

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



**DATA SCIENCE FOR DISCOVERY IN CHEMICAL AND
MATERIALS SCIENCES**

**DOE NATIONAL LABORATORY PROGRAM ANNOUNCEMENT NUMBER:
LAB 19-2082**

ANNOUNCEMENT TYPE: AMENDMENT 000001

**This Amendment 000001 is to change the dates of the Pre-Proposal
Response Date and the Submission Deadline for Proposals.**

Announcement Issue Date:	February 7, 2019
Submission Deadline for Letter of Intent:	N/A
Submission Deadline for Pre-Proposal:	March 8, 2019 at 5:00 PM Eastern Time A Pre-Proposal is required
Pre-Proposal Response Date:	April 12, 2019
Submission Deadline for Proposals:	May 22, 2019 at 5:00 PM Eastern Time

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REGISTRATIONS

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

The Department of Energy (DOE) Office of Science (SC) 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 SC 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 submissions and inquiries about this DOE National Laboratory Announcement should reference .

LAB 19-2082.

UPDATES AND REMINDERS

RECOMMENDATION

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

PRE-PROPOSAL REVIEW

Pre-proposals will be comparatively reviewed by DOE SC program managers to determine which pre-proposals may yield the most competitive proposals. Interested lead applicants are required to submit a pre-proposal in accordance with the instructions provided in Section IV.B.2, and to receive notification from DOE that they are encouraged to submit a proposal. Proposals received from an applicant who has not submitted the required pre-proposal, or who has received notification from DOE that they are discouraged from submitting a proposal, may be declined without further review.

All applicants must submit pre-proposals.

DATA MANAGEMENT PLAN

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

ACKNOWLEDGMENT OF FEDERAL SUPPORT

SC 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 SC awards.

- Please ensure that the research narrative is comprised of one and only one Portable Document Format (PDF) file, including all appendices, when it is uploaded.
- When using the PAMS website at <https://pamspublic.science.energy.gov>, please avoid using the back-arrow button in your web browser to navigate.
- Please ensure that the proposal 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:

Technical/Scientific Program Contacts:

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Biosciences Division

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SUMMARY

The DOE SC program in Basic Energy Sciences (BES) announces its interest in receiving new proposals in Data Science for Knowledge Discovery for Chemical and Materials Research with the aim of advancing the use of modern data science approaches (artificial intelligence, machine learning, graph theory, uncertainty quantification, etc.) to accelerate discovery in chemical and materials sciences. This funding opportunity is the first in this topical area sponsored by BES.

The program will support efforts (up to \$1,000,000 per year) for research with a focus on applying data science approaches and tools for experimental, theoretical/computational, or synergistic experimental/theoretical/computational research in areas supported by BES. Although the research may involve the development of new data science approaches, the focus of the effort should be on advancing understanding of fundamental properties and processes in chemical and materials systems.

SUPPLEMENTARY INFORMATION

BACKGROUND

Data science combines computer science, applied mathematics, and statistics with domain science to discover new knowledge from often complex (such as unstructured) data sets generated from experimental and/or computational studies. As part of data science, machine learning and artificial intelligence methods are rapidly evolving and leading to more accurate predictions and trustworthy decisions and actions. Thus, these methods are being applied widely in society. While scientific research has benefited greatly in many areas such as the chemical and materials sciences as well as bioinformatics, medicine, drug discovery, systems control, astronomy and particle physics, many opportunities remain for data science to accelerate the rate of fundamental discovery for complex chemical processes and materials. Recent public reports outline some of the emerging opportunities, such as the National Academies report titled [Data](#)

[Science: Opportunities to Transform Chemical Sciences and Engineering](#); some of the DOE-BES [Basic Research Needs Workshops](#); the NSF-sponsored report on [Framing the Role of Big Data and Modern Data Science in Chemistry](#); and the multi-agency sponsored report on the [Materials Acceleration Platform: Accelerating Advanced Energy Materials Discovery by Integrating High-Throughput Methods with Artificial Intelligence](#). These reports and other publications conclude that data science is contributing to a new paradigm in scientific research methodology.

Synergistically complementing theory, experimentation, and simulation, data science has already demonstrated some success in accelerating molecular and materials discovery. The next goal for this methodology is to generate new fundamental understanding of physical and chemical behavior, leading to successful predictions well outside the range of the original data, and possibly forcing modifications to the theoretical approaches. One specific area of interest to BES-supported research is that of complex chemical and materials processes, defined as those whose macroscopic properties, reaction mechanisms and dynamic behavior cannot be predicted from a known combination of the properties of the individual components, hence are outside the scope of existing theoretical approaches. Complex systems involve massive combinatorial spaces and nonlinear processes, which are being slowly tackled with large experimental, theoretical and computational efforts. Data science approaches, in combination with standard experimental and theoretical methods, are expected to accelerate the discovery of fundamentally new chemical mechanisms and material systems with exceptional properties and dynamic behavior, as well as new physical principles or laws. The specific energy-related topics of interest for this FOA, and those excluded, are mentioned below.

ADDITIONAL REQUIREMENTS

To be considered, a proposal must address the specific Eligibility requirements in Section III and the Review Criteria in Section V. In addition, proposals must:

- Focus on innovative applications of modern data science approaches (artificial intelligence, machine learning, graph theory, uncertainty quantification, etc.) to the research of complex energy-relevant chemical and materials systems to develop new and/or more accurate description of emergent behavior, processes, and mechanisms. A priority outcome from this research should be novel, robust, data-driven, hypothesis-based models that lead to improved understanding. Use of these data models should fill knowledge gaps, correct erroneous predictions based on existing models, extract knowledge from noisy data, and ideally extrapolate beyond the range of the available datasets. Identifying new physical descriptors may be important to manage the complexity of multidimensional datasets and enable inverse or statistically driven design concepts.
- Propose experimental, theoretical/computational, or synergistic experimental/theoretical/computational research that fits within the scope and priorities of core research activities within the BES Chemical Sciences, Geosciences, and Biosciences Division and/or Materials Sciences and Engineering Division. The proposed activity must be aligned with the existing BES portfolio at the National Laboratory leading the proposal. Of special interest is accurate modeling of the mechanisms of chemical and materials processes under exposure to thermal or radiative environments or driven excitations, with the purpose of predicting long-term dynamics.
- Address at least one of the following topics:

- Reaction chemistry across multiple scales in complex environments important in geosciences, catalysis, biochemistry or electrochemistry
- Synthesis science including nucleation, growth and restructuring of hybrid, hierarchical or other complex materials
- Far from equilibrium phenomena where dynamics is fast, such as in transport and separation in complex systems
- Behavior of properties and processes in extreme environments (e.g., radiation, corrosion, stress, pressure, temperature, electric and magnetic fields)
- Discovery of quantum materials and/or their collective, coherent, and strong correlation phenomena

Applicants are referred to relevant Basic Research Needs Workshop reports and the described priority research directions, in particular Quantum Materials, Synthesis Science, Energy and Water, Catalysis Science, and Future Nuclear Energy:

<https://science.energy.gov/bes/community-resources/reports/>.

This lab announcement will NOT consider proposals in certain topics or areas including:

- Quantum computing or quantum systems for quantum information science; energy storage; “omics” data and systems biology approaches; applied research, such as design or optimization of instruments, devices, tools or processes; an exclusive focus on database development and management; studies demonstrating the feasibility or performance of methods as the main or only goal; developments contributing to proprietary products; and research that could be supported by other programs, such as SBIR/STTR.
- Areas covered by the BES Scientific User Facilities Division, such as the development of data science approaches for reduction or analysis of large volumes of data from scientific user facilities as the main goal.
- Streaming data analytics, data management, visualization, and software and computational technologies such as supported by the Office of Advanced Scientific Computing Research and mentioned in the [FY 2019 Continuation of Solicitation from the Office of Science](#) (pp. 5-6).

The proposed efforts should integrate the appropriate types of expertise necessary to advance the state-of-the-art in the basic science of the chosen chemical or material challenges as well as in the proposal of data science to pursue those challenges. New data science approaches are expected to accelerate discovery, design, synthesis, characterization, modeling, and simulation for materials science and chemistry.

Open Science

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

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

Collaboration

Collaborative proposals, e.g. submissions of identical proposals by different institutions, will not be accepted. Proposals involving multiple institutions must be submitted by a single lead national laboratory.

Section II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT

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

DOE will consider funding multi-institution collaborations under this lab announcement. Entities proposing as a team must designate a lead organization. Pre-proposals and proposals must be submitted on behalf of the team members by the lead organization. Only one pre-proposal and one proposal is to be submitted for each team.

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

It is anticipated that up to \$20,000,000 (approximately \$6,667,000 annually for up to 3 years) will be available under this DOE National Laboratory Announcement, contingent on satisfactory peer review and the availability of appropriated funds. Up to 7 awards are expected. Proposers should request project support for three years.

Following the first year award, out-year support will be contingent on the availability of appropriated funds, progress of the research, and programmatic needs. Awards are expected to begin in fiscal year 2019.

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

C. MAXIMUM AND MINIMUM AWARD SIZE

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

Ceiling: \$1,000,000 per year

Floor: \$300,000 per year

D. EXPECTED NUMBER OF AWARDS

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

E. ANTICIPATED AWARD SIZE

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

F. PERIOD OF PERFORMANCE

DOE anticipates making authorizations with a project period of three 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 only 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. SC 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. A parallel, companion funding opportunity announcement (DE-FOA-0002082) is available for proposals led by other eligible institutions.

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 Principal Investigator (PI) 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. LIMITATIONS ON SUBMISSIONS

Limitation on Number of Proposals per Laboratory

A national laboratory may not submit more than three pre-proposals or proposals as the lead organization. If more than three proposals or pre-proposals are received from a national laboratory, DOE will consider only those proposals that match a qualified pre-proposal (as described below in Section IV.B.2). The remaining proposals will be declined without further review. However, there is no limitation on the number of proposals in which a national laboratory may participate as a team member or subawardee.

Lead PI

Proposals with more than one investigator, including proposals with multiple institutions, must designate one and only one investigator as the Lead Principal Investigator, who will exercise overall scientific control and direction of the proposed research. The Lead PI must be employed by or have a written agreement in place to be hired by the applicant institution. If the proposed Lead PI will not be employed by the lead organization at the time of award, the proposal will be declined without further review.

Limitation on Number of Proposals per Lead PI

An individual may be the lead PI on no more than one proposal. If more than one proposal is received with the same individual identified as the Lead PI, the last received proposal that matches a qualified pre-proposal (as described in Section IV, Part B.2, below) will be accepted: All other proposals will be declined without review.

Note that there is no limitation on the number of proposals in which an individual may participate in other roles: the limitation is only on serving as the Lead PI on more than one proposal. A Lead PI may serve as a co-investigator on other proposals.

Section IV – PROPOSAL AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST PROPOSAL PACKAGE

Proposal submission instructions are available in this Announcement on the DOE SC 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

Not applicable.

2. Pre-proposal

A pre-proposal is required.

PRE-PROPOSAL DUE DATE

March 8, 2019 at 5:00 PM Eastern Time

ENCOURAGE/DISCOURAGE DATE

April 12, 2019

A pre-proposal must be submitted by the date and time listed above. The pre-proposal must be submitted electronically through the DOE SC Portfolio Analysis and Management System (PAMS) website <https://pamspublic.science.energy.gov/>.

Entities proposing as a team must designate a lead organization. Pre-proposals must be submitted on behalf of the team members by the lead organization. Pre-proposals will be reviewed as outlined below. DOE will send a response by email to each applicant encouraging or discouraging the submission of a proposal by the date shown above. Applicants who have not received a response regarding the status of their pre-proposal by this date are responsible for contacting the program to confirm this status. Only those applicants that receive notification from DOE encouraging a proposal are encouraged to submit a proposal. Other proposals may be declined without review.

Note that a national laboratory can submit only three pre-proposals as the lead organization. If more than three pre-proposals are received that include the required signature from a senior laboratory official, the PAMS timestamp will be used to determine the pre-proposals eligible for further review. Pre-proposals are required.

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

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

Title of Preproposal
Lead Principal Investigator Name, Job Title
Institution
Lead PI Phone Number, Email Address
Laboratory Announcement Number: LAB 19-2082
Estimated Annual Budget Request:
Estimated Annual Budget Request by Each Institution:
Signature of the Laboratory Official*:

* A signature of a senior laboratory official who is authorized to commit the Laboratory to perform research is required. This signature on the pre-proposal also indicates that partner institutions have been appropriately engaged in the preparation of the pre-proposal.

Note: All the information above is required. Pre-proposals that are missing any of the above will be considered non-responsive and declined without review.

If a pre-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 pre-proposal will be deemed non-responsive and rejected without further review.

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

The pre-proposal must describe how the research will advance research described in Section I of this announcement, Supplementary Information. Applicants must describe how the research fits within the scope and priorities of the BES research divisions and are encouraged to review the descriptions of the BES Core Research Activities, which can be found on the BES website at: <https://science.energy.gov/bes/research/>.

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

1. On a separate page, the pre-proposal must include a list of the names and institutional affiliations of all participating investigators, including funded collaborators and consultants on the proposed project (one name per line with institutional affiliation, i.e., last name, first

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

PRE-PROPOSAL REVIEW

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

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

The review will be conducted by no less than three federal program managers chosen for their topical knowledge and diversity of perspective. Reviews will be comparative for pre-proposals within topical areas with priority given to scientifically innovative and forward-looking basic research with the highest likelihood of success as a proposal, including consideration of BES programmatic priorities. The results of the review will be documented.

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

SC is committed to ensuring that a sufficient number of applicants will be encouraged to submit proposals to foster a competitive merit review of the proposals. DOE expects to allow approximately 22 proposals, with the exact number based on the review. The intent in discouraging submission of certain proposals is to save the time and effort of applicants in preparing and submitting proposals with a negligible likelihood of success.

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

PRE-PROPOSAL SUBMISSION

It is important that the pre-proposal be a single file with extension .pdf, .docx, or .doc. The filename must not exceed 50 characters. The pre-proposal must be submitted electronically through the DOE SC Portfolio Analysis and Management System (PAMS) website

<https://pamspublic.science.energy.gov/>. The Principal Investigator and anyone submitting on behalf of the Principal Investigator must register for an account in PAMS before it will be possible to submit a pre-proposal. All PIs and those submitting pre-proposals on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays.

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

Please see **A. DOE Office of Science Portfolio Analysis and Management System (PAMS)** under Registrations, above, for instructions about how to register in PAMS.

Submit Your Pre-Proposal:

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

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

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

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this National Laboratory Announcement should reference LAB 19-2082.

Preproposals submitted outside PAMS will not be considered. Preproposals may not be submitted through grants.gov or www.FedConnect.net.

C. CONTENT AND PROPOSAL FORMS

PROPOSAL DUE DATE

May 22, 2019 at 5:00 PM Eastern Time.

Files that are attached to the forms must be PDF files 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.

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

RESUBMISSION OF PROPOSALS

Proposals submitted under this Announcement may be withdrawn from consideration by using SC’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.

SC 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.

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 organizational commitment are required for each organization participating as a team member. Letters stating commitment to the project are required of any unfunded collaborator. (See Appendix 7: Letters of Commitment).

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

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 (required for each team member)
- 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)
- 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
- Appendix 8: List of Collaborators
- Appendix 9: Other Attachment

SUBMISSION INSTRUCTIONS

Completed proposals must be submitted into the DOE SC 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 19-2082**. Proposals submitted in response to this Program Announcement must be submitted to PAMS May 22, 2019.

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. SC 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 19-2082**.

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 must 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 must be a self-contained document that identifies the name of the applicant, the Lead 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 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 must 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.

- Project title:
- Applicant/Institution:
- Street Address/City/State/Zip:
- Postal Address:
- Lead PI name, telephone number, email:
- Administrative Point of Contact name, telephone number, email:
- DOE National Laboratory Announcement Number: **LAB 19-2082**
- DOE/SC Program Office: Basic Energy Sciences
- PAMS Preproposal Number:

- Signature of the Laboratory Official*:

(*)A signature of a senior laboratory official who is authorized to commit the Laboratory to perform research is required. This signature on the proposal also indicates that partner institutions have been appropriately engaged in the preparation of the proposal.

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

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

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

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 and the associated principal investigator list and budget summary table, 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.”

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.

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

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

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

Management Plan and Timeline of Activities: For all proposals, this section should include a timeline for all major research tasks. Note that letters of commitment are required for all funded partner institutions and unfunded collaborators (Appendix 7). For multi-investigator research, this section should also 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.

Project Performance Site(s) [Required for teams involving more than one institution]: Identify and describe the site(s) where the work will be performed. Work sites at all partner institutions should be briefly described. Appendix 4 should include detailed information about facilities, equipment, and capabilities available for the research. Costs for new construction (including new buildings or additions to existing buildings) will not be allowed in the award.

APPENDIX 1: BIOGRAPHICAL SKETCH

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

- Provide the biographical sketch information as an appendix to your project narrative.
- Do not attach a separate file.
- The biographical sketch appendix will not count in the project narrative page limitation.
- The biographical information (curriculum vitae) for each person must not exceed 2 pages when printed on 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point. The biographical information (curriculum vitae) must include the following items within its page limit:
 - **Education and Training:** Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.
 - **Research and Professional Experience:** Beginning with the current position list, in chronological order, professional/academic positions with a brief description.
 - **Publications:** Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same

sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications. An abbreviated style such as the Physical Review Letters (PRL) convention for citations (list only the first author) may be used for publications with more than 10 authors.

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

In addition, DOE requires information to identify individuals who are conflicted with or potentially biased (favorably or unfavorably) against the investigators. **Include this information in Appendix 8 as a single list for all PIs.**

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

APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support (both Federal and non-Federal) for the PI and senior/key persons, including subawardees, for ongoing projects and pending 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 lead PI of the award or activity
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The total cost or value of funds supporting the individual submitting the current and pending support
- The award period (start date – end date).
- The person-months of effort per year being dedicated to the award or activity
- Briefly describe the research being performed and explicitly identify any overlaps or synergies with the proposed research.

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

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

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

APPENDIX 5: EQUIPMENT

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

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

APPENDIX 6: DATA MANAGEMENT PLAN

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

1. DMPs should describe whether and how data generated in the course of the proposed research will be shared and preserved. If the plan is not to share and/or preserve certain data, then the plan must explain the basis of the decision (for example, cost/benefit considerations, other parameters of feasibility, scientific appropriateness, or limitations discussed in #4). At

a minimum, DMPs must describe how data sharing and preservation will enable validation of results, or how results could be validated if data are not shared or preserved.

2. DMPs should provide a plan for making all research data displayed in publications resulting from the proposed research 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 SC User Facilities, researchers should consult the published description of data management resources and practices at that facility and reference it in the DMP. Information about other SC facilities can be found in the additional guidance from the sponsoring program.
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 SC research proposal merit review process. Applicants are encouraged to consult the SC website for further information and suggestions for how to structure a DMP: <http://science.energy.gov/funding-opportunities/digital-data-management/>

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

APPENDIX 7: LETTERS OF COMMITMENT

If applicable, a single organizational letter of commitment is required from each organization participating as a team member. Each organizational letter of commitment is limited to one page, must be specific to the proposal, and must be signed by a person authorized to commit the participating organization to a legally binding agreement for this project. (For DOE National Laboratories, the person authorized to legally commit the institution to participate in the proposal will be a senior laboratory official. If this letter is signed by a person who is not authorized to commit the national lab to the research, the proposal will be declined without peer review.)

Letters of commitment from unfunded collaborators are also required; these letters are limited to one-page and must be specific to the proposed research.

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

APPENDIX 8: LIST OF COLLABORATORS

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

- All persons who are, or who have been, collaborators or co-authors of papers, book or book articles, reports, or abstracts, during the 48 months preceding the submission of this proposal. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the PI interacted on a regular basis while the research was being done.
- Include any individuals who are currently, or have been, co-editors with any PI on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of this proposal.
- Include graduate and postdoctoral advisors and past advisees, including the names and current organizational affiliations of the PIs' graduate advisor(s) and principal postdoctoral sponsor(s) as well as the names and current organizational affiliations of past graduate students and postdoctoral associates.

APPENDIX 9: 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 must 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 must be included after the budget pages. The justification must cover labor, domestic travel, equipment, materials and supplies, and anything else that will be covered with project funds.

All DOE National Laboratories receiving funding as part of the proposed work must be proposed as subawards to the applicant institution. The applicant institution and any other DOE National Laboratory may propose an unlimited number of other subawards. All proposed first-tier subawards (those to be funded by the applicant institution or broken out for separate funding by DOE) must be accompanied by a complete subaward budget in the PAMS website. Second- and third-tier subawards (those to be funded by an institution other than the applicant institution) do not require a complete PAMS subaward budget, but their details must be explained in the budget

justification. The explanation of costs for second- and third-tier subawards must include a listing of the costs at the same budget categories as the main (or first-tier) budgets: Senior/Key Personnel, Other Personnel (by category), Equipment, Travel, Participant/Trainee Costs, Other Direct Costs (materials and supplies, publications, consultants).

The budget justification must be attached as one file, including a detailed justification for the applicant institution, a detailed justification for all first-tier subawards, and a summary explanation of the costs for all second- and third-tier subawards.

Proposals that do not include detailed budgets and justifications for first-tier subawards, including all participating DOE National Laboratories, will be considered incomplete.

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 (i.e., Lead PI and PIs), 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, provide detailed information on how the funding would be

distributed by the subcontractor (e.g., level of effort for PIs and other types of participants, equipment, materials, travel, etc.) in text or a simple table.

- **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

Not applicable

2. Pre-proposal Due Date

March 8, 2019 at 5:00 PM Eastern Time

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

3. Proposal Due Date

May 22, 2019 at 5:00 PM Eastern Time

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

4. Late Submissions

Delays in submitting 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.

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 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.

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. SC 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 Program Announcement should **reference LAB 19-2082**.

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 FOA has been submitted; (3) all mandatory requirements are satisfied; and (4) the proposed project is responsive to the objectives of the funding opportunity announcement (See Section I, Supplementary Information). In addition to the criteria required by regulation, DOE will apply the following criteria in its initial review of proposals: (5) the proposed project is not duplicative of current programmatic work; (6) for multi-institutional proposals, the lead institution is performing the largest percentage of the effort as determined by the budget allocations (proposals that do not include budget information for all participating institutions will be considered non-responsive); and (7) there is a corresponding, qualified pre-proposal for the proposal. Proposals that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

Be advised that proposals with a primary focus on advancing data science (e.g., applied mathematics and algorithm development) without application to fundamental science issues under investigation by BES-supported researchers are out of the scope of this Announcement. All proposals must have an encouraged pre-proposal and must be submitted by the same institution that submitted the pre-proposal. All proposals must have a Data Management Plan. Proposals for which the lead institution does not receive the largest percentage of funding compared to partnering institutions will be considered non-responsive.

2. Merit Review Criteria

Proposals will be subjected to scientific merit review (peer review). The proposal will be evaluated against the following criteria, with the first four listed in descending order of importance.

- 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, DOE will ask its merit reviewers to evaluate:

- 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 a proposal constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

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

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 Data Science related research?
- 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 the broader team of researchers?
- 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 proposal's management plan, including the proposed timeline?
- For multi-investigator research, how will synergy be achieved 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 SC-BES priorities (see <https://science.energy.gov/bes/csgb/> and <https://science.energy.gov/bes/mse/>)
- Ensuring an appropriate balance and diversity for activities within SC-BES programs
- Performance under current awards
- Delineation of the scope of the proposed research from other research activities in which the principal investigators are involved, particularly those supported by DOE and by other federal agencies
- 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

It is anticipated that the award selection will be completed by September 2019. It is expected that awards will be made in Fiscal Year 2019.

Section VI - AWARD ADMINISTRATION INFORMATION

A. AWARD NOTICES

1. Notice of Selection

Selected Applicants Notification: DOE will notify applicants selected for award. This notice of selection is not an authorization to begin performance.

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 period.

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 Program Announcement should reference **LAB 19-2082**.

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 sc.pams-helpdesk@science.doe.gov
Program Managers Scientific Contacts	Dr. Raul Miranda, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division, (301)-903-8014 raul.miranda@science.doe.gov Dr. Matthias Graf, Basic Energy Sciences, Materials Sciences and Engineering Division, (301)-903-0874 matthias.graf@science.doe.gov

C. DEPARTMENT OF ENERGY, OFFICE OF INSPECTOR GENERAL HOTLINE:

The Office of Inspector General (OIG) maintains a Hotline to facilitate the reporting of allegations of fraud, waste, abuse, or mismanagement in DOE programs or operations. If you wish to report such allegations, you may call, send a letter, or email the OIG Hotline ighotline@hq.doe.gov. Allegations may be reported by DOE employees, DOE contractors, or the general public. OIG contact information is available at <http://energy.gov/ig/services>.

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 proposer, 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.