

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



COMPUTATIONAL CHEMICAL SCIENCES RESEARCH

**FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER:
DE-FOA-0001912**

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Submission Deadline for Letters of Intent:	May 16, 2018 at 5 PM Eastern Time A Letter of Intent is Required
Submission Deadline for Pre-Applications:	Not Applicable
Submission Deadline for Applications:	June 18, 2018 at 5 PM Eastern Time

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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 letters of intent and applications well before the deadline.

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 Portfolio Analysis and Management System (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>.

DATA MANAGEMENT PLAN

Applications submitted under this Funding Opportunity Announcement (FOA) are subject to the SC Statement on Digital Data Management, published at <https://science.energy.gov/funding-opportunities/digital-data-management/>. Compliance with this statement is detailed in Section 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:

Scientific Program Contact:

Dr. Mark R. Pederson, Basic Energy Sciences (BES), Chemical Sciences, Geosciences,
and Biosciences (CSGB) Division
PHONE: (301)-903-9956
Mark.Pederson@science.doe.gov

STATUTORY AUTHORITY

Public Law 95-91, U.S. 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, SC Financial Assistance Program Rule, codified at 10 CFR 605

SUMMARY

The DOE SC program in Basic Energy Sciences (BES) announces its interest in receiving applications from single principal investigators (PIs), small groups (2-3 PIs), and centers (integrated multidisciplinary teams typically from multiple institutions) in Computational Chemical Sciences (CCS). CCS will support efforts to develop validated, public access codes and databases, and research to develop new approaches to enhance the use of large data sets for deriving new fundamental knowledge from calculations and advanced characterization of chemical systems. CCS will continue to support the DOE Exascale Computing Initiative (ECI), which was announced in September 2013. The ECI aims to accelerate the research and development needed to overcome key exascale challenges and maximize benefits of high-performance computing. This FOA continues the BES commitment to ECI by developing open source codes that can take full advantage of today's petascale and future exascale leadership computing facilities.

SUPPLEMENTARY INFORMATION

BES Mission and Objectives

The mission of the BES program is to support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security. BES also supports world-class, open-access scientific user

facilities consisting of a complementary set of intense x-ray sources, neutron sources, and research centers for nanoscale science.

Further information about BES programs can be found at:

Chemical Sciences, Geosciences, and Biosciences: <https://science.energy.gov/bes/csgb/>

Materials Sciences and Engineering: <https://science.energy.gov/bes/mse/>

Background

Software solutions and infrastructure provide the enabling tools for an effective scientific strategy to address the nation's energy challenges. BES-supported activities are entering a new era in which chemical reactions and molecular systems can be controlled and matter can be built with atom-by-atom precision. At the foundation of this new era are computational models that can accurately predict the behavior of molecules and materials based on theoretical calculations prior to their experimental synthesis. CCS will leverage U.S. leadership in computational chemistry codes in preparation for exascale computing. A systematic effort to modify or replace existing computational chemistry codes with codes well-adapted to anticipated exascale architectures is essential for the U.S. to compete in this high impact area. These codes will enable high-fidelity simulations to inform models for the improvement and acceleration of research, design, demonstration, and deployment phases of the energy innovation cycle. Open source and commercial codes have established U.S. dominance in computational chemistry. However, that dominance is being challenged with the transition to predominantly massively parallel high-performance computing platforms. Many of today's best chemical simulation codes are currently unable to use efficiently more than one percent of the processors available on existing leadership-class supercomputers. While recent breakthroughs in computational chemistry provide a strong foundation for future success, coordinated single-investigator, small-group and center efforts are crucial to modify or replace existing computational chemistry codes with codes that are well-adapted to current petascale and anticipated exascale architectures.

The CCS activity will support basic research to produce open source codes that design chemical and molecular processes and assemblies, including codes that take full advantage of the future generation of exascale leadership computing capabilities. The report from the foundational workshop for this activity, [Computational Materials Science and Chemistry](#) (2010), and the follow-on community-based workshops that occurred in 2011–2015, such as the [BES Computing and Data Requirements in the Exascale Age](#), identified a number of applications that could effectively utilize future exascale computing resources.

The CCS effort will deploy new, advanced capabilities in major open source chemical-simulation software used by the community to take advantage of gains in massively parallel computing platforms and systematically alleviate the need to employ semi-empirical case-by-case corrections. CCS will also support the design of algorithms to efficiently implement data-science approaches such as machine and deep learning on exascale computers. The goal of data-science efforts must be to advance the state-of-the-art capabilities from data curation and analysis to data-based discovery of new fundamental knowledge. These complex challenges will require coordinated research efforts, as described in foundational reports (see references section), that combine theoretical, computational and algorithmic advances with a goal of increasing by at

least 1,000 times the speed of accurate molecular and chemical design. Open source modular software tools will be developed that can be reused as plug-and-compute tools for the basic energy sciences community in preparation for the arrival of exascale computing facilities and for the optimized usage of existing petascale computers, augmenting U.S. leadership in the development of computational chemistry codes. This FOA is the second solicitation for proposals to support CCS.

Additional Information:

There is a separate Program Announcement to the DOE National Laboratories for proposals led by a DOE National Laboratory (See LAB 18-1912 in the PAMS website at <https://pamspublic.science.energy.gov>.) Multi-institutional team applications must be submitted by a single, lead institution. Collaborative proposals submitted in parallel by multiple institutions will not be accepted for this FOA. See Section III, D. for additional requirements for multi-institutional applications.

Note that only one application per entity, as lead organization, is permitted.

SUMMARY CRITERIA

To be considered, an application must meet the eligibility requirements in Section III and address the review criteria in Section V. In addition, an application must:

- Focus on development of open source, community-based codes that can be deployed on current petascale and future exascale computers to model systems of relevance to the BES mission, specifically those related to chemical sciences, geosciences, and biosciences.
- Focus on research leading to open source software for description of chemical and molecular processes. Suitable types of software will emphasize strong correlations, excited states, transport, dynamics, and/or electronic or optical properties, or will accurately describe the performance of molecule-based quantum-information systems that are based upon high-fidelity processing of light, charge or spin. Explicitly excluded are proposals that are limited to use of existing quantum-based methods in their traditional regimes of application. Efforts aimed at extending currently attainable length/time scales or increasing attention to complexity and that algorithmically match efficiency enhancements offered by next generation computers will receive priority.
- Describe a plan to deliver validated research codes and the associated data to academia, National Laboratories, and industry. Software developed under this FOA should have broad applicability. All efforts should describe how their efforts will develop and deploy modular capabilities. Center efforts must also describe how their plan to distribute the software as open source.
- Provide a detailed plan for the full utilization of today's petascale and tomorrow's exascale national leadership computing facilities.

Research and methodological developments appropriate for this FOA include but are not limited to:

- General quantum-mechanically implicitly or explicitly informed methods for improving the description of BES-relevant solvents and solute-solvent interactions.
- Fundamentally improved methods for predicting energetically efficient, field-driven control of chemical, electronic, magnetic and spin-dependent processes.
- Approaches to account for competing dissipative mechanisms or quantitatively predict the onset or effects of decoherence or non-idealities in molecular systems.
- Multi-scale methods for describing natural and artificial photochemistry to unlock the potential of solar driven energy conversion and storage.
- Fundamental methods for predictively creating collective or emergent functionalities of natural and artificially designed molecules, including molecules containing heavy atoms.
- Approaches for computationally assessing nondestructive spectroscopies that can either externally control molecular function or deduce changes in state.
- Methods for modeling membranes and molecular complexes composed of interfaces, which are critical for separation technologies for energy and water applications.

Successful proposals will include strategies for realizing the full potential of exascale machines and for implementing algorithms for reducing the explicit complexity. Proposals will deploy methods that go beyond those in use today.

Centers (integrated, multidisciplinary teams) comprising experts in quantum chemical theory, modeling, computation and applied mathematics must present a clear management plan that ensures a coherent team approach and that provides for the maintenance and long-term accessibility of software and data. Centers must also articulate mechanisms for community input to software and database development and validation from single-investigators and small-group CCS efforts.

Applications that are not programmatically aligned with BES research (see <https://science.energy.gov/bes/mse/> and <https://science.energy.gov/bes/csgeb/>) will be considered non-responsive.

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)

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.

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).

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).

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

Harnessing the Department of Energy's High-Performance Computing Expertise to Strengthen the US Chemical Enterprise (US DOE BES/ASCR and Council for Chemical Research, March 2011; (http://www.pnnl.gov/main/publications/external/technical_reports/PNNL-20896.pdf).
Basic Energy Sciences Roundtable on Opportunities for Quantum Computing in Chemical and Materials Sciences,
(https://science.energy.gov/~media/bes/pdf/reports/2018/Quantum_computing.pdf).

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).

<p>All entities submitting applications to this FOA must recognize the legal obligations to comply with export controls. Please see 10 CFR 810 for further information. This FOA is to support scientific endeavors that could be described in scholarly publications. Do not submit applications containing restricted data or unclassified nuclear information as defined in the Atomic Energy Act of 1954, as amended, 42 USC 2011 et seq., 10 CFR 1017, 10 CFR 1045.</p>
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Section II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT

DOE anticipates awarding Grants under this FOA.

B. ESTIMATED FUNDING

Research Grant Awards are expected to be made for a period of up to four years at a funding level appropriate for the proposed scope, with out-year support contingent on the availability of funds and satisfactory progress. DOE anticipates that the total value of grants made under this FOA will be between \$12 million and \$18 million. DOE expects that, subject to the availability of future year appropriations, \$21 million will be used to support Grants, National Laboratory authorizations, and interagency awards under this FOA and its companion program announcement (LAB 18-1912).

DOE is under no obligation to pay for any costs associated with the preparation or submission of an application. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this FOA.

C. MAXIMUM AND MINIMUM AWARD SIZE

(See B. Estimated Funding section above.)

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

Ceiling
\$2,000,000 per year

Floor
\$150,000 per year

D. EXPECTED NUMBER OF AWARDS

(See B. Estimated Funding Section above.)

Up to 15 awards are expected for both this FOA and the companion program announcement for DOE National Laboratories.

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

E. ANTICIPATED AWARD SIZE

(See B. Estimated Funding Section above.)

It is anticipated that award sizes may range from \$150,000 per year to \$2,000,000 per year. 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.

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 applications under this FOA.

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

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

I. RESPONSIBILITY

For multi-institution efforts, 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 sub-awardee.

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

If an award is made to another Federal agency or its Federally Funded Research and Development Center (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.

Applicants that are not domestic organizations should be advised that:

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

UNINCORPORATED CONSORTIA

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

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

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

Note that a consortium submits only one application, which would result in one award; consortium members receive sub-awards from the lead institution.

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 PIs are invited to work with their organizations, and other institutions, 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

Applicant institutions are limited to no more than one Letter of Intent (LOI) and no more than one application as a lead organization. DOE will consider the latest received submissions to be the institution's intended submission.

- Letters of intent in excess of the limited number of submissions will be discouraged.
- Applications in excess of the limited number of submissions will be declined without review.

An institution may participate in any number of applications as a team member.

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 Code of Federal Domestic Assistance (CFDA) number (81.049) and/or the funding opportunity number (**DE-FOA-0001912**) shown on the cover of this FOA and then follow the prompts to download the application package.

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

B. LETTER OF INTENT AND PRE-APPLICATION

1. Letter of Intent:

Letters of Intent (LOIs) are required.

LETTER OF INTENT DUE DATE:

May 16, 2018

LIMITATION ON NUMBER OF LETTERS OF INTENT SUBMITTED BY EACH LEAD ORGANIZATION

An entity may submit only one letter of intent as the lead organization. If more than one qualified LOI is received from a lead organization, DOE will consider the first qualified LOI received based on the PAMS date and time stamp. **Subsequent LOIs will be deemed non-responsive and any applications associated with the subsequent LOIs will also be deemed non-responsive to this FOA.** However, there is no limitation on the number of LOIs or applications in which an entity may participate as a team member or subcontractor.

LETTER OF INTENT CONTENTS

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

- 1) A cover sheet containing:
 - a. The planned title of the research application;
 - b. The name and mailing address of the sponsoring institution;
 - c. The name, institution, e-mail address, and telephone number of the Principal Investigator (PI) and any co-PIs;
 - d. Funding Opportunity Announcement Number: **DE-FOA-0001912**
 - e. Topical area: List “Computational Chemical Sciences”
 - f. Grant type: indicate type of grant (Single PI grant, Small group grant, or Center grant)
 - g. Signature of the institutional representative with authority to commit the lead institution to the research application: (LOIs without this signature will not be considered)

- 2) A narrative of up to three pages.
 - a. A brief abstract
 - b. A description of the proposed research and proposed methods of accomplishment. Describe how the research will address the research opportunities identified in one or more of the BES reports listed in Section I of this FOA.)
 - c. Total project cost information.

- 3) **A tabular listing of collaborators** for the PI and any co-PIs. The list must be in the tabular form provided below.** This listing should include co-authors over the past 48 months; graduate and postdoctoral advisors of the PI and any co-PIs; personnel, graduate students and postdoctoral associates that have been supervised during the past 60 months; and, any other current close associations of the key personnel. **The table should exclude all personnel at any of the institutions participating in the application.** The table should include the following elements:

Collaborator		Institution
Last Name	First Name	Institution Name

- ** Applicants are strongly encouraged to follow the exact format of the sample table since the tabular information will be compiled across all applications. Include grid lines around each cell.
- Do not merge name or institution cells, even if individuals share the same institution.
- Do not change the order of the columns.
- Do not include any additional information (e.g. “PI”, “Co-PI”, or footnote symbols) under “Last Name” and “First Name”.
- Do not include departmental affiliations under Institutions.
- If an individual has a joint appointment, separate the institutions with a “/” (i.e. “University of X / National Lab Y”).

This listing will not count in the page limitation

LETTER OF INTENT SUBMISSION

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

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

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

Create PAMS Account:

To register, click the “Create New PAMS Account” link on the website

<https://pamspublic.science.energy.gov/>.

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

PAMS will take you to the “Having Trouble Logging In?” page. (If you have been an 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.)

Register to Your Institution:

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

associate your profile with the new institution, and return you to the “Institutions – List” page when you are finished.

Submit Your Letter of Intent:

- Create your letter of intent outside the system and save it as a file with extension .docx, .doc, or .pdf. Make a note of the location of the file on your computer so you can browse for it later from within PAMS.
- Log into PAMS and click the Proposals tab. Click the “View / Respond to Funding Opportunity Announcements” link and find the current announcement in the list. Click the “Actions/Views” link in the Options column next to this announcement to obtain a dropdown menu. Select “Submit Letter of Intent” from the dropdown.
- On the Submit Letter of Intent page, select the institution from which you are submitting this LOI from the Institution dropdown. If you are associated with only one institution in the system, there will only be one institution in the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per LOI; to do so, click the “Select PI” button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the “Actions” link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose “Select PI.”
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the “Invite PI” link at the top left of the “Select PI” screen. You can enter an optional personal message to the PI in the “Comments” box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the LOI. Save the LOI for later work by clicking the “Save” button at the bottom of the screen. It will be stored in “My Letters of Intent” for later editing.
- Enter a title for your letter of intent.
- Select the appropriate technical contact from the Program Manager dropdown.
- To upload the LOI file into PAMS, click the “Attach File” button at the far right side of the screen. Click the “Browse” (or “Choose File” depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the “Upload” button to upload the file.
- At the bottom of the screen, click the “Submit to DOE” button to save and submit the LOI to DOE.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the LOI.

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-

1846 (toll free) or (301) 903-9610, email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this FOA should reference **DE-FOA-0001912**.

2. Pre-application

A pre-application is not required

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

You are required to use the compatible version of Adobe Reader software to complete a [Grants.gov](#) Adobe application package. To ensure you have the [Grants.gov](#) compatible version of Adobe Reader, visit the 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 in PDF unless otherwise specified in this announcement. Attached PDF files must be plain files consisting of text, numbers, and images

without editable fields, signatures, passwords, redactions, or other advanced features available in some PDF-compatible software. Do not use PDF portfolios or binders.

Please note 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 should have a unique file name.
- Please use only the following UTF-8 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 support are not required but may be included as an appendix to the application.

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 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 scientific program contracts 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 PII, 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 number fields on the SF-424 (R&R) form are used in PAMS to confirm the identity of the individual or organization submitting an application.

- Enter each number as a nine-digit number.
- Do not use hyphens or dashes.
- 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.

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

PUBLIC POLICY REQUIREMENTS

The applicant is made aware of generally applicable public policy requirements, including, but limited to the following:

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

2. Research and Related Other Project Information

Complete questions 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 name of the applicant, the project title, the Project Director/Principal Investigator(s) (PD/PI) and the PD/PI's institutional affiliation, any coinvestigators and their institutional affiliations, the objectives of the project, a description of the project, including methods to be employed, and the potential impact of the project (i.e., benefits, outcomes. A sample is provided below:

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

Text of abstract

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

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 to prepare public reports about supported research.

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

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

- The project title
- Applicant/Institution:
- Street Address/City/State/Zip:
- Postal Address:
- Lead PI name, telephone number, email:
- Administrative Point of Contact name, telephone number, email:
- Funding Opportunity FOA Number: **DE-FOA-0001912**
- DOE/SC Program Office: Basic Energy Sciences
- Topical Area of the Application: List “Computational Chemical Sciences”
- Grant type: indicate type of grant (Single PI grant, Small group grant, or Center grant)
- PAMS Letter of Intent or Preproposal tracking number: (applications without a corresponding LOI tracking number will be deemed non-responsive to the FOA)
- A table listing the annual and total funding to each institution participating in the application.

	Names	Institution	Year 1 Budget	Year 2 Budget	Year 3 Budget	Year 4 Budget	Total Budget
Lead PI							
Co-PI							
Co-PI							

Example budget table (\$ in thousands)

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 20 pages** of technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard 8.5” by 11” paper with 1 inch margins (top, bottom, left, and right). The font must not be smaller than 11 point. Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph. This page limit does not apply to the Cover Page, 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, D. for instructions on how to mark proprietary application information. To attach a Project Narrative, click “Add Attachment.”

Background/Introduction: Explanation of the importance and relevance of the proposed work in the context of relevant literature.

Project Objectives: This section should provide a clear, concise statement of the specific objectives/aims of the proposed project.

Proposed Research and Methods: Identify the hypotheses to be tested and details of the methods to be used.

Management Plan and Timeline of Activities: For all proposals, this section should include a timeline for all major research tasks. Note that letters of commitment are required for all funded collaborators (See Appendix 7). For the case of center proposals, this section should also describe the management structure, how effective collaborations among the participants will be fostered, and how integration of different research efforts will be attained.

The Project Narrative comprises the research plan for the project. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also 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.

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

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the PD/PI and each senior/key person 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 PD's/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 five professional and scholarly activities related to the effort proposed.

In addition, the biographical sketch must include information to permit DOE to identify individuals who are conflicted with or potentially biased (favorably or unfavorably) against the investigator. Include a section entitled "**Identification of Potential Conflicts of Interest or Bias**

in Selection of Reviewers” that will not count in a page limit. Provide the following information in this section:

- **Collaborators and Co-editors:** List in alphabetical order all persons, including their current organizational affiliation, who are, or who have been, collaborators or co-authors with you on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of this application. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the PI interacted on a regular basis while the research was being done. Also, list any individuals who are currently, or have been, co-editors with you on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of this application. If there are no collaborators or co-editors to report, state “None.”
- **Graduate and Postdoctoral Advisors and Advisees:** List the names and current organizational affiliations of your graduate advisor(s) and principal postdoctoral sponsor(s). Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates.

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 PD/PI’s and senior/key persons, including subawardees, for ongoing projects and pending applications. List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid.

For every activity, list the following items:

- The sponsor of the activity or the source of funding
- The award or other identifying number
- The title of the award or activity
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The 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 sub-awardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Computer 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 (local high-performance computing resources or, if appropriate, access to national leadership-class computing facilities) and the extent to which they would be available to the project. Please provide the Facility and Other Resource information as an appendix to your project narrative.

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

APPENDIX 5: EQUIPMENT

List 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 #5). 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 additionally provide an Open Source Software Distribution Plan. 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 Full Application. Guidance for preparing an Open source Software Distribution Plan is included in Section VIII of the FOA.
3. 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 SC 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.
4. 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 SC 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 SC facilities can be found in the additional guidance from the sponsoring program.
5. DMPs must protect confidentiality, personal privacy, PII, 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>

- This appendix should not exceed two pages 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)
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 7: LETTERS OF COMMITMENT FROM CO-PIs AND COLLABORATORS

Letters of commitment from each funded co-PI/collaborator must be endorsed by the co-PI/collaborator and an appropriate member of the institutional administration authorized to commit the institution to performance of the research. Letters of support from any additional unfunded collaborators should be included here also.

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

APPENDIX 8: OTHER ATTACHMENT

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

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

3. Research and Related Budget

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

Budget Fields

<p>Section A Senior/Key Person</p>	<p>For each Senior/Key Person, enter the requested information. List personnel, base salary, the number of months that person will be allocated to the project, requested salary, fringe benefits, and the total funds requested for each person. The requested salary must be the product of the base salary and the effort. Include a written narrative in the budget justification that justifies the need for requested personnel.</p>
<p>Section B Other Personnel</p>	<p>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.</p>
<p>Section C Equipment</p>	<p>For the purpose of this budget, equipment is designated as an item of property that has an acquisition cost of \$5,000 or more and an expected service life of more than one year. (Note that this designation applies for proposal budgeting only and differs from the DOE definition of capital equipment.) List each item of equipment separately and justify each in the budget justification section. Do not aggregate items of equipment. Allowable items ordinarily will be limited to research equipment and apparatus not already available for the conduct of the work. General-purpose office equipment is not eligible for support unless primarily or exclusively used in the actual conduct of scientific research.</p>
<p>Section D Travel</p>	<p>For purposes of this section only, travel to Canada or to Mexico is considered domestic travel. In the budget justification, list each trip's destination, dates, estimated costs including transportation and subsistence, number of staff traveling, the purpose of the travel, and how it relates to the project. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). To qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results. Domestic travel is to be justified separately from foreign travel.</p>
<p>Section E Participant/Trainee Support Costs</p>	<p>If applicable, submit training support costs. Educational projects that intend to support trainees (precollege, college, graduate and post graduate) must list each trainee cost that includes stipend levels and amounts, cost of tuition for each trainee, cost of any travel (provide the same information as needed under the regular travel category), and costs for any related training expenses. Participant costs are those costs associated with conferences, workshops, symposia or institutes and breakout items should indicate the number of participants, cost for each participant, purpose of the conference, dates and places of meetings and</p>

	<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"> • Materials and Supplies: Enter total funds requested for materials and supplies in the appropriate fields. In the budget justification, indicate general categories such as glassware, and chemicals, including an amount for each category (items not identified under “Equipment”). Categories less than \$1,000 are not required to be itemized. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). • Publication Costs: Enter the total publication funds requested. The proposal budget may request funds for the costs of documenting, preparing, publishing or otherwise making available to others the findings and products of the work conducted under the award. In the budget justification, include supporting information. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). • Consultant Services: Enter total funds requested for all consultant services. In the budget justification, identify each consultant, the services he/she will perform, total number of days, travel costs, and total estimated costs. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). • ADP/Computer Services: Enter total funds requested for ADP/Computer Services. The cost of computer services, including computer-based retrieval of scientific, technical and education information may be requested. In the budget justification, include the established computer service rates at the proposing organization if applicable. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). • Subawards/Consortium/Contractual Costs: Enter total costs for all subawards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details. • Equipment or Facility Rental/User Fees: Enter total funds requested for Equipment or Facility Rental/User Fees. In the budget justification, identify each rental/user fee and justify. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). • Alterations and Renovations: Enter total funds requested for Alterations and Renovations. In the budget justification, itemize by category and justify the costs of alterations and renovations,

	<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"> • Other: Add text to describe any other Direct Costs not requested above. Enter costs associated with “Other” item(s). Use the budget justification to further itemize and justify.
Section G Direct Costs	This represents Total Direct Costs (Sections A through F)
Section H Other Indirect Costs	Enter the Indirect Cost information for each field. Only four general categories of indirect costs are allowed/requested on this form, so please consolidate if needed. Include the cognizant Federal agency and contact information if using a negotiated rate agreement.
Section I Total Direct and Indirect Costs	This is the total of Sections G and H

BUDGET JUSTIFICATION (FIELD 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 should not exceed 50 characters.

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

Applicants should consult their local information technology (“IT”) support resources for any necessary assistance in converting the 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:

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

May 16, 2018 at 5:00 PM Eastern Time.

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

2. Pre-application Due Date

Not applicable.

3. Application Due Date

June 18, 2018 at 5:00 PM Eastern Time.

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

4. Late Submissions

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

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

- Unavailability of administrative personnel.
- An upper respiratory infection (a “cold”) the week of the deadline.

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

Applicants must contact the Scientific Program Contacts listed in this FOA to discuss the option of a late submission. Contacting the Scientific Program Contacts 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 four 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. 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. If you have problems completing the registration process or submitting your application, call Grants.gov at 1-800-518-4726 or send an email to support@grants.gov.

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

4. DOE SC Portfolio Analysis and Management System (PAMS)

After you submit your application through Grants.gov, the application will automatically transfer into the 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>. 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. All submission and inquiries about this FOA should reference **DE-FOA-0001912**.

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 SC.” These three people are the Principal Investigator (Block 14), Authorized Representative (Block 19), and Point of Contact (Block 5). In PAMS notation, applications are known as proposals, the Principal Investigator is known as the PI, the Authorized Representative is known as the Sponsored Research Officer/Business Officer/Administrative Officer (SRO/BO/AO), and the Point of Contact is known as the POC.

There will be a period of time between the application’s receipt at Grants.gov and its assignment to a DOE 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. All submission and inquiries about this FOA should reference **DE-FOA-0001912**.

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. In addition to the criteria required by regulation, DOE will apply the following criteria in its initial review of applications: (5) the proposed project is not duplicative of current programmatic work; and (6) there is a corresponding, qualified letter of intent for the application. An institution may only submit one application as lead organization.

In particular, to be responsive to the objectives of this FOA, the research proposed in the application **must**:

- (1) Focus on Research Opportunities identified in BES Roundtable or Basic Research Needs (BRN) Reports
- (2) Address research that is programmatically aligned with BES research (see <https://science.energy.gov/bes/mse/> and <https://science.energy.gov/bes/csgb/>)
- (3) Have a management plan that includes a timeline for the major activities for large team proposals.

Applications that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

2. Merit Review Criteria

Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria, with the first four listed in descending order of importance as found in 10 CFR 605.10 (d), the SC Financial Assistance Program Rule.

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

In addition to the merit review criteria established by regulation, DOE will ask its merit reviewers to provide commentary about:

- Adequacy of the Management Plan

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 on the criteria established by regulation:

SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROPOSED RESEARCH

- What is the scientific innovation of the proposed research?
- What is the likelihood of achieving valuable and impactful results?
- How does the proposed research advance computational chemical sciences and enable software that can exploit future exascale computer systems?
- Is the Data Management Plan suitable for the proposed research?

APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

- How logical are the hypotheses and how feasible are the research approaches to test these hypotheses?
- How innovative is the proposed method or approach?
- How well does the applicant recognize significant potential problems and consider alternative strategies?

COMPETENCY OF APPLICANT'S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES

- What is the past performance and qualifications of the principal investigator (PI) and, if appropriate the broader team of researchers?
- How likely is the plan for accessing the required facilities to be successful?
- How does the proposed work take advantage of unique facilities and capabilities?

REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET

- How adequate are the proposed budget and staffing levels to carry out the proposed research?
- How reasonable and appropriate is the budget for the scope?

ADEQUACY OF THE MANAGEMENT PLAN

- What are the strengths and weaknesses of the application's management plan, including the proposed timeline?
- If appropriate, comment on how the team will achieve synergy among the participants, including integration of experimental and theoretical work (if both are included in the proposed research)?

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 "SC 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 priorities
- Ensuring an appropriate balance of activities within SC programs
- Performance under current awards
- Current or previous DOE support

3. Selection

The DOE 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

DOE is interested in projects supported under this FOA beginning work by September 30, 2018.

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., 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

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

For DOE Grants and Cooperative Agreements made to universities, non-profits and other entities subject to Title 2 CFR, research awards made under this FOA will be subject to the Government-wide Research Terms and Conditions published at https://www.nsf.gov/pubs/policydocs/rtr/rcoverlay_march17.pdf and the DOE Agency Specific Standard Research Terms and Conditions published at https://www.nsf.gov/pubs/policydocs/rtr/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 at the 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. 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 Requirements Checklist, DOE F 4600.2, attached to the Financial Assistance 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. DOE cannot answer these questions.

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this FOA should reference **DE-FOA-0001912**.

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

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

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

B. AGENCY CONTACTS

Grants.gov Customer Support	800-518-4726 (toll-free) support@grants.gov
PAMS Customer Support	855-818-1846 (toll-free) 301-903-9610 sc.pams-helpdesk@science.doe.gov
Scientific Program Contact	Dr. Mark R. Pederson (301)-903-9956 Mark.Pederson@science.doe.gov

Section VIII - OTHER INFORMATION

A. MODIFICATIONS

Notices of any modifications to this FOA will be posted on Grants.gov and the FedConnect portal. You can receive an email when a modification or an FOA message is posted by registering with FedConnect as an interested party for this FOA. It is recommended that you register as soon after release of the FOA as possible to ensure you receive timely notice of any modifications or other FOAs. More information is available at <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 Financial Assistance 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 DOE Contracting Officer for this award and until the awardee receives notice of such availability, to be confirmed in writing by the DOE 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. 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."