

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



COMPUTATIONAL MATERIALS SCIENCES

**DOE NATIONAL LABORATORY PROGRAM ANNOUNCEMENT NUMBER:
LAB 19-2040**

ANNOUNCEMENT TYPE: INITIAL

Announcement Issue Date:	November 26, 2018
Submission Deadline for Letter of Intent:	N/A
Submission Deadline for Pre-Proposal:	December 21, 2018 at 12:00 PM (noon) Eastern Time A Pre-Proposal is required for new <i>and</i> renewal proposals
Pre-Proposal Response Date:	January 18, 2019
Submission Deadline for Proposals:	February 28, 2019 at 5:00 PM Eastern Time

Table of Contents

REGISTRATIONS	I
UPDATES AND REMINDERS.....	III
SECTION I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION	1
SECTION II – AWARD INFORMATION.....	5
A. TYPE OF AWARD INSTRUMENT.....	5
B. ESTIMATED FUNDING	5
C. MAXIMUM AND MINIMUM AWARD SIZE.....	5
D. EXPECTED NUMBER OF AWARDS.....	5
E. ANTICIPATED AWARD SIZE	6
F. PERIOD OF PERFORMANCE.....	6
G. TYPE OF PROPOSAL	6
SECTION III – ELIGIBILITY INFORMATION	7
A. ELIGIBLE APPLICANTS AND TOPICS	7
B. COST SHARING.....	7
C. ELIGIBLE INDIVIDUALS.....	7
D. LIMITATIONS ON SUBMISSIONS.....	7
SECTION IV – PROPOSAL AND SUBMISSION INFORMATION	8
A. ADDRESS TO REQUEST PROPOSAL PACKAGE.....	8
B. LETTER OF INTENT AND PRE-PROPOSAL.....	8
C. CONTENT AND PROPOSAL FORMS	12
D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS.....	27
E. SUBMISSION DATES AND TIMES	27
F. FUNDING RESTRICTIONS	28
G. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS	28
SECTION V - PROPOSAL REVIEW INFORMATION	30
A. CRITERIA	30
B. REVIEW AND SELECTION PROCESS	32
C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES	33
SECTION VI - AWARD ADMINISTRATION INFORMATION	34
A. AWARD NOTICES.....	34
B. REPORTING	34

SECTION VII - QUESTIONS/AGENCY CONTACTS.....	35
A. QUESTIONS	35
B. AGENCY CONTACTS.....	35
SECTION VIII - OTHER INFORMATION	36
A. MODIFICATIONS	36
B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE.....	36
C. COMMITMENT OF PUBLIC FUNDS.....	36
D. PROPRIETARY PROPOSAL INFORMATION.....	36
E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL.....	36
F. AVAILABILITY OF FUNDS.....	37

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 19-2040**.

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. To be considered eligible for an award under this Announcement, potential lead organizations 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 allowed to submit a full proposal. Proposals received from an applicant who has not submitted the required pre-proposal, or who has received notification from DOE that they are disallowed from submitting a full proposal, will be deemed non-responsive and will be rejected without further review.

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

RENEWAL PROPOSALS

Renewal proposals must be submitted from the institution that currently leads the research and that submitted the proposal that is currently supported. Changes in the Lead PI should be discussed with the program manager prior to submission of the renewal proposal.

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:

Dr. James Davenport

301-903-0035

james.davenport@science.doe.gov

SUMMARY

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

The program will support Large Team awards that must focus on the creation of computational codes and associated experimental/ computational databases by fully integrated teams, combining the skills of experts in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication. The research may involve the development of new ab initio theory, mining data from both experimental and theoretical databases, performing advanced in situ/operando characterization to generate the specific parameters needed to validate computational models, and well-controlled synthesis to confirm the predictions of the codes.

This effort is part of the DOE BES research related to the Materials Genome Initiative for Global Competitiveness as well as the DOE Office of Science Exascale activities. BES funded three large team Computational Materials Sciences awards in FY 2015 and two additional large team awards in FY 2016. Additional information on these awards can be found at the website listed in the references below. See the Summary Criteria section for more information on excluded research areas for this funding opportunity.

SUPPLEMENTARY INFORMATION

BACKGROUND

Major strides in materials synthesis, processing, and characterization, combined with concurrent advances in computational science enabled by enormous improvements in high-performance computing capabilities-have opened an unprecedented opportunity to design new materials with specific functions and properties. The goal is to leap beyond simple extensions of current theory and models of materials towards a paradigm shift in which specialized computational codes and

software enable the design, discovery, and development of new materials, and in turn, create new advanced, innovative technologies. Given the importance of materials to virtually all technologies, computational materials sciences are critical for American competitiveness and global leadership in innovation.

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

Research and development to create these computational codes require a fully integrated, multi-investigator team approach, combining the skills of experts in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication. The range of the research includes development of new ab initio theory, advanced materials modeling, mining data from both experimental and theoretical databases, performing advanced in situ/operando characterization to generate the specific parameters needed for computational models, and well controlled synthesis to confirm the predictions of the codes. Many of the underlying phenomena require understanding the material dynamics at ultrafast time scales and with near atomic resolution - requiring effective use of the unique world leading tools and instruments at DOE's user facilities, from ultrafast free electron lasers to aberration corrected electron microscopes to the best tools for controlled synthesis.

An ideal end product would be open source, robust, validated, user friendly software (and the associated experimental and computational data) that captures the essential physics and chemistry of relevant systems and can be used by the broader research community and by industry to dramatically accelerate the design of new functional materials. As appropriate, multiple software approaches can be incorporated, for example, software that uses the most advanced supercomputers coupled with derivative software for more general, routine use on computer clusters.

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 functional materials research. Suitable classes of functional materials include, for example, quantum materials, materials related to quantum information science, topological materials, wide-bandgap semiconductors, transition metal oxides, and magnetic, superconducting, photovoltaic, optoelectronic, and thermoelectric materials. Explicitly excluded are proposals on cold atoms, structural materials, isolated molecules, ionic liquids, and catalysts.
- Focus on research leading to open source software. Software developed under this Announcement should have broad applicability. Proposers must describe how the

software will be distributed as open source in an Open Source Software Distribution Plan. This plan should describe the maintenance and long-term accessibility of the software.

- Suitable types of software will emphasize strong correlations, multiscale properties, excited states, transport, electronic or optical properties. Explicitly excluded are proposals that emphasize density functional methods as currently implemented.
- Provide a detailed plan for the full utilization of today's petascale and pre-exascale, and tomorrow's exascale leadership computing facilities.
- Proposals must have integrated, multi-investigator teams combining expertise in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication. These proposals must articulate a clear management plan that ensures a coherent team approach.
- Include a Data Management Plan. This plan should describe the maintenance and long-term accessibility of data.
- The proposal should provide mechanisms for research community input to software and database development and validation.
- Multiple national laboratories and other organizations proposing as a team must designate a lead organization. Only one pre-proposal and one proposal is to be submitted for each team. The designated lead organization must perform a greater percentage of the effort, as determined by the budget distribution by institution, than any other partner organization or subawardee.

References:

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

([https://science.energy.gov/~media/bes/pdf/reports/files/Computational Materials Science and Chemistry_rpt.pdf](https://science.energy.gov/~media/bes/pdf/reports/files/Computational_Materials_Science_and_Chemistry_rpt.pdf))

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

From Quanta to the Continuum: Opportunities for Mesoscale Science

(https://science.energy.gov/~media/bes/pdf/reports/files/From_Quanta_to_the_Continuum_rpt.pdf)

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

(https://science.energy.gov/~media/bes/besac/pdf/Reports/Challenges_at_the_Frontiers_of_Matter_and_Energy_rpt.pdf)

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

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

(https://science.energy.gov/~media/bes/pdf/reports/2018/Quantum_systems.pdf).

Previous CMS Awards:

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

MGI 2014 Strategic Plan

https://www.mgi.gov/sites/default/files/documents/mgi_strategic_plan_-_dec_2014.pdf

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 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.

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 approximately \$8,000,000 per year will be available under this DOE National Laboratory Announcement and the companion FOA DE-FOA-0002040, contingent on satisfactory peer review and the availability of appropriated funds. Up to 4 national laboratory awards are expected. Proposers should request project support for four 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 an 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

(See B. Estimated Funding section above.)

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

Ceiling: \$2,500,000 per year

Floor: \$1,000,000 per year

For renewal proposals, notwithstanding the “Floor” identified above, DOE may consider limited-term renewal awards to allow for the completion of research projects and orderly closeout of CMS awards that do not merit long-term continued support. Annual funding for such awards could fall below the \$1,000,000 floor.

D. EXPECTED NUMBER OF AWARDS

(See B. Estimated Funding Section above.)

The exact number of awards will depend on the number of meritorious proposals and the

availability of appropriated funds.

E. ANTICIPATED AWARD SIZE

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

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

F. PERIOD OF PERFORMANCE

(See B. Estimated Funding section above.)

DOE anticipates making awards with a project period of four years. For renewal proposals, DOE may consider limited-term renewal awards to allow for the completion of research projects and orderly closeout of CMS renewals that do not merit long-term continued support. The duration of such awards would not exceed two years.

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

G. TYPE OF PROPOSAL

DOE will accept new and renewal 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-0002040) is available for applications 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

The Lead Organization and Limitation on Number of Proposals

A national laboratory may not submit more than **two** pre-proposals or proposals as the lead organization. If more than two proposals or pre-proposals are received from a national laboratory, DOE will consider only the proposal that matches a qualified pre-proposal (as described below in Section IV.B.2). The remaining proposals will be deemed non-responsive and rejected 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 and Limitation on Number of Proposals

The Lead Principal Investigator must be employed or have an agreement in place to be hired by the lead organization. **An individual may not be named as the Lead PI on more than one proposal.** If the proposed Lead PI will not be employed by the lead organization at the time of the award, the proposal will be deemed non-responsive and will be rejected without further review. Further, if more than one proposal is received from an applicant identifying the same individual as the Lead PI, DOE will consider only the application (if any) that matches a qualified Pre-Application (as described in Section IV.B.2). The remaining proposals will be deemed non-responsive and rejected without further review. However, there is no restriction on the number of proposals in which an individual may participate as a Principal Investigator (this is not the Lead Principal Investigator).

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

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

ENCOURAGE/DISOURAGE DATE

January 18, 2019

A pre-proposal must be submitted by **December 21, 2018 at 12:00 PM (noon) Eastern Time**. 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 **January 18, 2019**. 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 full proposal may submit full proposal.** No other full proposals will be considered.

Note that a national laboratory can submit only two pre-proposals as the lead organization. If more than two 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 for new and renewal proposals.

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-proposals 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, PI Email Address
Laboratory Announcement Number: LAB 19-2040
Type of Proposal: New or Renewal
Estimated Annual Budget Request:
Estimated Annual Budget Request by 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.

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 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 full application.

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

Applicants with the highest rated pre-proposal will be encouraged to submit full applications; others will be discouraged from submitting full 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 applications to foster a competitive merit review of the proposals. DOE expects to allow approximately 15 full proposals, with the exact number based on the review. The intent in discouraging submission of certain applications is to save the time and effort of applicants in preparing and submitting proposals with a negligible likelihood of success.

The PI will be automatically notified when the pre-application is encouraged or discouraged. The DOE SC Portfolio Analysis and Management System (PAMS) will send an email to the PI from PAMS.Autoreply@science.doe.gov, 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 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.

<p>WARNING: The PAMS website at https://pampspublic.science.energy.gov will permit you to edit a previously submitted preproposal in the time between your submission and</p>

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 Funding Opportunity Announcement should reference **LAB 19-2040**.

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

February 28, 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 recommendation are discouraged and will not be reviewed by the DOE.

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 8: Letters of Commitment).

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: Open Source Software Distribution Plan

- Appendix 8: Letters of Commitment
- Appendix 9: Renewal Proposals
- Appendix 10: List of Collaborators
- Appendix 11: 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 19-2040**. Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than **February 28, 2019**, at 5:00 PM Eastern Time.

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

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

- Log into PAMS. From the proposals tab, click the “View DOE National Laboratory Announcements” link and find the current announcement in the list. Click the “Actions/Views” link in the Options column next to this Announcement to obtain a dropdown menu. Select “Submit Proposal” from the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per proposal; to do so, click the “Select PI” button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the “Actions” link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose “Select PI.”
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the “Invite PI” link at the top left of the “Select PI” screen. You can enter an optional personal message to the PI in the “Comments” box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the proposal. Save the proposal for later work by selecting “Save” from the dropdown at the bottom of the screen and then clicking the “Go” button. It will be stored in “My Proposals” for later editing. As a minimum, you must complete all the required fields on the PAMS cover page before you can save the proposal for the first time.

- The cover page, budget, and attachments sections of the lab proposal are required by PAMS before it can be submitted to DOE.
- Complete the sections in PAMS one at a time, starting with the cover page and following the instructions for each section.
- Click the “+View More” link at the top of each section to expand the onscreen instructions. On the budget section, click the “Budget Tab Instructions” link to obtain detailed guidance on completing the budget form.
- Save each section by selecting either “Save” (to stay in the same section) or “Save... and Continue to the Next Section” (to move to the next section) from the dropdown menu at the bottom of the screen, followed by clicking the “Go” button.
- If you save the proposal and navigate away from it, you may return later to edit the proposal by clicking the “View My Existing Proposals” or “My Proposals” links within PAMS.
- You must enter a budget for each annual budget period.
- You must also enter a budget for each proposed sub-award. The sub-award section can be completed using the same steps used for the budget section.
- In the attachments section of the lab proposal, the abstract, the budget justification, and the proposal narrative are required and must be submitted as separate files.
- You must bundle everything other than the budget, abstract, and budget justification into one single PDF file to be attached under “Proposal Attachment.”
- Do not attach anything under “Other Attachments.”
- To upload a file into PAMS, click the “Attach File” button at the far right side of the screen. Click the “Browse” (or “Choose File” depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the “Upload” button to upload the file.
- Once you have saved all of the sections, the “Submit to DOE” option will appear in the dropdown menu at the bottom of the screen.
- To submit the proposal, select “Submit to DOE” from the dropdown menu and then click the “Go” button.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the proposal.
- The proposal will also appear under My Proposals with a Proposal Status of “Submitted to DOE.”

Please only submit a PAMS lab technical proposal in response to this Announcement; do not submit a DOE Field Work Proposal (FWP) at this time. 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 19-2040**.

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:
- Administrative Point of Contact name, telephone number, email:
- Lead PI name, telephone number, email:
- DOE National Laboratory Announcement Number: **LAB 19-2040**
- DOE/SC Program Office: Basic Energy Sciences
- DOE/SC Program Office Technical Contact: James Davenport
- PAMS Preproposal Number:
- Type of Proposal : New or Renewal

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 will be deemed non-responsive and will be rejected without further review. The Lead PI should not be changed unless unavoidable (discuss with the program manager) and only minor edits should be made, if necessary, to the title.

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

1. A list of all principal investigators with institution (postdoctoral staff and support staff need not be listed by name)
2. A table that lists the budget allocated to all partner institutions. Provide the total costs of the budget request in each year for each institution and totals for all rows and columns. **If 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 30 PAGES LONG)

The project narrative **must not exceed 30 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.

Research Focus: Proposals must address predictive design of functional materials, excluding cold atoms, structural materials, isolated molecules, ionic liquids, and catalysts. Proposals must propose research that leads to open source software, excluding density functional methods as currently implemented; proposals related to this topic will not be reviewed. Proposals must

provide a plan for full utilization of today's petascale and pre-exascale, and tomorrow's exascale leadership class computing.

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

- Briefly sketch the background, critically evaluate existing knowledge, and specifically identify the scientific gaps for functional materials that the project is intended to fill;
- Describe the role the proposed computational materials research could play in advancing the scientific field;
- Clearly state the four-year scientific research, software development, and data goals;
- Provide an account of any preliminary studies that may be pertinent to the proposed research or any currently available software that will be incorporated;
- State concisely the importance of the research described in the proposal and its potential scientific impact;
- Include any information that will help to establish the experience and competence of the principal investigators to pursue the proposed research, including experience in development and management of community software and data resources;
- Discuss the relevant experience of the lead organization, Lead PI, and, as appropriate, other principal investigators.
- **Renewal proposals:** This section must include a summary of the research performed in the prior award period. Note that a listing of the papers, software releases, and other research products is requested as Appendix 9.

Proposed Research: Applicants must provide detailed information regarding the proposed research. This section should demonstrate the close integration of the proposed research activities aimed at meeting the four-year scientific goals and how these will result in capabilities for design and discovery of functional materials. This section, which may be organized in subtasks, must clearly describe the proposed research by including the following:

- Describe a balanced and comprehensive program of basic research that, as needed, supports experimental, theoretical, and computational efforts and the development of new capabilities and approaches in these areas; include a clear statement of the open science questions to be addressed, a detailed research plan, an assessment of the potential scientific impact of the research, and a description of how the research plan will attain the 4-year scientific goals;
- Describe the scientific basis for the software to be developed and how it will be further developed;
- Describe how the proposed research will include development of software that will fully exploit the capabilities of today's petascale and pre-exascale, and tomorrow's exascale leadership computing facilities;
- Describe the role and intellectual contribution of the Lead PI, and, as appropriate, other PIs in the proposal;
- Briefly outline the resources available including access to existing research space, instrumentation, computational capabilities, and other facilities both within the partner institutions and external to the team (Appendix 4 should include detailed information about facilities, equipment, and capabilities available for the research);
- Describe plans for development and utilization of unique facilities, capabilities or approaches to address the scientific goals;

- Describe the plan and process that will be used to generate, verify, validate, and utilize computational and experimental data; and
- Describe how the software will be verified and experimentally validated and the role of the experimental component of the proposed research.

Management Plan: This section must provide a clear, substantive overview of the vision, management, and organization of the proposed Team by including the following:

- Describe the strategy and plan for project operations, the means of achieving an integrated research and development team, and plans for leadership and guidance for the scientific and technical direction of the project;
- Describe how the potential community that will use the software and associated data will be engaged to provide input to the research team;
- Describe how codes and data will be developed, maintained and shared; how will users gain access?
- Define an organizational structure that delineates the roles and responsibilities of senior/key personnel and describes the means of providing internal and external oversight and guidance for scientific and technical direction of the research and software development program, including but not limited to an **advisory committee (required)**, executive committees, program committees, or their equivalent; Advisory committee members need not be named unless project is awarded.
- Define proposed management processes for evaluation of research progress, decision making across the team, handling of intellectual property; and intra-team communication;
- Describe the availability of the Lead PI and other PIs, including discussion of their potential involvement in other major projects; and
- Include a brief (less than one page) overview of environmental, safety, health, and quality assurance (ES&H and QA) practices and oversight at each participating institution, including any required permits, licenses, and approvals that must be obtained.

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

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 and must include:

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

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

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

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

APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support (both Federal and non-Federal) for the PI and senior/key persons, including subawardees, for ongoing projects and pending applications. List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid.

For every activity, list the following items:

- The sponsor of the activity or the source of funding
- The award or other identifying number
- The title of the award or activity
- The lead PI of the award or activity
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The total cost or value of funds supporting the individual submitting the current and pending support
- The award period (start date – end date).
- The person-months of effort per year being dedicated to the award or activity

- Briefly describe the research being performed and explicitly identify any overlaps or synergies with the proposed research.

Provide the Current and Pending Support as an appendix to your project narrative. Concurrent submission of an application to other organizations for simultaneous consideration will not prejudice its review.

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

APPENDIX 3: BIBLIOGRAPHY & REFERENCES CITED

Provide a bibliography of any references cited in the Project Narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. For research areas where there are routinely more than ten coauthors of archival publications, you may use an abbreviated style such as the Physical Review Letters (PRL) convention for citations (listing only the first author). For example, your paper may be listed as, “A Really Important New Result,” A. Aardvark et. al. (MONGO Collaboration), PRL 999. Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the 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: OPEN SOURCE SOFTWARE DISTRIBUTION PLAN

Applicants are required to submit an Open Source Software Distribution Plan as part of their proposal. This plan describes how software produced under this Announcement will be distributed. Submission of an Open Source Software Distribution Plan is required; failure to submit a complete Plan may result in a determination of non-compliance for your proposal. For a DOE National Laboratory or a FFRDC, the data rights clause, including rights and requirements pertaining to computer software, in its M&O Contract shall apply and shall take precedence over any requirement set forth in this Appendix.

The plan must include the following elements:

1. A complete description of any existing software that will be modified or incorporated into software produced under this Announcement, 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 Announcement, and how that choice furthers the goals of this Announcement. 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 Announcement requires that the software or other information be shared or disseminated to others.

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

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

APPENDIX 8: 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 9: RENEWAL PROPOSALS

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

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

APPENDIX 10: LIST OF COLLABORATORS

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

- All persons who are, or who have been, collaborators or co-authors of papers, book or book articles, reports, or abstracts, during the 48 months preceding the submission of this application. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the PI interacted on a regular basis while the research was being done.
- Include any individuals who are currently, or have been, co-editors with any PI on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of this 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 11: OTHER ATTACHMENT

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

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

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

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

3. Proposal Due Date

February 28, 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 19-2040**.

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 to determine that (1) the applicant is eligible for the award; (2) the information required by the Announcement has been submitted; (3) all mandatory requirements are satisfied; (4) the proposed project is responsive to the objectives of the funding opportunity announcement, 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.

Be advised that proposals focused on cold atoms, structural materials, isolated molecules, ionic liquids, and catalysts will be considered non-responsive. Research that emphasizes density functional methods as currently implemented will be considered non-responsive. All 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 and Open Source Software Distribution Plan. Proposals that do not provide a detailed plan for the full utilization of petascale, pre-exascale, and future exascale leadership class computing facilities will be considered non-responsive. Proposals without a management plan will be considered non-responsive. 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, the first five of which will be weighted more heavily than the final two. The first five criteria are of equal value with each other. The final two criteria are of equal value with each other. The questions after each are intended to guide the reviewers; reviewers will not be required to provide written responses to each of these questions.

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

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

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

SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROPOSED RESEARCH

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

APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

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

COMPETENCY OF APPLICANT'S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES

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

REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET

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

STRENGTH OF THE MANAGEMENT PLAN

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

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

- Comment on how the applicant's approach addresses the scientific and software development goals in an integrated and coherent manner.

- Team proposals: Comment on the likelihood that the proposed team will work together in a cohesive and integrated manner.

DEVELOPMENT AND UTILIZATION OF UNIQUE FACILITIES, CAPABILITIES, OR APPROACHES

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

B. REVIEW AND SELECTION PROCESS

1. Merit Review

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
- Ensuring an appropriate balance and diversity for activities within SC-BES programs
- Performance under current awards
- Commitment to sharing the results of research and managing open source software for broad community access
- Delineation of the scope of the proposed research from other research activities in which the principal investigators are involved, particularly those supported by DOE and by other federal agencies
- Diversity of research activities that will address the scientific grand challenges and use-inspired basic research as articulated in the Basic Energy Sciences Advisory Committee (BESAC) and BES workshop reports
- Potential for developing synergies between the proposed project and other ongoing BES research activities, including but not limited to the Energy Frontier Research Centers, Energy Innovation Hubs, and the core research activities within the BES Materials Sciences and Engineering or Chemical Sciences, Geosciences, and Biosciences Divisions

3. Selection

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

4. 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.

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 19-2040**.

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 Manager Scientific Contact	James Davenport, 301-903-0035 james.davenport@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.