

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



COMPUTATIONAL CHEMICAL SCIENCES RESEARCH

**PROGRAM ANNOUNCEMENT TO THE DOE NATIONAL LABORATORIES
LABORATORY ANNOUNCEMENT NUMBER: LAB 18-1912
ANNOUNCEMENT TYPE: INITIAL**

Issue Date:	April 13, 2018
Submission Deadline for Letters of Intent:	May 16, 2018 at 5 PM Eastern A Letter of Intent is required
Submission Deadline for Pre-Proposals:	Not Applicable
Submission Deadline for Proposals:	June 18, 2018 at 5 PM Eastern

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REGISTRATIONS

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

The DOE Office of Science performs many functions for DOE national laboratory proposals in the Portfolio Analysis and Management System (PAMS), which is available at <https://pamspublic.science.energy.gov>.

You must register in PAMS to submit a pre-proposal, letter of intent, or DOE national laboratory proposal.

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

Notifications sent from the PAMS system will come from the PAMS email address <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 the “Having Trouble Logging In?” page. (Note: If you reviewed for or were listed as PI on a prior submission to the Office of Science but have not previously created an account, you may already be linked to an institution in PAMS. If this is the case, PAMS will take you to the PAMS home page.)

2. REGISTER TO YOUR INSTITUTION:

- Click the link labeled “Option 2: I know my institution and I am here to register to the institution.” (Note: If you previously created a PAMS account but did not register to an institution at that time, you must click the Institutions tab and click the “Register to Institution” link.)

- PAMS will take you to the “Register to Institution” page.
- Type a word or phrase from your institution name in the field labeled, “Institution Name like,” choose the radio button next to the item that best describes your role in the system, and click the “Search” button. A “like” search in PAMS returns results that contain the word or phrase you enter; you need not enter the exact name of the institution, but you should enter a word or phrase contained within the institution name. (Hint: If your institution has an acronym, such as ANL for Argonne National Laboratory or UCLA for the Regents of the University of California, Los Angeles, you may search for the acronym under “Institution Name like.” Many institutions with acronyms are listed in PAMS with their acronyms in parentheses after their names.)
- Find your institution in the list that is returned by the search and click the “Actions” link in the Options column next to the institution name to obtain a dropdown list. Select “Add me to this institution” from the dropdown. PAMS will take you to the “Institutions – List” page.
- If you do not see your institution in the initial search results, you can search again by clicking the “Cancel” button, clicking the Option 2 link, and repeating the search.
- All DOE National Laboratories have established profiles in PAMS, so please keep searching until you find your laboratory.

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 DOE National Laboratory Announcement should reference **LAB 18-1912**.

UPDATES AND REMINDERS

RECOMMENDATION

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

DATA MANAGEMENT PLAN

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

ACKNOWLEDGMENT OF FEDERAL SUPPORT

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

AVOIDING ERRORS

The following advice is compiled from actual experiences of applicants for Office of Science awards.

- Please ensure that the research narrative is comprised of one and only one PDF file, including all appendices, when it is uploaded.
- When using the Office of Science 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.

Section I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS ANNOUNCEMENT SHOULD BE DIRECTED TO:

Scientific Program Contacts:

Dr. Mark Pederson, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division

PHONE: (301)-903-9956

Mark.Pederson@science.doe.gov

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 funding opportunity 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 Announcement is the second solicitation for proposals to support CCS.

Additional Information:

There is a separate companion Funding Opportunity Announcement (FOA) for universities and other eligible institutions. See DE-FOA-0001912 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 Announcement. 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 Announcement 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.
- 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 Announcement 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 to 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.

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).

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

Section II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT

DOE anticipates awarding laboratory work authorizations under this DOE National Laboratory Announcement.

Any awards made under this Announcement will be subject to the provisions of the contract between DOE and the awardee National Laboratory.

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 authorizations made under this Announcement 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 national laboratory authorizations, grants, and interagency awards under this Announcement and its companion FOA.

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 program announcement.

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

\$300,000 per year

D. EXPECTED NUMBER OF AWARDS

(See B. Estimated Funding Section above.)

Up to 15 awards are expected for both this Announcement and the companion FOA.

The exact number of awards will depend on the number of meritorious proposals 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 \$300,000 per year to \$1,500,000 per year.

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

F. PERIOD OF PERFORMANCE

(See B. Estimated Funding section above.)

DOE anticipates making awards with a project 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 proposal; (3) submission of required reports; and (4) compliance with the terms and conditions of the award.

G. TYPE OF PROPOSAL

DOE will accept new DOE National Laboratory Proposals under this DOE National Laboratory Announcement. Please only submit a PAMS lab proposal in response to this Announcement; do not submit a DOE Field Work Proposal (FWP) at this time. The Office of Science will request FWPs later from those selected for funding consideration under this Announcement.

Section III – ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS AND TOPICS

This is a DOE National Laboratory-only Announcement. FFRDCs from other Federal agencies are not eligible to submit in response to this Program Announcement.

B. COST SHARING

Cost sharing is not required.

C. ELIGIBLE INDIVIDUALS

Eligible individuals with the skills, knowledge, and resources necessary to carry out the proposed research as a Lead Principal Investigator/Principal Investigator are invited to work with their organizations to develop a proposal. Individuals from underrepresented groups as well as individuals with disabilities are always encouraged to apply.

D. OTHER ELIGIBILITY REQUIREMENTS

Limitation on Number of Letters of Intent and Proposals Submitted by a Lead Organization: An entity may submit only one letter of intent as the lead organization, and as a result, may submit only one proposal. An institution may participate in any number of proposals as a team member. See [Section IV B.](#) for further details.

Team proposals: Entities proposing as a team must designate a lead organization. Letters of intent and proposals must be submitted on behalf of the team members by the lead organization. Only one letter of intent and one proposal is to be submitted for each team. The designated lead organization must perform a greater percentage of the effort than any other partner organization or subawardee. The percentage of effort will be determined by reviewing the total budget for each participating organization as a percentage of proposed total project costs. **If a proposal is received in which the lead organization is not performing a greater percentage of the effort than each of the other institutional partners, team members, or subawardees, as determined by the budget, the proposal will be deemed non-responsive and rejected without further review.**

Section IV – PROPOSAL AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST PROPOSAL PACKAGE

Proposal submission instructions are available in this Announcement on the DOE Office of Science Portfolio Analysis and Management System (PAMS). Screenshots showing the steps in DOE National Laboratory proposal submission are available in the PAMS External User Guide, accessible by navigating to <https://pamspublic.science.energy.gov> and clicking on the “PAMS External User Guide” link.

Proposals submitted outside of PAMS will not be accepted.

B. LETTER OF INTENT

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. If more than one qualified LOIs are received from a lead organization, DOE will consider the first one qualified LOIs 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.** 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. DOE National Laboratory Announcement Number: LAB 18-1912
 - e. Topical area: List “Computational Chemical Sciences”
 - f. Authorization 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 Announcement)
- 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. “Univ 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 Office of Science Portfolio Analysis and Management System (PAMS) website <https://pamspublic.science.energy.gov/>. It is important that the LOI be a single file with extension .pdf, .docx, or .doc. The 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 the “Having Trouble Logging In?” page. (If you have been an Office of Science merit reviewer or if you have previously submitted a proposal, 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 / View / Respond to DOE National Laboratory 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 scientific contact from the Program Manager dropdown.
- To upload the LOI file into PAMS, click the “Attach File” button at the far right side of the screen. Click the “Browse” (or “Choose File” depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the “Upload” button to upload the file.
- At the bottom of the screen, click the “Submit to DOE” button to save and submit the LOI to DOE.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the LOI.

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846

(toll free) or (301) 903-9610, email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this Laboratory Announcement should reference LAB 18-1912

2. Pre-application

A pre-application is not required

C. CONTENT AND PROPOSAL FORMS

PROPOSAL DUE DATE

June 18, 2018 at 5:00 PM Eastern Time or [See Section IV, Part E](#).

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

RESUBMISSION OF PROPOSALS

Proposals submitted under this Announcement may be withdrawn from consideration by using the Office of Science's PAMS website at <https://pamspublic.science.energy.gov>. Proposals may be withdrawn at any time between when the Laboratory submits the application and when DOE makes the application available to merit reviewers. Such withdrawals take effect immediately and cannot be reversed.

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

The Office of Science will usually consider the last submission, according to its timestamp, to be the intended version. Please consult with the Scientific Program Contact to resolve any confusion about which version of a proposal should be considered.

IMPROPER CONTENTS OF PROPOSALS

Proposals submitted under this Announcement will be stored in controlled-access systems, but they may be made publicly available if an award is made, and they will be made available to merit reviewers. As such, it is critical that Laboratories follow these guidelines:

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

- Clearly mark all proprietary or trade-secret information.

LETTERS

Letters of support are not required but may be included as an appendix to the application.

1. Summary of Proposal Contents and Information about PAMS

Each DOE National Laboratory proposal will contain the following sections:

- Budget, entered into PAMS as structured data using the PAMS budget form
- Abstract (one page), entered into PAMS as a separate pdf
- Budget justification, entered into PAMS as a separate pdf
- Proposal, combined into a single pdf containing the following information:
 - Proposal Cover Page
 - Table of Contents
 - Project Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel – 10 page limit)
 - Appendix 1: Biographical Sketch(es)
 - Appendix 2: Current and Pending Support
 - Appendix 3: Bibliography and References Cited
 - Appendix 4: Facilities and Other Resources
 - Appendix 5: Equipment
 - Appendix 6: Data Management Plan
 - Appendix 7 Letters of Commitment from co-PIs and Collaborators
 - Appendix 8: Other Attachments (optional)

SUBMISSION INSTRUCTIONS

Completed proposals must be submitted into the DOE Office of Science Portfolio Analysis and Management System (PAMS). 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 number) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this Program Announcement should reference **LAB 18-1912**. Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than **June 18, 2018**, at 5:00 PM Eastern Time.

All PIs and those submitting on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to ensure timely submissions. To register, click “Create New PAMS Account” on the website <https://pamspublic.science.energy.gov/> and follow the instructions for creating an account.

The following information is provided to help with proposal submission. Detailed instructions and screen shots can be found in the user guide. To find the user guide, click the “External User Guide” link on the PAMS home page. Onscreen instructions are available within PAMS.

- Log into PAMS. From the proposals tab, click the “View DOE National Laboratory 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 Proposal” from the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per proposal; 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 proposal. Save the proposal for later work by selecting “Save” from the dropdown at the bottom of the screen and then clicking the “Go” button. It will be stored in “My Proposals” for later editing. As a minimum, you must complete all the required fields on the PAMS cover page before you can save the proposal for the first time.
- The cover page, budget, and attachments sections of the lab proposal are required by PAMS before it can be submitted to DOE.
- Complete the sections in PAMS one at a time, starting with the cover page and following the instructions for each section.
- Click the “+View More” link at the top of each section to expand the onscreen instructions. On the budget section, click the “Budget Tab Instructions” link to obtain detailed guidance on completing the budget form.
- Save each section by selecting either “Save” (to stay in the same section) or “Save... and Continue to the Next Section” (to move to the next section) from the dropdown menu at the bottom of the screen, followed by clicking the “Go” button.
- If you save the proposal and navigate away from it, you may return later to edit the proposal by clicking the “View My Existing Proposals” or “My Proposals” links within PAMS.
- You must enter a budget for each annual budget period.
- You must also enter a budget for each proposed sub-award. The sub-award section can be completed using the same steps used for the budget section.
- In the attachments section of the lab proposal, the abstract, the budget justification, and the proposal narrative are required and must be submitted as separate files.
- You must bundle everything other than the budget, abstract, and budget justification into one single PDF file to be attached under “Proposal Attachment.”
- Do not attach anything under “Other Attachments.”

- To upload a 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.
- Once you have saved all of the sections, the “Submit to DOE” option will appear in the dropdown menu at the bottom of the screen.
- To submit the proposal, select “Submit to DOE” from the dropdown menu and then click the “Go” button.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the proposal.
- The proposal will also appear under My Proposals with a Proposal Status of “Submitted to DOE.”

Please only submit a PAMS lab technical proposal in response to this Announcement; do not submit a DOE Field Work Proposal (FWP) at this time. The Office of Science will request FWPs later from those selected for funding consideration under this Announcement.

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 number) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this Program Announcement should reference **LAB 18-1912**.

2. Detailed Contents of the Proposal

BUDGET AND BUDGET EXPLANATION

The budget must be submitted into PAMS using the PAMS budget form. Research proposed under this Announcement may only have one annual budget period.

PAMS will calculate the cumulative budget totals for you.

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

PROJECT SUMMARY/ABSTRACT (NO MORE THAN ONE PAGE)

The project summary/abstract must contain a summary of the proposed activity suitable for dissemination to the public. It should be a self-contained document that identifies the name of the applicant, the Principal Investigator (PI), the project title, the objectives of the project, a description of the project, including methods to be employed, the potential impact of the project (i.e., benefits, outcomes). This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must not exceed one page when printed using standard 8.5” by 11” paper with 1” margins (top,

bottom, left and right) with font not smaller than 11 point. The one-page project summary/abstract should be placed in a separate, single pdf document and attached on the appropriate screen in PAMS.

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

DOE COVER PAGE
(PART OF PROJECT NARRATIVE)

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

- The project title:
- Applicant/Institution:
- Street Address/City/State/Zip:
- Postal Address:
- Administrative Point of Contact name, telephone number, email:
- Lead PI name, telephone number, email:
- DOE National Laboratory Announcement Number: **LAB 18-1912**
- DOE/Office of Science Program Office: Office of 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 Tracking Number: (applications without a corresponding LOI tracking number will be deemed non-responsive)
- 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	Total Budget
Lead PI						
Co-PI						
Co-PI						

Example budget table (\$ in thousands)

PROJECT NARRATIVE (NO MORE THAN 20 PAGES LONG)

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 proposal. Merit reviewers are not required to access Internet sites; however, Internet publications in a list of references will be treated identically to print publications. See Part VIII.D for instructions on how to mark proprietary proposal 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: This section should describe the management structure, how effective collaborations among the participants will be fostered, how integration of experimental and theoretical efforts (if both are included in the research) will be attained, and the timeline for all major research tasks. Note that letters of commitment are required for all funded collaborators from other institutions (see Appendix 7).

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

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the project director/principal investigator (PD/PI) and each senior/key person as an appendix to your technical narrative. As part of the sketch, provide information that can be used by reviewers to evaluate the PI’s potential for leadership within the scientific community. Examples of information of interest are invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society activities, special international or industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences. The biographical information (curriculum vitae) must not exceed 3 pages when printed on 8.5” by 11” paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include the following:

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

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

Publications: Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications. An abbreviated style such as the Physical Review Letters (PRL) convention for citations (list only the first author) may be used for publications with more than 10 authors.

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

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

- **Collaborators and Co-editors:** List in alphabetical order all persons, including their current organizational affiliation, who are, or who have been, collaborators or co-authors with you on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of this proposal. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the Principal Investigator interacted on a regular basis while the research was being done. Also, 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 proposal. 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 personally identifiable information such as a Social Security Number, date of birth, or city of birth. Do not include information that a merit reviewer should not consider.

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

APPENDIX 2: CURRENT AND PENDING SUPPORT

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

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 proposal. 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 (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. Explicitly discuss plans to access XFELs as required for the research. Please provide the Facility and Other Resource information as an appendix to your project narrative.

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

APPENDIX 5: EQUIPMENT

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

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

APPENDIX 6: DATA MANAGEMENT PLAN

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

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

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

- This appendix should not exceed 2 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 from other institutions 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 proposal. 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.

3. Detailed Instructions for the Budget

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

To edit a section on the budget, click the edit icon () for each section on the page. Remember to save all budget periods before moving on to the next section. You can save the budget periods by selecting “Save All Budget Periods” from the dropdown on the lower right corner of the PAMS budget entry screen and then clicking the “Go” button. You can also save any data entry page in PAMS using the blue diskette icon () in the floating toolbar on the bottom of the screen.

Section A. Senior/Key Person (Required)

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

Section B. Other Personnel

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

Section C. Equipment Description

For the purpose of this budget, equipment is designated as an item of property that has an acquisition cost of \$5,000 or more and an expected service life of more than one year. (Note that this designation applies for proposal budgeting only and differs from the DOE definition of capital equipment.) List each item of equipment separately and justify each in the budget justification section. Allowable items ordinarily will be limited to research equipment and apparatus not already available for the conduct of the work. General-purpose office equipment, such as a personal computer, is not eligible for support unless primarily or exclusively used in the actual conduct of scientific research.

Section D. Travel

In the budget justification, list each trip's destination, dates, estimated costs including transportation and subsistence, number of staff traveling, the purpose of the travel, and how it relates to the project. Indicate whether travel cost estimates are based upon quotes from travel agencies; upon past experience of similar number of trips to similar travel destinations; or something else (describe). To qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results.

Section E. Participant/Trainee Support Costs:

If applicable, submit training support costs. Educational projects that intend to support trainees (precollege, college, graduate and post graduate) must list each trainee cost that includes stipend levels and amounts, cost of tuition for each trainee, cost of any travel (provide the same information as needed under the regular travel category), and costs for any related training expenses. Participant costs are those costs associated with conferences, workshops, symposia or institutes and breakout items should indicate the number of participants, cost for each participant, purpose of the conference, dates and places of meetings and any related administrative expenses. In the budget justification, indicate whether trainee cost estimates are based upon past experience of support of similar number of trainees on similar projects; past experience of support of similar number of participants attending similar conferences/workshops/symposia; or something else (describe).

Section F. Other Direct Costs:

Enter Other Direct Costs information for each item listed.

- **Materials and Supplies:** Enter total funds requested for materials and supplies in the appropriate fields. In the budget justification, indicate general categories such as glassware, and chemicals, including an amount for each category (items not identified under "Equipment"). Categories less than \$1,000 are not required to be itemized. In the budget justification, indicate whether cost estimates are based upon past experience of purchase of similar or like items; quotes/catalog prices of similar or like items; or

something else (describe).

- **Publication Costs:** Enter the total publication funds requested. The proposal budget may request funds for the costs of documenting, preparing, publishing or otherwise making available to others the findings and products of the work conducted under the award. In the budget justification, include supporting information. In the budget justification, indicate whether cost estimates are based upon past experience of purchase of similar or like items; vendor quotes of similar publication services; or something else (describe).
- **Consultant Services:** Enter total funds requested for all consultant services. In the budget justification, identify each consultant, the services he/she will perform, total number of days, travel costs, and total estimated costs. In the budget justification, indicate whether consultant cost estimate is based upon previous experience/quotes for similar or like services; or something else (describe).
- **ADP/Computer Services:** Enter total funds requested for ADP/Computer Services. The cost of computer services, including computer-based retrieval of scientific, technical and education information may be requested. In the budget justification, include the established computer service rates at the proposing organization if applicable. In the budget justification, indicate whether cost estimates are based upon quotes/past experience of purchase of similar computer services; established computer service rates at the proposing institution; or something else (describe).
- **Sub-awards/Consortium/Contractual Costs:** Enter total costs for all sub-awards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details.
- **Equipment or Facility Rental/User Fees:** Enter total funds requested for Equipment or Facility Rental/User Fees. In the budget justification, identify each rental/user fee and justify. In the budget justification, indicate whether cost estimates are based upon past experience with similar or like items; vendor quotes of similar items; or something else (describe).
- **Alterations and Renovations:** Enter total funds requested for Alterations and Renovations.
- **In the budget justification,** itemize by category and justify the costs of alterations and renovations, including repairs, painting, removal or installation of partitions, shielding, or air conditioning. Where applicable, provide the square footage and costs.
- **Other:** Add text to describe any other Direct Costs not requested above. Enter costs associated with “Other” item(s). Use the budget justification to further itemize and justify.

Section G. Direct Costs

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

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.

Section I. Total Direct and Indirect Costs

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

D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS

If selected for award, DOE reserves the right to request additional or clarifying information.

E. SUBMISSION DATES AND TIMES

1. Required Letter of Intent Due Date

May 16, 2018 at 5 PM Eastern Time

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

2. Pre-proposal Due Date

Not Applicable

3. Proposal Due Date

June 18, 2018 at 5 PM Eastern Time

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

4. Late Submissions

Delays in submitting letters of intent and proposals 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 Contact listed in this Funding Opportunity Announcement to discuss the option of a late submission. Contacting the Scientific Program Contact 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.

F. FUNDING RESTRICTIONS

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

G. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS

1. Where to Submit

Proposals must be submitted through PAMS to be considered for award.

Please only submit a PAMS lab technical proposal in response to this Announcement; do not submit a DOE Field Work Proposal (FWP) at this time. The Office of Science will request FWPs via the Searchable FWP system later from those selected for funding consideration under this Announcement.

2. Registration Process

ONE-TIME REGISTRATION PROCESS

You must complete the one-time registration process (all steps) before you can submit your first proposal through PAMS. Registration instructions appear in the front matter of this Announcement.

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 DOE National Laboratory Announcement should reference **LAB 18-1912**.

3. Proposal Receipt Notices

Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the proposal.

4. Viewing Submitted Proposals

Upon submission, the proposal will appear under My Proposals for the PI and the Submitter with a Proposal Status of “Submitted to DOE.”

Section V - PROPOSAL 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 Announcement 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 Announcement, the research proposed in the application **must**:

- (1) Focus on Research Opportunities identified in BES Roundtable or 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?

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

Proposals that pass the initial review will be subjected to a formal merit review and will be evaluated based on the criteria above.

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 Office of Science priorities
- Ensuring an appropriate balance of activities within Office of Science programs
- Performance under current awards
- Current or previous DOE support
- Degree of engagement by the lead institution for team proposals

3. Selection

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

4. Discussions and Award

The Government may enter into discussions with a selected applicant for any reason deemed necessary. 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 Announcement 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.

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

2. Notice of Award

A work authorization/contract modification issued by the contracting officer is the authorizing award document.

B. REPORTING

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

Section VII - QUESTIONS/AGENCY CONTACTS

A. QUESTIONS

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 DOE National Laboratory Announcement should reference **LAB 18-1912**.

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 Scientific Program Contact shown below.

Please contact the program staff with all questions not directly related to the PAMS system.

B. AGENCY CONTACTS

PAMS Customer Support	855-818-1846 (toll-free) 301-903-9610 sc.pams-helpdesk@science.doe.gov
Scientific Program Contact	Dr. Mark R Pederson, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division, (301)-903-9956 Mark.Pederson@science.doe.gov

Section VIII - OTHER INFORMATION

A. MODIFICATIONS

Notices of any modifications to this DOE National Laboratory Announcement will be posted on the Grants and Contracts website (<http://science.energy.gov/grants/>).

B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE

DOE reserves the right, without qualification, to reject any or all proposals received in response to this DOE National Laboratory Announcement and to select any proposal, in whole or in part, as a basis for negotiation and/or award.

C. COMMITMENT OF PUBLIC FUNDS

The Contracting Officer is the only individual who can make awards or commit the Government to the expenditure of public funds. A commitment by other than the Contracting Officer, either explicit or implied, is invalid.

D. PROPRIETARY PROPOSAL INFORMATION

Patentable ideas, trade secrets, proprietary or confidential commercial or financial information, disclosure of which may harm the applicant, should be included in a proposal 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 proposal which are to be restricted:

“The data contained in pages _____ of this proposal have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes.”

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 proposal, consents to the use of non-Federal reviewers/administrators. Non-Federal reviewers must sign conflict of interest and non-disclosure agreements prior to reviewing a proposal. Non-Federal personnel conducting administrative activities must sign a non-disclosure agreement.

F. AVAILABILITY OF FUNDS

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