

**PROGRAM ANNOUNCEMENT  
TO DOE NATIONAL LABORATORIES**



**U. S. Department of Energy  
Office of Science  
Office of Basic Energy Sciences (BES)**

*Computational Chemical Sciences*

**DOE National Laboratory Announcement Number: LAB 17-1775  
Announcement Type: **Amendment 0001****

<b>Issue Date:</b>	<b>May 23, 2017</b>
<b>Letter of Intent Due Date</b>	<b>June 5, 2017 at 5:00 PM Eastern Time A Letter of Intent is required</b>
<b>Pre-Proposal Due Date:</b>	<b>Not Applicable</b>
<b>Proposal Due Date:</b>	<b>July 17, 2017 at 5:00 PM Eastern Time</b>
<b>Amendment:</b>	<b>This announcement is amended to correct typographical errors on pages 19 and 22.</b>

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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>.

There are many activities that you can perform in PAMS, and more functionality will be added throughout the near future. DOE national laboratories will submit pre-proposals, letters of intent, and proposals directly into PAMS.

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](mailto:PAMS.Autoreply@science.doe.gov)>. Please make sure your email server/software allows delivery of emails from the PAMS email address to yours.

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

#### 1. CREATE PAMS ACCOUNT:

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

- Click the “No, I have never had an account” link and then the “Create Account” button.
- You will be prompted to enter your name and email address, create a username and password, and select a security question and answer. Once you have done this, click the “Save and Continue” button.
- On the next page, enter the required information (at least one phone number and your mailing address) and any optional information you wish to provide (e.g., FAX number, website, mailstop code, additional email addresses or phone numbers, Division/Department). Click the “Create Account” button.
- Read the user agreement and click the “Accept” button to indicate that you understand your responsibilities and agree to comply with the rules of behavior for PAMS.
- PAMS will take you 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](mailto:sc.pams-helpdesk@science.doe.gov). All submission and inquiries about this DOE National Laboratory Announcement should reference **LAB 17-1775**.

## **Section I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION**

**GENERAL INQUIRIES ABOUT THIS ANNOUNCEMENT SHOULD BE DIRECTED TO:**

### **Technical/Scientific Program Contacts:**

Dr. Jeffrey L. Krause  
301-903-5827 [Jeff.Krause@science.doe.gov](mailto:Jeff.Krause@science.doe.gov)

### **SUMMARY**

The Office of Basic Energy Sciences (BES) of the Office of Science (SC), U.S. Department of Energy (DOE), announces its interest in receiving applications in Computational Chemical Sciences (CCS) that propose integrated, multidisciplinary teams to perform research to develop validated, public access codes and databases. Computational Chemical Sciences teams could also develop new approaches to enhance the use of large data sets derived from advanced characterization of chemical systems. Computational Chemical Sciences will 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 (HPC). 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 Basic Energy Sciences (BES) program is to support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security. 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/csgeb/>  
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 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 materials and molecules based on theoretical calculations prior to their experimental synthesis. This Funding Opportunity Announcement (FOA) initiates a new activity in Computational Chemical Sciences to 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. In addition, 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, a multidisciplinary team effort is needed to modify or replace existing computational chemistry codes with codes that are well-adapted to current petascale and anticipated exascale architectures.

The Computational Chemical Sciences activity will support basic research to produce open-source codes that design chemical 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 utilize effectively future exascale computing resources. These include: 1) new catalysts to improve the efficiency of chemical processes, make effective use of bioenergy, drive energy conversion processes, and mitigate environmental impact; 2) better models of solar photoconversion processes to improve efficiency of electricity generation by photovoltaics; 3) natural and artificial photosynthesis to unlock the potential of solar driven energy conversion and storage; 4) next generation molecular assemblies to create new functionalities; 5) membranes and molecular complexes composed of solid-gas/liquid interfaces, which are critical for separation technologies for energy and water applications.

In this effort, computational chemists will deploy advanced capabilities in all 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. Further advantages may be obtained by designing algorithms to implement efficiently the expected machine and deep learning capabilities of exascale computers. These complex challenges will require multi-investigator teams that combine theoretical, computational and algorithmic advances with a goal of increasing by at least 1,000 times the accuracy and speed of 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.

## SUMMARY CRITERIA

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

- Focus on computational chemical sciences research. Develop open-source, community based codes that can be deployed on current petascale and future exascale computers to model areas of relevance to BES and to perform accurate and efficient processes and reactions relevant to the BES mission, specifically those related to chemical sciences, geosciences, and biosciences (see section IV.C.2 – Project Narrative, Proposed Research and Methods).
- Explicitly excluded are proposals on quantum computing and areas of primary interest to materials sciences such as quantum materials.
- Focus on research leading to open-source software. Suitable types of software will emphasize strong correlations, excited states, transport, dynamics, and/or electronic or optical properties. Explicitly excluded are proposals that emphasize density functional methods as currently implemented or semi-empirical approaches, dynamical mean field theory, and classical and first principles molecular dynamics.
- Describe a plan to deliver validated research codes and the associated data to academia, National Laboratories, and industry. Software developed under this FOA should have broad applicability. Applicants must describe how the software will be distributed as open-source in an Open-Source Software Distribution Plan.
- Provide a detailed plan for the full utilization of today's petascale and tomorrow's exascale national leadership computing facilities.
- Use integrated, multi-investigator teams combining, where appropriate, expertise in quantum chemistry, theory, modeling, computation, and applied mathematics.
- Articulate a clear management plan that insures a coherent team approach and provides for the maintenance and long-term accessibility of software and data.
- Include a Data Management Plan.
- Provide mechanisms for community input to software and database development and validation.

### References:

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

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

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

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

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



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

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

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

*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](http://www.pnnl.gov/main/publications/external/technical_reports/PNNL-20896.pdf))*

### **Multi-Institutional Awards**

DOE expects a single proposal for each project to be submitted by the Lead Laboratory. Other participant institutions such as universities, industry, non-profit organizations and Federally Funded Research and Development Centers (FFRDCs) should not submit proposals. Funding for participants other than the Lead Laboratory will be by subcontract, except for DOE National Laboratories, which will be funded directly by DOE through the usual FWP process. However, National Laboratories should not submit an FWP to Searchable FWP unless selected for an award. National Laboratories are strongly encouraged to engage University partners.

This solicitation is for DOE National Laboratories only. Proposals from institutions other than DOE National Laboratories will not be accepted.

The Letter of Intent must list all participants and their affiliations. The proposal (not the Letter of Intent) must additionally contain detailed budgets and budget justifications for each participating institution.

### **Collaboration**

Collaborative proposals submitted from different institutions will not be accepted.

## **Section II – AWARD INFORMATION**

### **A. TYPE OF AWARD INSTRUMENT**

DOE anticipates awarding laboratory work authorizations under this DOE National Laboratory Program 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**

DOE expects to make multiple awards for a period of up to four years for each award. Total funding for four years, pending Congressional appropriations, is estimated at \$24,000,000.

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

### **C. MAXIMUM AND MINIMUM AWARD SIZE**

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

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

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

### **E. PERIOD OF PERFORMANCE**

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

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

## **F. TYPE OF PROPOSAL**

DOE will accept new DOE National Laboratory Proposals under this DOE National Laboratory Announcement. 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.

### **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.

## **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 AND PRE-PROPOSAL**

#### **1. Letter of Intent (LOI)**

A Letter of Intent is required and must be submitted by the due date.

**LETTER OF INTENT DUE DATE:  
JUNE 5, 2017 AT 5:00 PM EASTERN TIME**

All submission and inquiries about this Laboratory Announcement should reference LAB 17-1775

**To be considered eligible for an award under this National Laboratory Announcement, potential prime applicants (Lead Laboratories) are *required* to submit a Letter of Intent in accordance with the instructions provided below. Proposals received from an applicant who has not submitted the required Letter of Intent will be deemed non-responsive and will be declined without further review.**

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

**An individual may not be named as the Project Director on more than one Letter of Intent or proposal.** The Project Director is the Lead Principal Investigator and must be employed or have an agreement in place to be hired by the Lead Laboratory. If the proposed Project Director will not be employed by the Lead Laboratory, the proposal will be deemed non-responsive and will be rejected without further review. If more than one qualified LOI is received from an applicant identifying the same individual as the Project Director, DOE will consider only the first qualified LOI received based on the PAMS date and time stamp. The remaining LOIs will be deemed non-responsive and the applicant will not be allowed to submit full applications tied to

those LOIs.

Only one LOI should be submitted for the entire project by the Lead Laboratory/Project Director. The LOI should include, at the top of the first page, the following information:

Title of Letter of Intent  
Project Director Name, Job Title  
Lead Laboratory  
Project Director Phone Number, Email Address  
Laboratory Announcement Number: LAB 17-1775

In addition, the Lead Laboratory on the full proposal must be the same as on the LOI. If a proposal is received for which the Lead Laboratory has changed since submission, then the proposal will be deemed non-responsive and will be declined without further review. The Project Director should not be changed unless unavoidable and only minor edits should be made, if necessary, to the title. If necessary, the applicant may make changes to other senior/key personnel and other participating institutions, although DOE discourages extensive changes.

**This cover page must be signed by an official of the Lead Laboratory who has the authority to commit institutional support for the proposal and by the proposed Project Director.** For DOE National Laboratory applicants, the institutional official should be the Laboratory Director. **All applicants must include both of these signatures on the LOI.** Applicants that fail to provide both signatures will be required to provide a corrected LOI with both signatures within one week after June 5, 2017 in order for their full proposal to be considered for award.

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

The LOI is also used to help in planning the review and the selection of potential reviewers for the proposal.

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

**Table 1: Team Members (Project Director, PIs\*, Task Leaders and Senior/Key Personnel) on the proposal and institutional affiliations**

Team Members			Institution
Last Name	First Name	Title	Institution Name

\*Note: This category refers to PIs other than the Lead PI (Project Director) and includes institutional technical leads for other than the lead laboratory.

**Table 2: Collaborators of Team Members**

Collaborator			Institution
Last Name	First Name	Title	Institution Name

For all team members, Table 2 must include co-authors over the past 48 months, graduate and postdoctoral advisors, graduate students and postdoctoral associates that have been supervised during the past 60 months, and any other current close associations.

**Table 2 should exclude all personnel at any of the institutions listed in Table 1.**

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 LOI. **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 an 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 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](mailto: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](mailto:sc.pams-helpdesk@science.doe.gov).

## **2. Pre-proposal**

A Pre-proposal is not required or invited.

## **C. CONTENT AND PROPOSAL FORMS**

PROPOSAL DUE DATE

**July 17, 2017 at 5:00 PM Eastern Time**

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.

LETTERS

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

## RENEWAL APPLICATIONS

This announcement is for new applications only. Renewal applications will not be accepted.

## 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 proposal and when DOE makes the proposal 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 proposals. 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 your program manager to resolve any confusion about which version of a proposal should be considered.

## 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 – 20 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
  - 7
  - Appendix 7: Open-Source Software Distribution Plan
  - Appendix 8: Other Attachments (optional)

## SUBMISSION INSTRUCTIONS

Full 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](mailto:sc.pams-helpdesk@science.doe.gov). All submissions and inquiries about this Program Announcement should reference **LAB 17-1775**. Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than **July 17, 2017** 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](mailto: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](mailto:sc.pams-helpdesk@science.doe.gov). All submissions and inquiries about this Program Announcement should reference **LAB 17-1775**.

## 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.

The designated Lead Laboratory, i.e., the prime applicant, must perform a greater percentage of the effort than any other partner organization or subawardee. The percentage of effort will be determined by reviewing the total budget for each participating organization as a percentage of proposed total project costs. **If a proposal is received in which the prime applicant is not performing a greater percentage of the effort (based on budget distribution) than each of the other institutional partners, team members, or subawardees, the proposal will be deemed non-responsive and declined without further review.**

### 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 Project Director (PD), 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 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. 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:
- Project Director name, telephone number, email:
- DOE National Laboratory Announcement Number: **LAB 17-1775**
- DOE/Office of Science Program Office: Office of Basic Energy Sciences
- DOE/Office of Science Program Office Technical Contact: Jeffrey Krause
- PAMS Letter of Intent Tracking Number:

On separate pages, as a supplement to the cover page, include the following three tables providing personnel and budget information for the entire project (including all institutions). Note Tables 1 & 2 are the same (possibly updated) as those submitted in the LOI.

**Table 1: Team Members (Project Director, PIs\*, Task Leaders and Senior/Key Personnel) on the application and institutional affiliations**

Team Members			Institution
Last Name	First Name	Title	Institution Name

\*Note: This category refers to PIs other than the Lead PI (Project Director) and includes institutional technical leads for other than the lead laboratory.

**Table 2: Collaborators of Team Members**

Collaborator			Institution
Last Name	First Name	Title	Institution Name

For all team members, Table 2 must include co-authors over the past 48 months, graduate and postdoctoral advisors, graduate students and postdoctoral associates that have been supervised during the past 60 months, and any other current close associations.

**Table 2 should exclude all personnel at any of the institutions listed in Table 1.**

**Table 3: Budget by Institution**

Institution	Team Member	Role	Y1 Budget	Y2 Budget	Y3 Budget	Y4 Budget	Total Budget

<b>Total</b>							

Tables 1-3 will not count in the project narrative page limitation.  
**PROJECT NARRATIVE (NO MORE THAN 20 PAGES LONG)**

The Project Narrative comprises the research plan for the project. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The 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.

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 as well as a review of the relevant literature.

**Proposed Research and Methods:** Applicants must provide detailed information regarding the proposed research. This section should demonstrate the close integration of the proposed research activities aimed at meeting the four-year scientific goals and how these will result in new capabilities in computational chemical sciences. This section may be organized into subtasks and should include a description of:

- A balanced and comprehensive research program that develops open-source codes that can be deployed on future exascale computers, including algorithms that can efficiently use machine and deep learning capabilities. This software will model accurate and efficient processes and reactions relevant to the BES mission in chemical sciences, geosciences, and biosciences. Areas of interest include:

- 1) new catalysts to improve the efficiency of chemical processes, make effective use of bioenergy, drive energy conversion processes, and mitigate environmental impact;
  - 2) better models of solar photoconversion processes to improve efficiency of electricity generation by photovoltaics;
  - 3) natural and artificial photosynthesis to unlock the potential of solar driven energy conversion and storage;
  - 4) next generation molecular assemblies to create new functionalities; and
  - 5) membranes and molecular complexes composed of solid-gas/liquid interfaces, which are critical for separation technologies for energy and water applications.
- The scientific basis for the software to be developed and how it will be further developed;
  - How the software will be validated using existing data and/or data generated through this project (note that an experimental component is not required for this proposal);
  - How the software will exploit the capabilities of today's petascale and tomorrow's exascale national leadership computing facilities;
  - The role and intellectual contribution of the Project Director, task leaders, and each other senior /key person in the application;
  - The plans for development and/or utilization of unique facilities, capabilities, or approaches to address the scientific goals.

**Timetable of Activities:** Timeline for all major activities including milestones and deliverables.

**Project Management Plan:** Multi-institutional proposals must include a project management plan that clearly indicates the roles and responsibilities of each organization and indicates how activities will be coordinated and communicated among team members including the following:

- Describe the strategy and plan for project operations, the means of achieving an integrated research and development team, and plans for leadership and guidance for the scientific and technical direction of the project;
- Describe how the potential community that will use the software will be engaged;
- Describe how codes and data will be developed, maintained and shared;
- Define an organizational structure that delineates the roles and responsibilities of senior/key personnel and describes the means of providing oversight and guidance for scientific and technical direction of the project;
- Define proposed management processes for evaluation of research progress, decision making across the team, handling of intellectual property; and intra-team communication;
- Describe the availability of the Project Director, co-principal investigators, and other senior/key personnel, including their potential involvement in other major projects.

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

#### 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 2 pages when printed on 8.5" x 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 5 professional and scholarly activities related to the effort proposed.

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

- **Collaborators and Co-editors:** List in alphabetical order all persons, including their current organizational affiliation, who are, or who have been, collaborators or co-authors with you on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of this 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.

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

included in the two page limit for each biographical sketch.

**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 subawardees, for ongoing projects and pending proposals. List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid.

For every activity, list the following items:

- The sponsor of the activity or the source of funding
- The award or other identifying number
- The title of the award or activity
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The person-months of effort per year being dedicated to the award or activity
- A description of the similarities, differences, and synergies of the award or activity with the research described in the current proposal.

Provide the Current and Pending Support as an appendix to your project narrative. Concurrent submission of a proposal 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 subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. For proposed investigations requiring access to experimental user facilities maintained by institutions other than the applicant, please provide a document from the facility manager confirming that the researchers will have access to the facility. Please provide the Facility and Other Resource information as an appendix to your project narrative.

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

#### APPENDIX 5: 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: OPEN-SOURCE SOFTWARE DISTRIBUTION PLAN

Applicants are required to submit an Open-Source Software Distribution Plan as part of their Full Application. This plan describes how software produced under this Announcement will be distributed. Submission of an Open-Source Software Distribution Plan is required. Proposals that do not have an Open-Source Software Distribution Plan will be deemed non-responsive and will not be reviewed..

The plan must include the following elements:

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

or others when multiple parties will contribute to the development of the software or the FOA requires that the software or other information be shared or disseminated to others.

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

- Provide “Open-Source Software Distribution Plan” as Appendix 7 to the Project Narrative within the same file. Do not attach a separate file; and

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).
- **Subawards/Consortium/Contractual Costs:** Enter total costs for all subawards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details.

**Equipment or Facility Rental/User Fees:** Enter total funds requested for Equipment or Facility Rental/User Fees. In the budget justification, identify each rental/user fee and justify. In the budget justification, indicate whether cost estimates are based upon past experience with similar or like items; vendor quotes of similar items; or something else (describe).

- **Alterations and Renovations:** Enter total funds requested for Alterations and Renovations.
- **In the budget justification,** itemize by category and justify the costs of alterations and renovations, including repairs, painting, removal or installation of partitions, shielding, or air conditioning. Where applicable, provide the square footage and costs.
- **Other:** Add text to describe any other Direct Costs not requested above. Enter costs associated with “Other” item(s). Use the budget justification to further itemize and justify.

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

June 5, 2017 at 5:00 PM Eastern Time

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

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

A Pre-proposal is not required or invited.

### **3. Proposal Due Date**

July 17, 2017 at 5:00 PM Eastern Time

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

### **4. Late Submissions**

Delays in submitting letters of intent, pre-proposals, 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 Program Office/Manager listed in this Funding Opportunity Announcement to discuss the option of a late submission. Contacting the Program Office/Manager after the deadline may reduce the likelihood that a request will be granted.

DOE notes that not all requests for late submission will be approved.

You may be able to submit your proposal in response to the currently available Office of Science Annual Solicitation. Please contact the Program Office/Manager listed in this Laboratory Announcement to discuss this option.



## **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](mailto:sc.pams-helpdesk@science.doe.gov). All submission and inquiries about this DOE National Laboratory Program Announcement should reference **LAB 17-1775**.

### **3. Proposal Receipt Notices**

Upon submission, the PI will receive an email from the PAMS system <[PAMS.Autoreply@science.doe.gov](mailto:PAMS.Autoreply@science.doe.gov)> acknowledging receipt of the 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 to determine that (1) the applicant is eligible for the award; (2) the information required by the Program Announcement has been submitted; (3) all mandatory requirements are satisfied; (4) the proposed project is responsive to the objectives of the Program Announcement, and (5) the proposed project is not duplicative of programmatic work. Proposals 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**

The application will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria, which have approximately equal weight. The bulleted information after each are intended to guide the reviewers; reviewers will not be required to provide written responses to each of these.

- 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;
- Reasonableness and Appropriateness of the Proposed Budget;
- Strength of the Management Plan;
- Synergy and Integration Among the PIs;
- Development and Utilization of Unique Facilities, Capabilities or Approaches.

#### **SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROJECT**

- Assess how the results of the proposed work will impact the direction, progress, and thinking in relevant scientific fields of research. What is the likelihood of achieving influential results?
- Describe the science proposed by this collaboration that is not feasible now.
- Assess whether the plan for basic research is consistent with BES priorities as expressed in BES reports and the specific topics targeted by this Announcement.
- Is the Data Management Plan suitable for the proposed research; to what extent does it make the data available and useful to the scientific community?

#### **APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH**

- Assess the appropriateness of the proposed scientific methods and approaches detailed in the proposal to achieve the stated scientific goals.
- Assess the strategy and the plan for the development and operation of the project including the need for the proposed collaboration, the means for achieving an integrated

team of the indicated scientists and applied mathematicians or computer scientists, and plans for leadership and guidance for the scientific and technical direction.

- Evaluate the appropriateness of the performance metrics that will allow progress and contributions to be measured.
- Are the plans (if any) for external collaborations and partnerships reasonable and appropriate?
- Evaluate the proposed approach for making the code and any associated data available to general users from the research community, including the Open-Source Software Distribution Plan. Describe the plan for obtaining input from the community that would use the software and any associated data.

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

- Do the Project Director and the other Team Members have a proven record of research in the disciplines needed for success in this project?
- Will the Project Director and the other Team Members have sufficient time to devote to this project, taking into account their potential involvement in other major projects?
- How does the proposed research exploit existing resources or contribute new resources (e.g., algorithms, software) or would it result in a duplication of existing resources?

#### REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET

- Assess the appropriateness of the budget to support all elements of the collaboration.
- Does the collaboration rely upon efforts by unpaid contributors? If so, what evidence suggests that these collaborations will continue over the lifetime of the proposed research?
- How does the requested budget relate to the proposed project structure?

#### STRENGTH OF THE MANAGEMENT PLAN

- Is there a clear lead organization and a qualified Project Director?
- Evaluate the comprehensiveness of the management plan and the organizational structure that delineates the roles and responsibilities of the team members.
- Assess how the project timeline will allow progress and contributions to be measured over the course of the research.
- If needed, is there a well-defined strategy to use state-of-the-art technology and frequent virtual meetings to enable meaningful, efficient long distance collaboration?

#### SYNERGY AND INTEGRATION AMONG THE PIs

- Evaluate the proposed approach to create a well-integrated, interdisciplinary team in order to address the scientific and computational goals.
- Assess whether the proposed collaboration will result in advances that would not have been accomplished by those same researchers working separately. Have the applicants defined scientific problems that are likely to be addressed only through close collaboration among the researchers on the application?

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

- Will the proposed research accelerate scientific discovery through the effective use DOE High-Performance Computing (HPC)? Assess the proposed plan for the utilization of DOE HPC resources within the period of performance and the potential impact of these resources on the project.
- Can this project be completed on computing platforms that are currently available or are expected to be available?
- Evaluate the proposed development of unique facilities, capabilities, or approaches to achieve the stated scientific goals. How do these compare with similar developments in the field?

## 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. Selection

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

- Scientific and technical merit of the proposed activity as determined by merit review
- Availability of funds
- Relevance of the proposed activity to Office of Science priorities
- Ensuring an appropriate balance of activities within Office of Science programs
- Previous performance

### 3. 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

It is anticipated that the award selection will be completed by September 1, 2017. It is expected that awards will be made in Fiscal Year 2017.

DOE is interested in seeing projects supported under this Announcement begin work by September 30, 2017.

## **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](mailto:sc.pams-helpdesk@science.doe.gov). All submission and inquiries about this DOE National Laboratory Program Announcement should reference LAB 17-1775.

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 DOE National Laboratory Program Announcement or 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 <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>
Program Manager Scientific Contact	Basic Energy Sciences, SC-22 Dr. Jeffrey L. Krause 301-903-5827 <a href="mailto:Jeff.Krause@science.doe.gov">Jeff.Krause@science.doe.gov</a>

## **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.