	<b>November 26, 2018</b>
<b>Submission Deadline for Letters of Intent:</b>	<b>N/A</b>
<b>Submission Deadline for Pre-Applications:</b>	<b>December 21, 2018 at 12:00 PM (noon) Eastern Time A Pre-Application is required for new <i>and</i> renewal applicants</b>
<b>Pre-Application Response Date:</b>	<b>January 18, 2019</b>
<b>Submission Deadline for Applications:</b>	<b>February 28, 2019 at 5:00 PM Eastern Time</b>

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## UPDATES AND REMINDERS

### RECOMMENDATION

The Department of Energy (DOE) Office of Science (SC) encourages you to register in all systems as soon as possible. You are also encouraged to submit pre-applications, and applications well before the deadline.

### PRE-APPLICATION REVIEW

Pre-applications will be comparatively reviewed by DOE SC program managers to determine which pre-applications may yield the most competitive applications. To be considered eligible for an award under this FOA, potential lead organizations are required to submit a pre-application in accordance with the instructions provided in Section IV.B.2, and to receive notification from DOE that they are allowed to submit a full proposal. Applications received from an applicant who has not submitted the required pre-application, or who has received notification from DOE that they are disallowed from submitting a full application, will be deemed non-responsive and will be rejected without further review.

All applicants, both for new and renewal awards, must submit pre-applications.

### AVOIDING ERRORS

The following advice is compiled from actual experiences of applicants for SC financial assistance awards.

- Please ensure that the research narrative is comprised of one and only one Portable Document Format (PDF) file, including all appendices, when it is attached to the SF-424 (R&R) form.
- When using the PAMS website at <https://pamspublic.science.energy.gov>, please avoid using the back-arrow button in your web browser to navigate.
- Please ensure that the application contains no personally identifiable information (PII).
- Please ensure that the budget is calculated using the applicable negotiated indirect cost and fringe benefit rates.

### GRANTS.GOV WORKSPACE

Applications submitted through Grants.gov at <https://www.Grants.gov> must be submitted through a “Workspace.” Workspace permits members of a team to simultaneously work on their application in an online collaborative environment. Application forms may exist as both online webforms and downloadable forms. More information is available at <https://www.grants.gov/web/grants/applicants/workspace-overview.html>.

### RENEWAL APPLICATIONS

The Lead Principal Investigator (PI) for any application submitted for a **renewal** (an addition of a project period) of an existing award will be required to submit a Renewal Proposal Products

section through the PAMS website at <https://pamspublic.science.energy.gov>. The submitted product list will be sent for merit review as part of the application. The application will not be considered complete and cannot be sent for review until the product list has been submitted. Renewal applications must be submitted from the institution that holds the current award. Changes in the Lead PI should be discussed with the program manager prior to submission of the renewal proposal.

#### DATA MANAGEMENT PLAN

Applications submitted under this FOA are subject to the Office of Science Statement on Digital Data Management, published at <https://science.energy.gov/funding-opportunities/digital-data-management/>. Compliance with this statement is detailed in Part IV of this FOA.

#### ACKNOWLEDGMENT OF FEDERAL SUPPORT

SC published guidance about how its support should be acknowledged at <https://science.energy.gov/funding-opportunities/acknowledgements/>.

## **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](mailto: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 DOE SC program in Basic Energy Sciences (BES) announces its interest in receiving new and renewal applications in Computational Materials Sciences with the aim of producing widely applicable, validated community codes and the associated databases for the design of functional materials. Proposals must include plans for the utilization of DOE's Leadership Class Computing facilities including petascale, pre-exascale and future exascale machines. The research component should meet the standards and priorities of the BES research program as determined by BES community planning documents (see references below) and peer review.

The program will support both single investigator/small group and larger team awards. Larger awards must focus on the creation of computational codes and associated experimental/computational databases by fully integrated teams, combining the skills of experts in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication. The research may involve the development of new ab initio theory, mining data from both experimental and theoretical databases, performing advanced in situ/operando characterization to generate the specific parameters needed to validate computational models, and well-controlled synthesis to confirm the predictions of the codes. Smaller, single investigator or small group awards should address specific computational developments or techniques that can add functionality/capabilities to standard codes.

This effort is part of the DOE BES research related to the Materials Genome Initiative for Global Competitiveness as well as the DOE Office of Science Exascale activities. BES funded three large team Computational Materials Sciences awards in FY 2015 and two additional large team

awards in FY 2016. Additional information on these awards can be found at the website listed in the references below. See the Summary Criteria section for more information on excluded research areas for this funding opportunity.

## **SUPPLEMENTARY INFORMATION**

### **BACKGROUND**

Major strides in materials synthesis, processing, and characterization, combined with concurrent advances in computational science enabled by enormous improvements in high-performance computing capabilities have opened an unprecedented opportunity to design new materials with specific functions and properties. The goal is to leap beyond simple extensions of current theory and models of materials towards a paradigm shift in which specialized computational codes and software enable the design, discovery, and development of new materials, and in turn, create new advanced, innovative technologies. Given the importance of materials to virtually all technologies, computational materials sciences are critical for American competitiveness and global leadership in innovation.

This paradigm shift will accelerate the design of revolutionary materials to meet the Nation's energy security and enhance economic competitiveness. Development of fundamentally new design principles could enable stand-alone research codes and integrated software packages to address multiple length and time scales for prediction of the total functionality of materials over a lifetime of use. Examples include dynamics and strongly correlated matter, conversion of solar energy to electricity, and electrical and thermal transport in materials for improved electronics. Success will require extensive R&D with the goal of creating experimentally validated, robust community codes that will enable functional materials innovation.

Research and development to create these computational codes 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 includes development of new ab initio theory, advanced materials modeling, mining data from both experimental and theoretical databases, performing advanced in situ/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 addition, single investigator/small group efforts are required to bolster the larger team activities, taking on higher risk research that addresses specific computational developments or techniques that can add innovative software functionality/capabilities.

## **ADDITIONAL REQUIREMENTS**

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

- Focus on functional materials research. Suitable classes of functional materials include, for example, quantum materials, materials related to quantum information science, topological materials, wide-bandgap semiconductors, transition metal oxides, and magnetic, superconducting, photovoltaic, optoelectronic, and thermoelectric materials. Explicitly excluded are proposals on cold atoms, structural materials, isolated molecules, ionic liquids, and catalysts.
- Focus on research leading to open source software. 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. This plan should describe the maintenance and long-term accessibility of the software.
- Suitable types of software will emphasize strong correlations, multiscale properties, excited states, transport, electronic or optical properties. Explicitly excluded are proposals that emphasize density functional methods as currently implemented.
- Provide a detailed plan for the full utilization of today's petascale and pre-exascale, and tomorrow's exascale leadership computing facilities.
- For larger awards, applications must have integrated, multi-investigator teams combining expertise in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication. These proposals must articulate a clear management plan that ensures a coherent team approach.
- Include a Data Management Plan. This plan should describe the maintenance and long-term accessibility of data.
- The application should provide mechanisms for research community input to software and database development and validation.
- Entities proposing as a team must designate a lead organization. Only one pre-application and one application is to be submitted for each team. The designated lead organization must perform a greater percentage of the effort, as determined by the budget distribution by institution, than any other partner organization or subawardee.

### **References:**

*Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science*

([https://science.energy.gov/~media/bes/pdf/reports/files/Computational\\_Materials\\_Science\\_and\\_Chemistry\\_rpt.pdf](https://science.energy.gov/~media/bes/pdf/reports/files/Computational_Materials_Science_and_Chemistry_rpt.pdf))

BES Computing and Data Requirements in the Exascale Age (BES Exascale Requirements Review); [https://science.energy.gov/~media/bes/pdf/reports/2017/BES-EXA\\_rpt.pdf](https://science.energy.gov/~media/bes/pdf/reports/2017/BES-EXA_rpt.pdf)).

*From Quanta to the Continuum: Opportunities for Mesoscale Science*

([https://science.energy.gov/~media/bes/pdf/reports/files/From\\_Quanta\\_to\\_the\\_Continuum\\_rpt.pdf](https://science.energy.gov/~media/bes/pdf/reports/files/From_Quanta_to_the_Continuum_rpt.pdf))

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

([https://science.energy.gov/~media/bes/besac/pdf/Reports/Challenges\\_at\\_the\\_Frontiers\\_of\\_Matter\\_and\\_Energy\\_rpt.pdf](https://science.energy.gov/~media/bes/besac/pdf/Reports/Challenges_at_the_Frontiers_of_Matter_and_Energy_rpt.pdf))

DOE Exascale Initiative (<https://energy.gov/downloads/doe-exascale-initiative>).

Basic Energy Sciences Roundtable on Opportunities for Basic Research for Next-Generation Quantum Systems (2018),

([https://science.energy.gov/~media/bes/pdf/reports/2018/Quantum\\_systems.pdf](https://science.energy.gov/~media/bes/pdf/reports/2018/Quantum_systems.pdf)).

*Previous CMS Awards:*

<https://science.energy.gov/bes/funding-opportunities/closed-foas/computational-materials-sciences-awards-2016-foa/>

*MGI 2014 Strategic Plan*

[https://www.mgi.gov/sites/default/files/documents/mgi\\_strategic\\_plan\\_-\\_dec\\_2014.pdf](https://www.mgi.gov/sites/default/files/documents/mgi_strategic_plan_-_dec_2014.pdf)

## **Open Science**

SC is dedicated to promoting the values of openness in Federally-supported scientific research, including, but not limited to, ensuring that research may be reproduced and that the results of Federally-supported research are made available to other researchers. These objectives may be met through any number of mechanisms including, but not limited to, data access plans, data sharing agreements, the use of archives and repositories, and the use of various licensing schemes.

The use of the phrase “open-source” does not refer to any particular licensing arrangement, but is to be understood as encompassing any arrangement that furthers the objective of openness.

## **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.

DOE will consider funding multi-institution collaborations under this FOA. Entities proposing as a team must designate a lead organization. Pre-applications 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 pre-application and one application is to be submitted for each team.

### **B. ESTIMATED FUNDING**

It is anticipated that up to \$24,000,000 (\$6,000,000 annually for up to 4-years) will be available under this FOA, contingent on satisfactory peer review and the availability of appropriated funds. Up to 8 awards are anticipated, with a mix of single PI/small group and larger team awards. Applicants should request project support for four years, with the release of out-year support contingent on adequate progress of the research.

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 two kinds of awards, Large team awards (usually multi-institutional) and Individual/small group awards (1 or a few investigators).

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

**Individual/Small Group Awards:** Ceiling: \$750,000 per year; Floor: \$200,000 per year

**Large Team Awards:** Ceiling: \$2,000,000 per year; Floor: \$750,000 per year

For Large Team renewal proposals, notwithstanding the “Floor” identified above, DOE may consider limited-term renewal awards to allow for the completion of research projects and orderly closeout of CMS awards that do not merit long-term continued support. Annual funding for such awards could fall below the \$750,000 floor.

#### **D. EXPECTED NUMBER OF AWARDS**

(See B. Estimated Funding Section above.)

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

#### **E. ANTICIPATED AWARD SIZE**

(See B. Estimated Funding Section and C. Maximum and Minimum Award Size 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.)

Research grant awards are expected to be made for a period of up to four years as befitting the project. For renewal proposals, DOE may consider limited-term renewal awards to allow for the completion of research projects and orderly closeout of CMS renewals that do not merit long-term continued support. The duration of such awards would not exceed two years.

Continuation funding (funding for the second and subsequent budget periods) is contingent on: (1) availability of funds appropriated by Congress and future year budget authority; (2) progress towards meeting the objectives of the approved application; (3) submission of required reports; and (4) compliance with the terms and conditions of the award.

#### **G. TYPE OF APPLICATION**

DOE will accept new and renewal applications under this FOA.

For renewal applications only, the Lead PI is required to submit a Renewal Proposal Products section through SC's PAMS website at <https://pamspublic.science.energy.gov>. The Lead PI must enter into PAMS each product created during the course of the previous project period. The publication date (MM/YYYY) should be included in the data for each publication. Types of products include publications, intellectual property, technologies or techniques, and other products such as databases or software. As soon as the renewal application is assigned to a program manager, the Lead PI will receive an automated email from PAMS (<[PAMS.Autoreply@science.doe.gov](mailto:PAMS.Autoreply@science.doe.gov)>) instructing him or her to navigate to the PAMS Task tab to complete and submit the Renewal Proposal Products. The submitted product list will be sent for merit review as part of the application. The application will not be considered complete and cannot be sent for review until the product list has been submitted.

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

For grant awards, the value of, and funding for team members employed by a DOE/National Nuclear Security Administration (NNSA) National Laboratory contractor, a non-DOE/NNSA Federally Funded Research and Development Center (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 a subaward 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 management and operating (M&O) contract, as applicable, in consultation between DOE and the prime awardee.

If a subaward 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 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.

A parallel, companion announcement (LAB 19-2040) is available for applications led by DOE laboratories, including DOE/NNSA FFRDC Contractors. DOE/NNSA National Laboratory Contractors may be proposed as subawards under a prime application submitted under this FOA.

Other Federal agencies and their FFRDC contractors are not eligible to submit applications as prime applicants under this FOA but may be proposed as subawards under a prime application submitted under this FOA.

Applicants that are not domestic organizations should be advised that:

- Individual applicants are unlikely to possess the skills, abilities, and resources required 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.

Applications from for-profit organizations that propose research related to current commercial activity may be declined without merit review.

#### ***DOE/NNSA National Laboratory Contractors***

DOE/NNSA National Laboratory Contractor applicants are not eligible for a prime award under this FOA, but may be proposed as a team member on another entity's application if their cognizant DOE/NNSA Contracting Officer provides written authorization. This authorization should be submitted with the application as part of the Budget Justification for DOE/NNSA National Laboratory Contractor File. [This is not required for the National Energy Technology Laboratory because it is a Government Owned/Government Operated (GOGO).] **Please note that failure to provide this authorization may result in rejection of an application prior to merit review.** If a DOE/NNSA National Laboratory Contractor is proposed as a team member, the proposed work will be authorized under the DOE field work authorization system or other appropriate process and performed under the laboratory Contractor's management and operating (M&O) contract, as applicable. The following wording is acceptable for the authorization:

“Authorization is granted for the \_\_\_\_\_ Laboratory to participate in the proposed project. The work proposed for the laboratory is consistent with or complementary to the missions of the laboratory and will not adversely impact execution of the DOE/NNSA assigned programs at the laboratory.”

### ***Non-DOE/NNSA Federal Agencies and their FFRDC Contractors***

Non-DOE/NNSA Federal agencies and their FFRDC contractors are not eligible for a prime award under this announcement, but may be proposed as a team member on another entity's application subject to the following guidelines:

The prime applicant must obtain written authorization for non-DOE/NNSA FFRDC participation. The cognizant Contracting Officer for the Federal agency sponsoring the FFRDC contractor must authorize in writing the participation of the FFRDC contractor on the proposed project and this authorization should be submitted with the application. The written authorization must also contain a determination that the use of a FFRDC contractor is consistent with the contractor's authority under its award and does not place the FFRDC contractor in direct competition with the private sector, in accordance with FAR Part 17.5. **Please note that failure to provide this authorization may result in rejection of an application prior to merit review.** The following wording is acceptable for the authorization:

“Authorization is granted for the \_\_\_\_\_ Laboratory to participate in the proposed project. The work proposed for the laboratory is consistent with or complementary to the missions of the laboratory and will not adversely impact execution of the (insert agency) assigned programs at the laboratory. This laboratory is authorized to perform the work proposed in the application submitted under DOE Funding Opportunity Announcement # DE-FOA-0002040 by the following statutory authority (insert statute name, citation, and section).”

### **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 Principal Investigator (PI) 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. LIMITATIONS ON SUBMISSIONS**

#### **Lead PI and Limitation on Number of Applications**

The Lead PI must be employed or have an agreement in place to be hired by the lead organization. **An individual may not be named as the Lead PI on more than one application.** If the proposed Lead PI will not be employed by the lead organization at the time of the award, 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 Lead PI, DOE will consider only the application (if any) that matches a

qualified Pre-Application (as described in Section IV.B.2). 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 co-PI (this is not the Lead PI).

## **Section IV – APPLICATION AND SUBMISSION INFORMATION**

### **A. ADDRESS TO REQUEST APPLICATION PACKAGE**

Application forms and instructions are available at grants.gov. To access these materials, go to <https://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-0002040) shown on the cover of this FOA and then follow the prompts to download the application package.

Applications submitted through [www.FedConnect.net](http://www.FedConnect.net) will not be accepted.

### **B. LETTER OF INTENT AND PRE-APPLICATION**

#### **1. Letter of Intent**

Not applicable.

#### **2. Pre-application**

**A pre-application is required from all applicants, both for new and for renewal applications.**

PRE-APPLICATION DUE DATE

**December 21, 2018 at 12:00 PM (noon) Eastern Time**

ENCOURAGE/DISOURAGE DATE

**January 18, 2019**

A pre-application must be submitted by **December 21, 2018 at 12:00 PM (noon) Eastern Time**. The pre-application must be submitted electronically through the DOE SC Portfolio Analysis and Management System (PAMS) website <https://pamspublic.science.energy.gov/>.

Entities proposing as a team must designate a lead organization. **Pre-applications must be submitted on behalf of the team members by the lead organization.** Pre-applications will be reviewed as outlined below. DOE will send a response by email to each applicant encouraging or discouraging the submission of an application by **January 18, 2019**. Applicants who have not received a response regarding the status of their pre-application by this date are responsible for contacting the program to confirm this status. **Only those applicants that receive notification from DOE encouraging a full application may submit full applications.** No other full applications will be considered.

**Note that an individual can serve as the Lead PI on only one pre-application.** In the event that two or more pre-applications are received with the same individual as the lead PI, the PAMS timestamp will be used to determine the eligible pre-application and all others will be disqualified.

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

Title of Pre-application  
Lead Principal Investigator Name, Job Title  
Institution  
Lead PI Phone Number, Lead PI Email Address  
Funding Opportunity Announcement Number: DE-FOA-0002040  
Type of Application: Single Investigator/Small Group or Large Team  
Estimated Annual Budget Request:  
Estimated Annual Budget Request by Institution:

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

**The information described below on participating investigators, collaborators, advisors and advisees is required and does not count towards the three page limit for the pre-application.** Failure to include this information will result in the pre-application being discouraged from submitting a full application.

1. On a separate page, the pre-application must include a list of the names and institutional affiliations of all participating investigators, including funded collaborators and consultants on the proposed project (one name per line with institutional affiliation, i.e., last name, first name, institution – no titles are needed).
2. On a separate page(s), for each funded individual, provide a list (one name per line with institutional affiliation, i.e., last name, first name, institution – no titles are needed) of collaborative investigators and co-authors of the past 48 months, co-editors of the past 24 months, past graduate and postdoctoral advisors/advisees, and close associations. **Do not include individuals from the investigator's home institution**, as these individuals would not be asked to review the application regardless of their engagement as a collaborator/co-author.

#### PRE-APPLICATION REVIEW

Federal Program Managers will evaluate all pre-applications to determine their responsiveness to the requirements of the FOA and their competitiveness within a scientific topic. The review will be based on the following criteria:

1. Responsiveness to the objectives of the FOA.
2. Scientific and technical merit.
3. Appropriateness of the proposed research approaches.
4. Likelihood of scientific impact.

The review will be conducted by no less than three federal program managers chosen for their topical knowledge and diversity of perspective. Reviews will be a comparative review with

priority given to scientifically innovative and forward-looking basic research with the highest likelihood of success as a full application. The results of the review will be documented.

Applicants with the highest rated pre-applications will be encouraged to submit full applications; others will be discouraged from submitting full applications. Upon request, feedback from the comparative review will be provided after the deadline for the receipt of applications.

SC is committed to ensuring that a sufficient number of applicants will be encouraged to submit applications to foster a competitive merit review of the applications. DOE expects to allow approximately 30 full proposals, with the exact number based on the review. The intent in discouraging submission of certain applications is to save the time and effort of applicants in preparing and submitting applications with a negligible likelihood of success.

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

#### PRE-APPLICATION SUBMISSION

It is important that the pre-application be a single file with extension .pdf, .docx, or .doc. The filename must not exceed 50 characters. The pre-application must be submitted electronically through the DOE SC Portfolio Analysis and Management System (PAMS) website <https://pamspublic.science.energy.gov/>. The PI and anyone submitting on behalf of the PI must register for an account in PAMS before it will be possible to submit a pre-application. All PIs and those submitting pre-applications on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays.

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

**Please see Section IV, Part I, 4., DOE SC Portfolio Analysis and Management System (PAMS), below, for instructions about how to register in PAMS.**

#### **Submit Your Pre-Application:**

- Create your pre-application (called a preproposal in PAMS) outside the system and save it as a file with extension .docx, .doc, or .pdf. Make a note of the location of the file on your computer so you can browse for it later from within PAMS.
- Log into PAMS and click the Proposals tab. Click the “View / Respond to Funding Opportunity Announcements” link and find the current announcement in the list. Click the “Actions/Views” link in the Options column next to this announcement to obtain a dropdown menu. Select “Submit Preproposal” from the dropdown.
- On the Submit Preproposal page, select the institution from which you are submitting this preproposal from the Institution dropdown. If you are associated with only one institution in the system, there will only be one institution in the dropdown.

- Note that you must select one and only one PI per preproposal; to do so, click the “Select PI” button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the “Actions” link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose “Select PI.”
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the “Invite PI” link at the top left of the “Select PI” screen. You can enter an optional personal message to the PI in the “Comments” box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the preproposal. Save the preproposal for later work by clicking the “Save” button at the bottom of the screen. It will be stored in “My Preproposals” for later editing.
- Enter a title for your preproposal.
- Select the appropriate technical contact from the Program Manager dropdown.
- To upload the preproposal file into PAMS, click the “Attach File” button at the far right side of the screen. Click the “Browse” (or “Choose File” depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the “Upload” button to upload the file.
- At the bottom of the screen, click the “Submit to DOE” button to save and submit the preproposal to DOE.
- Upon submission, the PI will receive an email from the PAMS system <[PAMS.Autoreply@science.doe.gov](mailto:PAMS.Autoreply@science.doe.gov)> acknowledging receipt of the preproposal.

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

**WARNING:** The PAMS website at <https://pamspublic.science.energy.gov> will permit you to edit a previously submitted pre-application in the time between your submission and the deadline. If you choose to edit, doing so will remove your previously submitted version from consideration. If you are still editing at the time of the deadline, you will not have a valid submission. Please pay attention to the deadline.

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](mailto:sc.pams-helpdesk@science.doe.gov). All submission and inquiries about this FOA should reference **DE-FOA-0002040**.

Pre-applications submitted outside PAMS will not be considered. Pre-applications may not be submitted through [grants.gov](http://grants.gov) or [www.FedConnect.net](http://www.FedConnect.net).

### **C. GRANTS.GOV APPLICATION SUBMISSION AND RECEIPT PROCEDURES**

This section provides the application submission and receipt instructions for applications to SC.

Please read the following instructions carefully and completely.

## **1. Electronic Delivery**

SC is participating in the Grants.gov initiative to provide the grant community with a single site to find and apply for grant funding opportunities. SC requires applicants to submit their applications online through Grants.gov.

## **2. How to Register to Apply through Grants.gov**

a. Instructions: Read the instructions below about registering to apply for SC funds. Applicants should read the registration instructions carefully and prepare the information requested before beginning the registration process. Reviewing and assembling the required information before beginning the registration process will alleviate last-minute searches for required information.

Organizations must have a Data Universal Numbering System (DUNS) Number, active System for Award Management (SAM) registration, and Grants.gov account to apply for grants. If individual applicants are eligible to apply for this funding opportunity, then you may begin with step 3, Create a Grants.gov Account, listed below.

Creating a Grants.gov account can be completed online in minutes, but DUNS and SAM registrations may take several weeks. Therefore, an organization's registration should be done in sufficient time to ensure it does not impact the entity's ability to meet required application submission deadlines.

Complete organization instructions can be found on Grants.gov here:

<https://www.grants.gov/web/grants/applicants/organization-registration.html>

1) *Obtain a DUNS Number*: All entities applying for funding, including renewal funding, must have a DUNS Number from Dun & Bradstreet (D&B). Applicants must enter the DUNS Number in the data entry field labeled "Organizational DUNS" on the SF-424 form. For more detailed instructions for obtaining a DUNS Number, refer to:

<https://www.grants.gov/web/grants/applicants/organization-registration/step-1-obtain-duns-number.html>

2) *Register with SAM*: All organizations applying online through Grants.gov must register with SAM at <https://www.sam.gov>. Failure to register with SAM will prevent your organization from applying through Grants.gov. SAM registration must be renewed annually. For more detailed instructions for registering with SAM, refer to:

<https://www.grants.gov/web/grants/applicants/organization-registration/step-2-register-with-sam.html>

3) *Create a Grants.gov Account*: The next step is to register an account with Grants.gov. Follow the on-screen instructions or refer to the detailed instructions here:

<https://www.grants.gov/web/grants/applicants/registration.html>

4) *Add a Profile to a Grants.gov Account:* A profile in Grants.gov corresponds to a single applicant organization the user represents (i.e., an applicant) or an individual applicant. If you work for or consult with multiple organizations and have a profile for each, you may log in to one Grants.gov account to access all of your grant applications. To add an organizational profile to your Grants.gov account, enter the DUNS Number for the organization in the DUNS field while adding a profile. For more detailed instructions about creating a profile on Grants.gov, refer to: <https://www.grants.gov/web/grants/applicants/registration/add-profile.html>

5) *EBiz POC Authorized Profile Roles:* After you register with Grants.gov and create an Organization Applicant Profile, the organization applicant's request for Grants.gov roles and access is sent to the EBiz POC. The EBiz POC will then log in to Grants.gov and authorize the appropriate roles, which may include the AOR role, thereby giving you permission to complete and submit applications on behalf of the organization. You will be able to submit your application online any time after you have been assigned the AOR role. For more detailed instructions about creating a profile on Grants.gov, refer to: <https://www.grants.gov/web/grants/applicants/registration/authorize-roles.html>

6) *Track Role Status:* To track your role request, refer to: <https://www.grants.gov/web/grants/applicants/registration/track-role-status.html>

b. *Electronic Signature:* When applications are submitted through Grants.gov, the name of the organization applicant with the AOR role that submitted the application is inserted into the signature line of the application, serving as the electronic signature. The EBiz POC **must** authorize people who are able to make legally binding commitments on behalf of the organization as a user with the AOR role; **this step is often missed and it is crucial for valid and timely submissions.**

### 3. How to Submit an Application to SC via Grants.gov

Grants.gov applicants can apply online using Workspace. Workspace is a shared, online environment where members of a grant team may simultaneously access and edit different webforms within an application. For each FOA, you can create individual instances of a workspace.

Below is an overview of applying on Grants.gov. For access to complete instructions on how to apply for opportunities, refer to:

<https://www.grants.gov/web/grants/applicants/apply-for-grants.html>

1) *Create a Workspace:* Creating a workspace allows you to complete it online and route it through your organization for review before submitting.

2) *Complete a Workspace:* Add participants to the workspace, complete all the required forms, and check for errors before submission.

a. *Adobe Reader:* If you decide not to apply by filling out webforms you can download individual PDF forms in Workspace so that they will appear similar to other Standard forms. The

individual PDF forms can be downloaded and saved to your local device storage, network drive(s), or external drives, then accessed through Adobe Reader.

NOTE: Visit the Adobe Software Compatibility page on Grants.gov to download the appropriate version of the software at: <https://www.grants.gov/web/grants/applicants/adobe-software-compatibility.html>

b. Mandatory Fields in Forms: In the forms, you will note fields marked with an asterisk and a different background color. These fields are mandatory fields that must be completed to successfully submit your application.

c. Complete SF-424 Fields First: The forms are designed to fill in common required fields across other forms, such as the applicant name, address, and DUNS number. To trigger this feature, an applicant must complete the SF-424 information first. Once it is completed, the information will transfer to the other forms.

3) Submit a Workspace: An application may be submitted through workspace by clicking the Sign and Submit button on the Manage Workspace page, under the Forms tab. Grants.gov recommends submitting your application package at least 24-48 hours prior to the close date to provide you with time to correct any potential technical issues that may disrupt the application submission.

4) Track a Workspace: After successfully submitting a workspace package, a Grants.gov Tracking Number (GRANTXXXXXXXX) is automatically assigned to the package. The number will be listed on the Confirmation page that is generated after submission.

For additional training resources, including video tutorials, refer to:  
<https://www.grants.gov/web/grants/applicants/applicant-training.html>

Applicant Support: Grants.gov provides applicants 24/7 support via the toll-free number 1-800-518-4726 and email at support@grants.gov. For questions related to the specific grant opportunity, contact the number listed in the application package of the grant you are applying for.

If you are experiencing difficulties with your submission, it is best to call the Grants.gov Support Center and get a ticket number. The Support Center ticket number will assist SC with tracking your issue and understanding background information on the issue.

#### **4. Timely Receipt Requirements and Proof of Timely Submission**

Proof of timely submission is automatically recorded by Grants.gov. An electronic date/time stamp is generated within the system when the application is successfully received by Grants.gov. The applicant AOR will receive an acknowledgement of receipt and a tracking number (GRANTXXXXXXXX) from Grants.gov with the successful transmission of their application. Applicant AORs will also receive the official date/time stamp and Grants.gov Tracking number in an email serving as proof of their timely submission.

When SC successfully retrieves the application from Grants.gov, and acknowledges the download of submissions, Grants.gov will provide an electronic acknowledgment of receipt of the application to the email address of the applicant with the AOR role. Again, proof of timely submission shall be the official date and time that Grants.gov receives your application. Applications received by Grants.gov after the established due date for the program will be considered late and may not be considered for funding by SC.

Applicants using slow internet, such as dial-up connections, should be aware that transmission can take some time before Grants.gov receives your application. Again, Grants.gov will provide either an error or a successfully received transmission in the form of an email sent to the applicant with the AOR role. The Grants.gov Support Center reports that some applicants end the transmission because they think that nothing is occurring during the transmission process. Please be patient and give the system time to process the application.

## **D. CONTENT AND APPLICATION FORMS**

### APPLICATION PREPARATION

You must submit the application through Grants.gov at <https://www.grants.gov/>, using either the online webforms or downloaded forms. (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 software compatibility page at <https://www.grants.gov/web/grants/applicants/adobe-software-compatibility.html>.

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 PDF files unless otherwise specified in this FOA. 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 the following restrictions that apply to the names of all files attached to your application:

- Please limit file names to 50 or fewer characters
- Do not attach any documents with the same name. All attachments must have a unique name.
- Please use only the following characters when naming your attachments: A-Z, a-z, 0-9, underscore, hyphen, space, period, parenthesis, curly braces, square brackets, ampersand, tilde, exclamation point, comma, semi colon, apostrophe, at sign, number sign, dollar sign, percent sign, plus sign, and equal sign. 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. Letters stating commitment to the project are required of any unfunded collaborator. Letters of organizational commitment are required for each organization participating as a team member (See Appendix 8: Organizational Letters of Commitment).

## RENEWAL APPLICATIONS

Renewal applications must be submitted from the institution that holds the current award. Changes in the Lead PI should be discussed with the program manager prior to submission of the renewal proposal.

For renewal applications only, the Lead PI is required to submit a Renewal Proposal Products section through the PAMS website at <https://pamspublic.science.energy.gov>. The Lead PI must enter into PAMS each product created during the course of the previous project period. The publication date (MM/YYYY) should be included in the data for each publication. Types of products include publications, intellectual property, technologies or techniques, and other products such as databases or software. As soon as the renewal application is assigned to a program manager, the Lead PI will receive an automated email from PAMS (<[PAMS.Autoreply@science.doe.gov](mailto:PAMS.Autoreply@science.doe.gov)>) instructing him or her to navigate to the PAMS Task tab to complete and submit the Renewal Proposal Products. The submitted product list will be sent for merit review as part of the application. The application will not be considered complete and cannot be sent for review until the product list has been submitted.

## RESUBMISSION OF APPLICATIONS

Applications submitted under this FOA may be withdrawn from consideration by using the PAMS website at <https://pamspublic.science.energy.gov>. Applications may be withdrawn at any time between when the applicant submits the application and when DOE makes the application available to merit reviewers. Such withdrawals take effect immediately and cannot be reversed. Please exercise due caution. After the application is made available to merit reviewers, the applicant may contact the DOE program office identified in this FOA to request that it be withdrawn.

After an application is withdrawn, it may be resubmitted, if this FOA is still open for the submission of applications. Such resubmissions will only count as one submission if this FOA restricts the number of applications from an applicant.

Note that there may be a delay between the application's submission in Grants.gov and when it is available to be withdrawn in PAMS. SC will usually consider the last submission, according to its Grants.gov timestamp, to be the intended version. Please consult with your program manager to resolve any confusion about which version of an application should be considered.

## IMPROPER CONTENTS OF APPLICATIONS

Applications submitted under this FOA will be stored in controlled-access systems, but they may be made publicly available if an award is made. As such, it is critical that applicants follow these guidelines:

- Do not include information subject to any legal restriction on its open distribution, whether classified, export control, or unclassified controlled nuclear information.
- Do not include sensitive and protected personally identifiable information, including social security numbers, birthdates, citizenship, marital status, or home addresses. Pay particular attention to the content of biographical sketches and curriculum vitae.
- Do not include letters of support from Federal officials.
- Do not include letters of support on Federal letterhead. Letters that are not letters of support (such as letters confirming access to sites, facilities, equipment, or data; or letters from cognizant contracting officers) may be on Federal letterhead.
- Clearly mark all proprietary or trade-secret information.

#### CHANGE OF AWARDEE INSTITUTION

If an awardee chooses to relinquish an award made under this FOA to permit the transfer of the award to a new institution, the new institution must submit an application under the then-available SC “annual” or “open” FOA.

#### 1. SF-424 (R&R)

Complete this form first to populate data in other forms. Complete all the required fields in accordance with the pop-up instructions on the form. The list of certifications and assurances referenced in Field 17 is available on the DOE Financial Assistance Forms Page at <https://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 Employer Identification Number (EIN) 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.
- SC does not use the twelve-digit EIN format required by some other agencies.
- SC does not use the DUNS+4 format.

#### 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.

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.

## 2. Research and Related Other Project Information

### **Note regarding question 4.a. and 4.b.:**

If any environmental impact, positive or negative, is anticipated, indicate “yes” in response to question 4.a., “potential impact – positive or negative - on the environment.” Disclosure of the impact should be provided in response to question 4.b. First indicate whether the impact is positive or negative and then identify the area of concern (e.g., air, water, exposure to radiation, etc.). Should the applicant have any uncertainty, they should check “yes.”

DOE understands the phrase in field 4.a., “potential impact ... negative” to apply if the work described in the application could potentially have any of the impacts listed in (1) through (5) of 10 CFR 1021, Appendix B, Conditions that Are Integral Elements of the Classes of Action in Appendix B. (<http://www.ecfr.gov>)

Additionally, for actions which could have any other adverse impacts to the environment or have any possibility for adverse impacts to human health (e.g., use of human subjects, Biosafety Level 3-4 laboratory construction/operation, manufacture or use of certain nanoscale materials which are known to impact human health, or any activities involving transuranic or high level radioactive waste, or use of or exposure to any radioactive materials beyond de minimis levels), applicants should indicate a “negative” impact on the environment.

Lastly, 1) if there would be extraordinary circumstances (i.e., scientific or public controversy) related to the significance of environmental effects (10 CFR 1021.410 (b)(2)), 2) if the work is connected to other actions with potentially significant impacts (10 CFR 1021.410 (b)(3)), or 3) if the work is related to other nearby actions with the potential for cumulatively significant impacts (10 CFR 1021.410 (b)(3)), applicants should indicate a “negative” impact on the environment.

Complete questions in fields 1 through 6 of the SF-424(R&R) form 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 project title, name of the applicant (Lead PI), the PIs, 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:

<p>A Really Great Idea</p> <p>A. Smith, Lead Institution (Lead Principal Investigator) A. Brown, Institution (Principal Investigator) A. Jones, Institution (Principal Investigator)</p> <p>Text of abstract</p>
--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------

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.”

If an application is recommended for award, the project summary will be used in preparing a public abstract about the award. Award abstracts and titles form a Government document that describes the project and justifies the expenditure of Federal funds in light of the DOE and SC mission statements at <https://energy.gov/mission> and <https://science.energy.gov/about/>.

- 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 must 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-0002040
- DOE/SC Program Office: Basic Energy Sciences
- DOE/SC Program Office Technical Contact: James Davenport
- DOE Award Number (if Renewal Application):
- PAMS Preproposal (Pre-application) tracking number:
- Type of Application: Single Investigator/small group OR Large team

The lead applicant/awardee/recipient/organization must be the same as on the required pre-application. **If an application is received for which the lead organization has changed since submission of the pre-application, then the application will be deemed non-responsive and will be rejected without further review.** The Lead PI should not be changed unless unavoidable (discuss with the program manager) and only minor edits should be made, if

necessary, to the title.

On separate pages, also not counted towards the page limitation for the narrative, as a supplement to the cover page, include

1. A list of all principal investigators with institution (postdoctoral staff and support staff need not be listed by name)
2. A table that lists the budget allocated to all partner institutions. Provide the total costs of the budget request in each year for each institution and totals for all rows and columns. **If an application is received in which the lead organization 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.**

**Important Instructions to the Sponsored Research Office of Submitting Institutions:** SC requires that you create one single PDF file that contains the DOE Cover Page, project narrative, biographical sketch, current and pending support, bibliography and references cited, facilities and other resources, equipment, data management plan, and other attachments. This single PDF file must be attached in Field 8 on the Grants.gov form. Do not attach any of the items listed in this paragraph separately in any other field in Grants.gov. If you do, these additional attachments will not become part of the application in PAMS.

PROJECT NARRATIVE (FIELD 8 ON THE FORM)

The project narrative **must not exceed 30 pages for Large Team applications and must not exceed 20 pages for Single Investigator/Small Group applications.** The narrative should provide technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard 8.5” by 11” paper with 1 inch margins (top, bottom, left, and right). The font must not be smaller than 11 point. Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph. This page limit does not apply to the Cover Page and the associated principal investigator list and budget summary table; detailed Budget Page(s), Budget Justification, biographical material, publications and references, and appendices, each of which may have its own page limit.

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 Section VIII, Part D for instructions on how to mark proprietary application information. To attach a Project Narrative, click “Add Attachment.”

The Project Narrative comprises the research plan for the project. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the method to be used. It should also include a timeline for the major activities of the proposed project, and should indicate which project personnel will be responsible for which activities. There should be no ambiguity about which personnel will perform particular parts of the project,

and the time at which these activities will take place.

**Research Focus:** Applications must address predictive design of functional materials, excluding cold atoms, structural materials, isolated molecules, ionic liquids, and catalysts. Applications must propose research that leads to open source software, excluding density functional methods as currently implemented; applications related to this topic will not be reviewed. Applications must provide a plan for full utilization of today's petascale and pre-exascale, and tomorrow's exascale leadership class computing.

**Background/Introduction:** Explanation of the importance and relevance of the proposed work as well as a review of the relevant literature.

- Briefly sketch the background, 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 principal 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, Lead PI, and, as appropriate, other principal investigators.
- **Renewal applications:** This section must include a summary of the research performed in the prior award period. Note that a listing of the papers, software releases, and other research products is requested as Appendix 9.

**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 how the proposed research will include development of software that will fully exploit the capabilities of today's petascale and pre-exascale, and tomorrow's exascale leadership computing facilities;
- Describe the role and intellectual contribution of the Lead PI, and, as appropriate, other PIs 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;
- For Large team applications:
  - Describe the plan and process that will be used to generate, verify, validate, and utilize computational and experimental data; and
  - Describe how the software will be verified and experimentally validated and the role of the experimental component of the proposed research.

**Management Plan: Required for Large Team applications.** 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 Lead PI and other PIs, including discussion of their potential involvement in other major projects; and
- 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.

**Project Performance Site(s): Required for teams involving more than one institution.** Identify and describe the site(s) where the work will be performed. 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.

**Do not attach any of the requested appendices described below as files for fields 9, 10, 11, and 12 in Grants.gov. Follow the below instructions to include the information as appendices in the single, bundled project narrative file.**

## APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the Lead PI and other PIs listed in Section A on the R&R Budget form.

As part of the sketch, provide information that can be used by reviewers to evaluate the PI's potential for leadership within the scientific community. Examples of information of interest are invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society activities, special international or industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences.

- 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 must not exceed 2 pages when printed on 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include:

The biographical information (curriculum vitae) must include the following items within its page limit:

- **Education and Training:** Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.
- **Research and Professional Experience:** Beginning with the current position list, in chronological order, professional/academic positions with a brief description.
- **Publications:** Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications. An abbreviated style such as the Physical Review Letters (PRL) convention for citations (list only the first author) may be used for publications with more than 10 authors.
- **Synergistic Activities:** List no more than 5 professional and scholarly activities related to the effort proposed.

In addition, DOE requires information to identify individuals who are conflicted with or potentially biased (favorably or unfavorably) against the investigators. Include this information in Appendix 10 as a single list for all PIs.

**Personally Identifiable Information:** Do not include sensitive and protected personally identifiable information including social security numbers, birthdates, citizenship, marital status, or home addresses. Do not include information that a merit reviewer should not make use of.

## APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support (both Federal and non-Federal) for the 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 lead PI 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 total cost or value of funds supporting the individual submitting the current and pending support
- The award period (start date – end date).
- The person-months of effort per year being dedicated to the award or activity
- Briefly describe the research being performed and explicitly identify any overlaps or synergies with the proposed research.

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 & 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, Computer, Office, and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. For proposed investigations requiring access to experimental or computational user facilities maintained by institutions other than the applicant, please summarize the plans for accessing these capabilities and past experience with these or similar facilities.

Please provide the Facility and Other Resource information as an appendix to your project narrative.

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

#### APPENDIX 5: EQUIPMENT

List major items of equipment already available for this project and, if appropriate identify location and pertinent capabilities. Provide the Equipment information as an appendix to your project narrative.

- Do not attach a separate file.
- 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 (<https://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 at <https://science.energy.gov/user-facilities/>.

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 SC research proposal merit review process. Applicants are encouraged to consult the SC website for further information and suggestions for how to structure a DMP: <https://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.
- This appendix will not count in the project narrative page limitation.

## APPENDIX 8: ORGANIZATIONAL LETTERS OF COMMITMENT

If applicable, 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, must be specific to the application, and must be signed by a person authorized to commit the participating organization to a legally binding agreement for this project. (For DOE National Laboratories, the person authorized to legally commit the institution to participate in the proposal will be a senior laboratory official. If this letter is signed by a person who is not authorized to commit the national lab to the research, the application will be declined without peer review.)

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

## APPENDIX 9: RENEWAL APPLICATIONS

For renewal applications, a list of the published journal papers, software releases, and other research products from the prior award period should be included as an appendix. For convenience of the reviews, journal papers should be separated into two groups, those intellectually led by the grant and those for which the journal paper was collaborative with other funded activities. The PIs names should be highlighted in the listing for each paper.

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

## APPENDIX 10: LIST OF COLLABORATORS

To identify potential conflicts of interest or bias in selection of reviewers, for all PIs on the proposal, please provide a **single list in alphabetical order (last name, first name, institution – do not include titles or roles)** of potential conflicts. Do NOT include anyone from a partner institution since reviewers would NOT be considered from these institutions. Include:

- All persons who are, or who have been, collaborators or co-authors of papers, book or book articles, reports, or abstracts, 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 PI interacted on a regular basis while the research was being done.
- Include any individuals who are currently, or have been, co-editors with any PI on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of this application.
- Include graduate and postdoctoral advisors and past advisees, including the names and current organizational affiliations of the PIs' graduate advisor(s) and principal postdoctoral sponsor(s) as well as the names and current organizational affiliations of past graduate students and postdoctoral associates.

## 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.
- **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 Section IV, Part G).

The following advice will improve the accuracy of your budget request:

- Funds requested for personnel (senior, key, and other) must be justified as the product of their effort on the project and their institutional base salary.
- Funds requested for fringe benefits must be calculated as the product of the requested salary and, if present, the negotiated fringe benefit rate contained in an institution’s negotiated indirect cost rate agreement.
- Funds requested for indirect costs must be calculated using the correct indirect cost base and the negotiated indirect cost rate.
- You are encouraged to include the rate agreement used in preparing a budget as a part of the budget justification.

If you are proposing indirect costs and do not already have an Indirect Cost Rate Agreement with your Cognizant Federal Agency or documentation of rates accepted for estimating purposes by DOE or another Federal agency, it is recommended that you begin preparing an Indirect Cost Rate Proposal to be submitted, upon request, to the DOE contract specialist/grants management specialist who will evaluate your application if you are selected for award.

For your convenience in preparing an Indirect Cost Rate proposal, a link to applicant resources, including indirect rate model templates, has been provided below:

Budget Fields

Section A Senior/Key Person	For each Senior/Key Person (i.e., principal investigators), 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 <b>each</b> item of equipment separately and justify each in the budget justification section. Do not aggregate items of equipment. Allowable items ordinarily will be limited to research equipment and apparatus not already available for the conduct of the work. General-purpose office equipment is not eligible for support unless primarily or exclusively used in the actual conduct of scientific research.
Section D Travel	For purposes of this section only, travel to Canada or to Mexico is considered domestic travel. In the budget justification, list each trip's destination, dates, estimated costs including transportation and subsistence, number of staff traveling, the purpose of the travel, and how it relates to the project. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). To qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results. Domestic travel is to be justified separately from foreign travel.
Section E Participant/Trainee Support Costs	If applicable, submit training support costs. Educational projects that intend to support trainees (precollege, college, graduate and post graduate) must list each trainee cost that includes stipend levels and amounts, cost of tuition for each trainee, cost of any travel (provide the same information as needed under the regular travel category), and costs for any related training expenses. Participant costs are those costs associated with conferences, workshops, symposia or institutes and breakout items should indicate the number of participants, cost for each participant, purpose of the conference, dates and places of meetings and

	<p>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"> <li>• <b>Materials and Supplies:</b> 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).</li> <li>• <b>Publication Costs:</b> Enter the total publication funds requested. The proposal budget may request funds for the costs of documenting, preparing, publishing or otherwise making available to others the findings and products of the work conducted under the award. In the budget justification, include supporting information. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).</li> <li>• <b>Consultant Services:</b> Enter total funds requested for all consultant services. In the budget justification, identify each consultant, the services he/she will perform, total number of days, travel costs, and total estimated costs. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).</li> <li>• <b>ADP/Computer Services:</b> Enter total funds requested for ADP/Computer Services. The cost of computer services, including computer-based retrieval of scientific, technical and education information may be requested. In the budget justification, include the established computer service rates at the proposing organization if applicable. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).</li> <li>• <b>Subawards/Consortium/Contractual Costs:</b> Enter total costs for all subawards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details.</li> <li>• <b>Equipment or Facility Rental/User Fees:</b> Enter total funds requested for Equipment or Facility Rental/User Fees. In the budget justification, identify each rental/user fee and justify. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).</li> <li>• <b>Alterations and Renovations:</b> Enter total funds requested for Alterations and Renovations. In the budget justification, itemize by category and justify the costs of alterations and renovations,</li> </ul>

	<p>including repairs, painting, removal or installation of partitions, shielding, or air conditioning. Where applicable, provide the square footage and costs.</p> <ul style="list-style-type: none"> <li>• <b>Other:</b> Add text to describe any other Direct Costs not requested above. Enter costs associated with “Other” item(s). Use the budget justification to further itemize and justify.</li> </ul>
Section G 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 L 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 L.** The file automatically carries over to each budget year.

You may wish to include the indirect cost rate agreement as a part of the budget justification.

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

**Budgets for Subawardees:** 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 either e-mail it to each subawardee that is required to submit a separate budget or use the collaborative features of Workspace. After the subawardee has either e-mailed its completed budget back to you or completed it within Workspace, 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 must 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 L.

Applicants should consult their local information technology (“IT”) support resources for any necessary assistance in converting the forms downloaded from Grants.gov into plain PDF files that can be combined into one non-Portfolio PDF file (the Budget Justification).

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.

Note: If an application proposes subawards to a DOE National Laboratory, a Federal agency, or another Federal agency’s FFRDC, the value of such proposed subawards will be deducted from any resulting award: Those classes of organizations must be paid directly by SC. However, the details of such proposed budgets are an essential for understanding and analyzing the proposed research.

**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:

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

**E. 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

Applicants that are not institutions of higher education, that request indirect costs, and that do not already have an Indirect Cost Rate Agreement with their Cognizant Federal Agency or documentation of rates accepted for estimating purposes by DOE or another Federal agency, are advised to begin preparing an Indirect Cost Rate Proposal for submission, upon request, to the DOE contract specialist/grants management specialist who will evaluate your application if you are selected for award.

## **F. SUBMISSION DATES AND TIMES**

### **1. Letter of Intent Due Date**

Not applicable

### **2. Pre-application Due Date**

December 21, 2018 at 12:00 PM (noon) Eastern Time

You are encouraged to submit your pre-application well before the deadline.

### **3. Application Due Date**

February 28, 2019 at 5:00 PM Eastern Time

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

### **4. Late Submissions**

Delays in submitting 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.

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 FOA to discuss the option of a late submission. Contacting the Program Office/Manager after the deadline may reduce the likelihood that a request will be granted. DOE notes that not all requests for late submission will be approved.

## **G. INTERGOVERNMENTAL REVIEW**

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

## **H. FUNDING RESTRICTIONS**

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

**Cost Principles:** Costs must be allowable, allocable and reasonable in accordance with the applicable Federal cost principles referenced in 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.

## **I. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS**

### **1. Systems to Register In**

Applicants must complete a series of registrations and enrollments to submit applications in response to this FOA. Applicants not currently registered with SAM and grants.gov should allow **at least 4 weeks** to complete these requirements.

You should start the process as soon as possible.

You may not be able to use your preferred Internet browser: Each system has its own requirements.

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

Applicants must register with SAM at <https://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.pdf](https://www.sam.gov/sam/transcript/Quick_Guide_for_Grants_Registrations.pdf). SAM maintains a complete user guide at [https://www.sam.gov/sam/SAM\\_Guide/SAM\\_User\\_Guide.htm](https://www.sam.gov/sam/SAM_Guide/SAM_User_Guide.htm).

Applicants must provide a Taxpayer Identification Number (TIN) to complete their registration in SAM.gov. An applicant's TIN is an 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 <https://www.irs.gov/businesses/small-businesses-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 IRS using the website listed above.

Applicants must register with FedConnect at [www.fedconnect.net](http://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.fhrs.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, following the instructions at <https://www.grants.gov/web/grants/applicants/registration.html>.

## **3. Where to Submit an Application**

You must submit the application through Grants.gov at <https://www.grants.gov/>, using either the online webforms or downloaded forms. (Additional instructions are provided in Section IV A of this FOA.)

Submit electronic applications through the "Apply for Grants" function at [www.grants.gov](http://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](mailto: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 SC 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 SC. 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](mailto: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 SC 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](mailto:sc.pams-helpdesk@science.doe.gov). All submission and inquiries about this FOA should reference DE-FOA-0002040.

## 5. Viewing Submitted Applications

Each grants.gov application submitted to the DOE 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 PI (Block 14), Authorized Representative (Block 19), and Point of Contact (Block 5). In PAMS notation, applications are known as proposals, the PI 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 SC 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 SC 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 SC 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](mailto:sc.pams-helpdesk@science.doe.gov). All submissions and inquiries about this FOA should reference **DE-FOA-0002040**.

## **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 applications focused on cold atoms, structural materials, isolated molecules, ionic liquids, and catalysts will be considered non-responsive. Research that emphasizes density functional methods as currently implemented will be considered non-responsive. All applications MUST have an encouraged pre-application and must be submitted by the same institution that submitted the pre-application. All applications must have a Data Management Plan and Open Source Software Distribution Plan. Applications that do not provide a detailed plan for the full utilization of petascale, pre-exascale, and future exascale leadership class computing facilities will be considered non-responsive. Large team awards without a management plan will be considered non-responsive. Applications for which the lead institution does not receive the largest percentage of funding compared to partnering institutions will be considered non-responsive.

#### **2. Merit Review Criteria**

Applications will be subjected to scientific merit review (peer review) and will be evaluated in accordance with 10 CFR 605.10(d), the Office of Science Financial Assistance Program Rule. The application will be evaluated against the following criteria, the first five of which will be weighted more heavily than the final two. The first four criteria are of equal value with each other. The fifth criteria applies only to Large Team proposals, and will be weighed equally with the first four criteria. 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.

1. Scientific and/or Technical Merit of the Project;
2. Appropriateness of the Proposed Method or Approach;
3. Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
4. Reasonableness and Appropriateness of the Proposed Budget.
5. Strength of the Management Plan – Large Team proposals only
6. Synergy Among the PIs, including Cohesion and Integration of the Research and Software Development Activities
7. Development and Utilization of Unique Facilities, Capabilities or Approaches

Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

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

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

- What new capability/functionality will the proposed software provide to the materials research community? How will the research plan attain the 4-year research and software/data goals?
- Comment on the novelty and scientific value of the proposed research.
- How widespread would be the interest in the software within the materials research community?
- How does the proposed work compare with other efforts in its field, both in terms of scientific and/or technical merit and originality?
- For renewal applications, comment on the progress and impact for the first award period.

#### APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

- Comment on the balance among scientific research, software development and community outreach.
- Describe and assess the plans for verification and experimental validation.
- How does the applicant recognize significant potential problems and consider alternative strategies?

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

- Assess the record of research accomplishments and computational/experimental skills of the Lead PI and team members (if appropriate).
- Comment on experience/expertise of the PIs and institutions in the development and maintenance of community research codes and data

#### REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET

- Comment on the appropriateness of the proposed budget and the distribution of the funds/staffing among research tasks/themes, software development, and PIs/institution (if applicable).

#### STRENGTH OF THE MANAGEMENT PLAN – Large Team applications only

- Assess the management plan, including the description of the roles/responsibilities of the PIs, plans for communication and integration of the team, and experience of the Lead PI in managing similar sized teams.
- Assess the time available for the Lead PI.
- How will the community be engaged in software development and distribution?
- How will the advisory committee (which is required) be engaged to provide oversight and guidance for the research.
- Are there any concerns regarding the ES&H or QA plans?

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

- Comment on how the applicant’s approach addresses the scientific and software development goals in an integrated and coherent manner.
- Team applications: Comment on the likelihood that the proposed team will work together in a cohesive and integrated manner.

#### DEVELOPMENT AND UTILIZATION OF UNIQUE FACILITIES, CAPABILITIES, OR APPROACHES

- How will the team utilize current petascale, pre-exascale and future exascale computing facilities?
- Assess the quality and appropriateness of the Data Management Plan and Open Source Software Distribution Plan.

### **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: <https://science.energy.gov/grants/policy-and-guidance/merit-review-system/>.

#### **2. Program Policy Factors**

The Selection Official may consider any of the following program policy factors in making the selection, listed in no order of significance:

- Availability of funds
- Relevance of the proposed activity to SC-BES priorities
- Ensuring an appropriate balance and diversity for activities within SC-BES programs
- Performance under current awards
- Commitment to sharing the results of research and managing open source software for broad community access
- 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
- Potential for developing synergies between the proposed project and other ongoing BES research activities, 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

### **3. Selection**

The Selection Official will consider the findings of the merit review and may consider any of the Program Policy Factors described above.

### **4. 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.

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.

#### **REPORTING OF MATTERS RELATED TO RECIPIENT INTEGRITY AND PERFORMANCE (DECEMBER 2015)**

DOE, prior to making a Federal award with a total amount of Federal share greater than the simplified acquisition threshold, is required to review and consider any information about the applicant that is in the designated integrity and performance system accessible through SAM (currently FAPIIS) (see 41 U.S.C. 2313); The applicant, at its option, may review information in the designated integrity and performance systems accessible through SAM and comment on any information about itself that a Federal awarding agency previously entered and is currently in the designated integrity and performance system accessible through SAM; DOE will consider any written comments by the applicant, in addition to the other information in the designated integrity and performance system, in making a judgment about the applicant's integrity, business ethics, and record of performance under Federal awards when completing the review of risk posed by applicants as described in §200.205 Federal awarding agency review of risk posed by applicants.

### **5. 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 2019. It is expected that awards will be made in Fiscal Year 2019.

## **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 Section IV, Part 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; (7) General Terms and Conditions; and (8) Federal Assistance Reporting Checklist, which identifies the reporting requirements.

Research awards made under this funding opportunity will be subject to the government-wide Research Terms and Conditions published at [https://www.nsf.gov/pubs/policydocs/rtc/rtcoverlay\\_march17.pdf](https://www.nsf.gov/pubs/policydocs/rtc/rtcoverlay_march17.pdf) and the DOE Agency Specific Standard Research Terms and Conditions published at [https://www.nsf.gov/pubs/policydocs/rtc/agencyspecifics/doe\\_417.pdf](https://www.nsf.gov/pubs/policydocs/rtc/agencyspecifics/doe_417.pdf). These Terms and Conditions will be incorporated in the award by reference.

### **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).

#### **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: <https://www.ecfr.gov>). Prime awardees must keep their data in SAM current at <https://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: <https://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 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 <https://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:

<https://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 <https://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms> under Award Terms.

## **4. Statement of Substantial Involvement**

Not applicable.

## **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 FOA. Publications and other methods of public communication describing any work based on or developed under an award resulting from this FOA must contain an acknowledgment of SC support. The format for such acknowledgments is provided at <https://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 (OSTI) 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 <https://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](mailto: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](mailto:sc.pams-helpdesk@science.doe.gov). All submission and inquiries about this FOA should reference **DE-FOA-0002040**.

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) <a href="mailto:support@grants.gov">support@grants.gov</a>
PAMS Customer Support	855-818-1846 (toll-free) 301-903-9610 <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>
Program Manager Scientific Contact	James Davenport, 301-903-0035 <a href="mailto:james.davenport@science.doe.gov">james.davenport@science.doe.gov</a>

## **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 <https://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 <https://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.

## **J. ENVIRONMENTAL, SAFETY AND HEALTH (ES&H) PERFORMANCE OF WORK AT DOE FACILITIES**

With respect to the performance of any portion of the work under this award which is performed at a DOE-owned or controlled site, the recipient agrees to comply with all state and Federal ES&H regulations, and with all other ES&H requirements of the operator of such site.

Prior to the performance on any work at a DOE-Owned or controlled site, the recipient shall contact the site facility manager for information on DOE and site specific ES&H requirements.

The recipient shall apply this provision to all subawardees at any tier.

## **K. FEDERAL, STATE, AND LOCAL REQUIREMENTS**

With respect to the performance of any portion of the work under this award, the recipient agrees to comply with all applicable local, state, and Federal ES&H regulations. The recipient shall apply this provision to all sub awardees at any tier.

## **L. NATIONAL ENVIRONMENTAL POLICY ACT (NEPA) COMPLIANCE**

If question 4.a. on the "Research and Related Other Project Information" document indicates "potential impact on the environment", or if DOE's own review indicates it, DOE may ask the applicant to provide additional information on those impacts in order to prepare an environmental critique/synopsis per 10 CFR 1021.216. Note that this pre-award environmental critique/synopsis process would be separate from the preparation of a NEPA document such as an environmental impact statement (EIS) or an environmental assessment (EA). If DOE determines the latter documentation is necessary, this process would need to be completed, funded by and with the participation of the awardee, prior to them taking any action on the proposed project that could have adverse environmental effects or that could limit the choice of reasonable alternatives. The inability to satisfy the NEPA requirements after an award would result in cancellation of the award. Note that in most cases, even where potential impact on the environment exists, preparation of such NEPA documents is rarely necessary, but DOE has the expectation that the Applicant will disclose the potential, which would serve to initiate dialog with DOE if necessary. Should the applicant have any uncertainty, they should check "yes."