

**PROGRAM ANNOUNCEMENT
TO DOE NATIONAL LABORATORIES**



**U. S. Department of Energy
Office of Science**

**Computational Materials Sciences
DOE National Laboratory Announcement Number: LAB 16-1528
Announcement Type: **Amendment 000002****

Issue Date: 02/09/2016

Issue Date of Amendment 000002: 03/25/2016

**Letter of Intent Due Date: 03/07/2016 at 5 PM Eastern Time
(A Letter of Intent is required)**

Pre-Proposal Due Date: Not Applicable

Proposal Due Date: 04/25/2016 at 5 PM Eastern Time

The application due date will not be extended as a result of this amendment.

AMENDMENTS:

Amendment 1: Page 24. In Individual Commitment Statement “this page is not included in the three page limit for each biographical sketch” is changed to “two page limit for each biographical sketch”

Amendment 2:

Page 3, first bullet, “structural properties; and synthesis of 2-d layered materials” is changed to “structural properties and synthesis of 2-d layered materials”

Page 16, Summary of Proposal contents and Information about PAMS, Appendix list is corrected to reflect additional appendices on pages 23 to 28.

Amendment 2 provides the following changes to the text of this Announcement:

On Page 3, a grammatical correction

Delete the semicolon after the highlighted word ‘properties’ in the first bullet.

- Focus on functional materials research. Suitable classes of functional materials include, for example, semiconductors, transition metal oxides, magnetic or superconducting materials, metal-halide perovskites, and heterogeneous catalysts. Explicitly excluded are proposals on structural, thermoelectric, and energy storage materials; structural **properties**; and synthesis of 2-d layered materials, assemblies of nanoparticles, isolated molecules, liquids (including ionic liquids), and homogeneous catalysts.

On Page 16, an inconsistency was resolved

The summary contents does not match the actual list of appendices on pages 23 to 28.

1. Summary of Proposal Contents and Information about PAMS

Each DOE National Laboratory proposal will contain the following sections:

- Budget, entered into PAMS as structured data using the PAMS budget form
- Abstract (one page), entered into PAMS as a separate pdf
- Budget justification, entered into PAMS as a separate pdf
- Proposal, combined into a single pdf containing the following information:
 - Proposal Cover Page
 - Table of Contents
 - Project Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel – 30 page limit)
 - Appendix 1: Biographical Sketch(es)
 - Appendix 2: Current and Pending Support
 - Appendix 3: Bibliography and References Cited

- Appendix 4: Facilities, Equipment & Resources
- Appendix 5: Additional Funding
- Appendix 6: Data Management Plan
- Appendix 7 : Open Source Software Distribution Plan
- Appendix 8: Statement of Conflict of Interest
- Appendix 9: Organizational Letters of Commitment
- Appendix 10: List of Collaborators and Possible Conflicts of Interest
- Appendix 11: Other Attachment

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REGISTRATIONS

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

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

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

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

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

Notifications sent from the PAMS system will come from the PAMS email address <PAMS.Autoreply@science.doe.gov>. Please make sure your email server/software allows delivery of emails from the PAMS email address to yours.

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

1. CREATE PAMS ACCOUNT:

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

- Click the “No, I have never had an account” link and then the “Create Account” button.
- You will be prompted to enter your name and email address, create a username and password, and select a security question and answer. Once you have done this, click the “Save and Continue” button.
- On the next page, enter the required information (at least one phone number and your mailing address) and any optional information you wish to provide (e.g., FAX number, website, mailstop code, additional email addresses or phone numbers, Division/Department). Click the “Create Account” button.
- Read the user agreement and click the “Accept” button to indicate that you understand your responsibilities and agree to comply with the rules of behavior for PAMS.
- PAMS will take you the “Having Trouble Logging In?” page. (Note: If you reviewed for or were listed as PI on a prior submission to the Office of Science but have not previously created an account, you may already be linked to an institution in PAMS. If this is the case, PAMS will take you to the PAMS home page.)

2. REGISTER TO YOUR INSTITUTION:

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this DOE National Laboratory Announcement should reference **LAB FY-1528**.

RECOMMENDATION

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

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 applications in Computational Materials Sciences proposing integrated, multidisciplinary teams that will perform research to develop validated community codes and data bases for predictive design of functional materials, excluding structural materials. Computational Materials Sciences Teams could also involve new approaches to enhance the use of large data sets derived from advanced characterization of materials, materials synthesis, processing, and properties assessments and the parallel data that are generated by large scale computational efforts that model materials phenomena. Computational Materials Sciences will support the Materials Genome Initiative for Global Competitiveness (MGI) that was announced by the President in June 2011. The goal of the MGI is to reduce the time from discovery to deployment of new materials by a factor of two and is tied to advancement of American manufacturing capability. This funding opportunity continues the BES commitment to the MGI and the development of open source codes that can take full advantage of today's petascale and future exascale leadership computing facilities.

In FY 2015, the first Computational Materials Sciences awards were made. Additional information on these awards can be found at the website listed in the references below. Projects selected in 2016 will support research for functional materials topics and types of software not supported in 2015. See the Summary Criteria section for more information on excluded research areas for this funding opportunity.

SUPPLEMENTARY INFORMATION

BACKGROUND

Recent major strides in materials synthesis, processing, and characterization, combined with concurrent advances in computational science – enabled by improvements in high performance computing capabilities – have opened an unprecedented opportunity to design new materials with targeted properties. The opportunity is to leap beyond simple extensions of current theory and models of materials towards a paradigm shift in which specialized computational codes and software, coupled with innovative availability and use of experimental and theoretical data, enable the ability to design, discover, and develop new materials, and in turn, create new advanced, innovative technologies. Given the importance of materials to virtually all

technologies, computational materials science is a critical area in which the United States needs to be competitive.

If successful, this paradigm shift of integration would significantly accelerate the design of revolutionary materials to meet the Nation's energy goals and enhance economic competitiveness. Development of fundamentally new design principles could enable stand-alone research codes and software packages to address multiple length and time scales for prediction of the total functionality of materials over a lifetime of use. Recent scientific workshops and National Research Council studies have identified enticing scientific challenges that would advance these goals. Examples include dynamics and strongly correlated matter, conversion of solar energy to electricity, design of new catalysts for a wide range of industrial uses, and electron transport in materials for improved electronics. Success will require extensive research and development with the goal of creating and experimentally validating, robust community codes that will enable functional materials innovation. Utilization of today's petascale leadership class computers and planning for algorithms and software codes that can be implemented for exascale computing are critical aspects of the required software.

Research and development to create the computational codes will 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 will include development of new ab initio theory, advanced materials modeling, mining the data from both experimental and theoretical databases, performing advanced in situ/in 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.

In FY 2015, the first Computational Materials Sciences awards were made. Additional information on these awards can be found at the website listed in the references below. Projects selected in 2016 will support research for functional materials topics and types of software not supported in 2015. See the Summary Criteria section for more information on excluded research areas for this funding opportunity.

SUMMARY CRITERIA

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

- Focus on functional materials research. Suitable classes of functional materials include, for example, semiconductors, transition metal oxides, magnetic or superconducting materials, metal-halide perovskites, and heterogeneous catalysts. Explicitly excluded are proposals on structural, thermoelectric, and energy storage materials; structural properties and synthesis of 2-d layered materials, assemblies of nanoparticles, isolated molecules, liquids (including ionic liquids), and homogeneous catalysts.
- Focus on research leading to open source software. Suitable types of software will emphasize strong correlations, excited states, transport, electronic or optical properties. Explicitly excluded are proposals that emphasize density functional methods as currently implemented or semi-empirical approaches, dynamical mean field theory, and classical and first principles molecular dynamics.
- Describe a plan to deliver experimentally validated research codes and the associated experimentally and theoretically derived data for the design of functional materials to academia, National Laboratories, and industry. Software developed under this FOA should have broad applicability. Applicants must describe how the software will be distributed as open source in an Open Source Software Distribution Plan.
- Provide a detailed plan for the full utilization of today's petascale and tomorrow's exascale leadership computing facilities.
- Use integrated, multi-investigator teams combining expertise in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication.
- Articulate a clear management plan which insures a coherent team approach and provides for the maintenance and long-term accessibility of software and data.
- Include a Data Management Plan.
- Provide mechanisms for community input to software and database development and validation.

References:

Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science (<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#CMSC>)

From Quanta to the Continuum: Opportunities for Mesoscale Science
(<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#OFMS>)

Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science
http://science.energy.gov/~media/bes/besac/pdf/Reports/CFME_rpt_print.pdf

FY 2015 Awards:

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

MGI Strategic Plan

https://www.whitehouse.gov/sites/default/files/microsites/ostp/NSTC/mgi_strategic_plan_-_dec_2014.pdf

Collaboration

Collaborative proposals will not be accepted under this announcement.

Section II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT

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

B. ESTIMATED FUNDING

DOE expects to make multiple Computational Materials Sciences awards for a period of up to four years for each award. Total funding, estimated at a maximum of \$4,000,000 annually across all awards with the potential for additional annual funding in future fiscal years, is expected to be available to support the awards from this National Laboratory Announcement and FOA DE-FOA-0001528, subject to appropriation of funds by Congress. DOE is under no obligation to pay for any costs associated with preparation or submission of proposals. DOE reserves the right to fund, in whole or in part, any, all, or none of the proposals submitted in response to this announcement.

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

C. MAXIMUM AND MINIMUM AWARD SIZE

(See B. Estimated Funding section above.)

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

DOE does not expect to receive applications that fall outside of the maximum and minimum amounts stated above.

Ceiling

\$2,500,000 per year

Floor

\$1,500,000 per year

D. EXPECTED NUMBER OF AWARDS

(See B. Estimated Funding Section above.)

The number of awards will depend on the number of meritorious proposals and the availability of appropriated funds. DOE reserves the right to fund, in whole or in part, any, all, or none of the proposals submitted in response to this Announcement.

E. ANTICIPATED AWARD SIZE

(See B. Estimated Funding Section 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.)

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

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

G. TYPE OF PROPOSAL

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

Section III – ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS AND TOPICS

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

Institutions that received prime awards made under FOA DE-FOA-0001276 (Computational Materials Sciences, FY2015) are not eligible to submit applications as prime applicants under this Funding Opportunity Announcement (DE-FOA-0001528) and its companion Laboratory Announcement (LAB 16-1528). Current prime awardees may participate as subawardees other prime applicant institutions.

Institutions participating as subawardees in awards made under FOA DE-FOA-0001276 (Computational Materials Sciences, FY2015) are eligible to submit applications as prime applicants under this Funding Opportunity Announcement (DE-FOA-0001528) and its companion Laboratory Announcement (LAB 16-1528).

UNINCORPORATED CONSORTIA

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

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

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

Note that a consortium is applied for in one application and results in one award with subawards to consortia members. Collaborations are applied for separately with identical applications and result in multiple awards to the collaborating 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 Lead Principal Investigator/Principal Investigator are invited to work with their organizations to develop a proposal. Individuals from underrepresented groups as well as individuals with disabilities are always encouraged to apply.

D. OTHER ELIGIBILITY REQUIREMENTS

Letter of Intent (LOI)

To be considered eligible for an award under this FOA, potential prime applicants (lead organizations) are *required* to submit a LOI in accordance with the instructions provided in Section IV.B.1 of this Announcement below. Proposals received from an applicant who has not submitted the required LOI will be deemed non-responsive and will be rejected without further review.

The lead organization on an proposal must be the same as on the required LOI. **If a proposal is received for which the lead organization has changed since submission of the LOI, then the proposal will be deemed non-responsive and will be rejected without further review.** The Lead Principal Investigator (PI) or Project Director should not be changed unless unavoidable and only minor edits should be made, if necessary, to the title. If necessary, the applicant may make changes to other senior/key personnel and other participating institutions, although DOE discourages extensive changes.

The Lead Organization and Limitation on Number of Applications

An entity may not submit more than **one** application as the lead organization. If more than one application is received from an entity, DOE will consider only the application that matches a qualified LOI (as described below in Section IV.B.1). The remaining applications will be deemed non-responsive and rejected without further review. However, there is no limitation on the number of applications in which an entity may participate as a team member or subawardee.

The Project Director and Limitation on Number of Applications

The Project Director is the Lead Principal Investigator and must be employed or have an agreement in place to be hired by the lead organization. **An individual may not be named as the Project Director on more than one application.** If the proposed Project Director will not be employed by the lead organization, the application will be deemed non-responsive and will be rejected without further review. Further, if more than one application is received from an applicant identifying the same individual as the Project Director, DOE will consider only the application (if any) that matches a qualified LOI (as described in Section IV.B.1). The remaining applications will be deemed non-responsive and rejected without further review. However, there is no restriction on the number of applications in which an individual may participate as a Principal Investigator (This is not the Lead Principal Investigator/Project Director).

Team Arrangements

Entities proposing as a team must designate a lead organization. LOIs and applications must be submitted on behalf of the team members by the lead organization and DOE will enter into a prime award relationship with the designated lead organization. Only one LOI and one application are to be submitted for each team. The designated lead organization, i.e., the prime applicant, must perform a greater percentage of the effort than any other partner organization or subawardee. The percentage of effort will be determined by reviewing the total budget for each participating organization as a percentage of proposed total project costs. **If an application is received in which the prime applicant 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 application will be deemed non-responsive and rejected without further review.**

Eligible/Ineligible Entities

If a proposal is received that includes an ineligible entity, or an employee of an ineligible entity performing activities as a team member and/or subawardee, the proposal will be deemed non-responsive and rejected without further review. Note, however, that otherwise ineligible entities are not precluded from serving as vendors of materials, supplies, equipment, and providing scientific and technical advisory services to a proposed Team, if they are acting purely in that role. Scientific and technical advisory services allow for the provision of scientific and technical expertise without actually performing research activities; examples of such services include serving as members of advisory committees and technical peer review panels or participation in scientific workshops or conferences.

Performance of Work in the United States

DOE requires all work performed by the prime recipient under funding agreements resulting from this FOA to be performed in the United States except as discussed below: – i.e., a prime recipient must expend its total project costs in the United States.

This requirement does not apply to travel or to equipment, materials and supply purchases. Like all proposed costs, proposed travel, equipment, and material and supply costs will be evaluated to determine whether they are necessary and appropriate for the conduct of the effort. Furthermore, it is the sense of Congress that, to the greatest extent practicable, all equipment and products purchased with funds made available under awards resulting from this FOA should be American-made.

Work funded as a subaward from the prime recipient may be performed outside of the United States.

DATA MANAGEMENT PLAN

A Data Management Plan as described in Section IV C. “Proposal Contents and Forms” - Appendix 6, is required. Proposals that do not have a Data Management Plan will be deemed nonresponsive and will be not reviewed.

OPEN SOURCE SOFTWARE DISTRIBUTION PLAN

An Open Source Software Distribution Plan as described in Section IV C. “Proposal Contents and Forms” - Appendix 7, is required. Proposals that do not have an Open Source Software Distribution Plan will be deemed nonresponsive and will be not reviewed.

RESEARCH FOCUS

Proposals must address predictive design of functional materials, excluding structural, thermoelectric, and energy storage materials; structural properties; and synthesis of 2-d layered materials, assemblies of nanoparticles, isolated molecules, liquids (including ionic liquids), and homogeneous catalysts. Proposals related to these topics will not be reviewed.

Proposals must propose research that leads to open source software, excluding density functional methods as currently implemented or semi-empirical approaches, dynamical mean field theory, and classical and first principles molecular dynamics. Proposals related to these topics will not be reviewed.

Section IV – PROPOSAL AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST PROPOSAL PACKAGE

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

Proposals submitted outside of PAMS will not be accepted.

B. LETTER OF INTENT AND PRE-PROPOSAL

1. Letter of Intent

LETTER OF INTENT DUE DATE

March 7, 2016 at 5 PM Eastern Time

A Letter of Intent is required and must be submitted by March 7, 2016 at 5 PM Eastern Time. **Any application received for which there is not an associated LOI will be deemed non-responsive and will be rejected without further review.** In addition, the lead organization on the application must be the same as on the LOI. If an application is received for which the lead organization has changed since submission of the LOI, then the application will be deemed non-responsive and will be rejected without further review. The Lead PI or Project Director should not be changed unless unavoidable and only minor edits should be made, if necessary, to the title. If necessary, the applicant may make changes to other senior/key personnel and other participating institutions, although DOE discourages extensive changes.

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

- Letter of Intent Title (this is the Project Name)
- Lead Principal Investigator Name, Job Title (this is the Project Director)
- Lead Organization
- Lead Principal Investigator Phone Number and Email Address
- Funding Opportunity Announcement Number: DE-FOA-0001528

This cover page must be signed by an official of the lead organization who has the authority to commit institutional support for the application and by the proposed Project Director. For DOE National Laboratory applicants, the institutional official should be the Laboratory Director. For other applicants, this official should be someone who has authority over research activities for the entire institution, such as the Vice President for Research, Chief Technology Officer, or the equivalent. **All applicants must provide both of these signatures on the LOI.** Applicants that fail to provide both signatures on the LOI will be required to provide a corrected LOI with both signatures on or before March 19, 2016 in order for their full

application associated with the LOI to be considered for award.

The cover page must be followed by a clear and concise description of the goals, objectives, and technical approaches of the proposed research. The description of the proposed research may not exceed two pages when printed on 8.5 X 11 inch paper, with a minimum text font size no smaller than Times New Roman 12 point and margins no smaller than one inch on all sides. The required header information and any figures and references, if included, must fit within the two-page limit.

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

Table 1: Senior/key personnel on the application and institutional affiliations

Senior/Key Personnel			Institution
Last Name	First Name	Title	Institution Name

Table 2: Collaborators for senior/key personnel on the application

Collaborator			Institution
Last Name	First Name	Title	Institution Name

** Table 2 must include co-authors over the past 48 months, graduate and postdoctoral advisors of the senior/key personnel, graduate students and postdoctoral associates that have been supervised by the senior/key personnel during the past 60 months, and any other current close associations of the senior/key personnel. Table 2 should exclude all personnel at any of the institutions listed in Table 1.

- Table 1 and Table 2 will not count in the LOI page limitation.

The Lead Organization and Limitation on Number of Letters of Intent

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

The Project Director/Lead Principal Investigator and Limitation on Letters of Intent

The Project Director is the Lead Principal Investigator and must be employed or have an agreement in place to be hired by the lead organization in the event an award is made. An individual may not be named as the Project Director on more than one LOI. If more than one qualified LOI is received from an applicant identifying the same individual as the Project Director, DOE will consider the first qualified LOI received based on the PAMS date and time stamp. The remaining LOIs will be deemed non-responsive and the applicant will not be allowed to submit full applications tied to those LOIs.

All LOIs received by DOE will be acknowledged by an automated email to the Project Director. Any individual named as the Project Director on a LOI that is found to be non-responsive to the LOI requirements will be notified by March 21, 2016 and will be ineligible to submit a full application associated with that LOI. LOIs deemed responsive will receive no additional notification.

The LOI must be submitted electronically through the DOE Office of Science Portfolio Analysis and Management System (PAMS) website <https://pamspublic.science.energy.gov/>. It is important that the LOI be a single file with extension .pdf, .docx, or .doc. The Principal Investigator (PI) and anyone submitting on behalf of the PI must register for an account in PAMS before it will be possible to submit a letter of intent. **All PIs and those submitting LOIs on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays.**

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

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

Create PAMS Account:

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

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

PAMS will take you the “Having Trouble Logging In?” page. (If you have been an Office of Science merit reviewer or if you have previously submitted an proposal, you may already be

linked to an institution in PAMS. If this happens, you will be taken to the PAMS home page.

Register to Your Institution:

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

Submit Your Letter of Intent:

- Create your letter of intent outside the system and save it as a file with extension .docx, .doc, or .pdf. Make a note of the location of the file on your computer so you can browse for it later from within PAMS.
- Log into PAMS and click the Proposals tab. Click the “View / View / Respond to DOE National Laboratory Announcements” link and find the current announcement in the list. Click the “Actions/Views” link in the Options column next to this announcement to obtain a dropdown menu. Select “Submit Letter of Intent” from the dropdown.
- On the Submit Letter of Intent page, select the institution from which you are submitting this LOI from the Institution dropdown. If you are associated with only one institution in the system, there will only be one institution in the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per LOI; to do so, click the “Select PI” button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the “Actions” link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose “Select PI.”

- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the “Invite PI” link at the top left of the “Select PI” screen. You can enter an optional personal message to the PI in the “Comments” box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the LOI. Save the LOI for later work by clicking the “Save” button at the bottom of the screen. It will be stored in “My Letters of Intent” for later editing.
- Enter a title for your letter of intent.
- Select the appropriate technical contact from the Program Manager dropdown.
- To upload the LOI file into PAMS, click the “Attach File” button at the far right side of the screen. Click the “Browse” (or “Choose File” depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the “Upload” button to upload the file.
- At the bottom of the screen, click the “Submit to DOE” button to save and submit the LOI to DOE.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the LOI.

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

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

2. Pre-proposal

A pre-proposals is not required or invited.

C. CONTENT AND PROPOSAL FORMS

PROPOSAL DUE DATE

April 25, 2016 at 5 PM Eastern Time.

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

LETTERS

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

1. Summary of Proposal Contents and Information about PAMS

Each DOE National Laboratory proposal will contain the following sections:

- Budget, entered into PAMS as structured data using the PAMS budget form
- 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 – 30 page limit)
 - Appendix 1: Biographical Sketch(es)
 - Appendix 2: Current and Pending Support
 - Appendix 3: Bibliography and References Cited
 - Appendix 4: Facilities, Equipment & Other Resources
 - Appendix 5: Additional Funding
 - Appendix 6: Data Management Plan
 - Appendix 7: Open Source Software Distribution Plan
 - Appendix 8: Statement of Conflict of Interest
 - Appendix 9: Organizational Letters of Commitment
 - Appendix 10: List of Collaborators and Possible Conflicts of Interest
 - Appendix 11: Other Attachment

SUBMISSION INSTRUCTIONS

Full proposals must be submitted into the DOE Office of Science Portfolio Analysis and Management System (PAMS). For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free number) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this Program Announcement should reference **LAB 16-1528**. Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than **April 25, 2016**, at 5:00 PM Eastern Time.

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

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

- Log into PAMS. From the proposals tab, click the “View DOE National Laboratory Announcements” link and find the current announcement in the list. Click the “Actions/Views” link in the Options column next to this Announcement to obtain a dropdown menu. Select “Submit Proposal” from the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per proposal; to do so, click the “Select PI” button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the “Actions” link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose “Select PI.”
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the “Invite PI” link at the top left of the “Select PI” screen. You can enter an optional personal message to the PI in the “Comments” box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the proposal. Save the proposal for later work by selecting “Save” from the dropdown at the bottom of the screen and then clicking the “Go” button. It will be stored in “My Proposals” for later editing. As a minimum, you must complete all the required fields on the PAMS cover page before you can save the proposal for the first time.
- The cover page, budget, and attachments sections of the lab proposal are required by PAMS before it can be submitted to DOE.
- Complete the sections in PAMS one at a time, starting with the cover page and following the instructions for each section.
- Click the “+View More” link at the top of each section to expand the onscreen instructions. On the budget section, click the “Budget Tab Instructions” link to obtain detailed guidance on completing the budget form.
- Save each section by selecting either “Save” (to stay in the same section) or “Save... and Continue to the Next Section” (to move to the next section) from the dropdown menu at the bottom of the screen, followed by clicking the “Go” button.
- If you save the proposal and navigate away from it, you may return later to edit the proposal by clicking the “View My Existing Proposals” or “My Proposals” links within PAMS.
- You must enter a budget for each annual budget period.
- You must also enter a budget for each proposed sub-award. The sub-award section can be completed using the same steps used for the budget section.
- In the attachments section of the lab proposal, the abstract, the budget justification, and the proposal narrative are required and must be submitted as separate files.
- You must bundle everything other than the budget, abstract, and budget justification into one single PDF file to be attached under “Proposal Attachment.”
- Do not attach anything under “Other Attachments.”
- To upload a file into PAMS, click the “Attach File” button at the far right side of the screen. Click the “Browse” (or “Choose File” depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the “Upload” button to upload the file.

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

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free number) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this Program Announcement should reference **LAB 15-1528**.

2. Detailed Contents of the Proposal

BUDGET AND BUDGET EXPLANATION

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

PAMS will calculate the cumulative budget totals for you.

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

PROJECT SUMMARY/ABSTRACT (NO MORE THAN ONE PAGE)

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

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

DOE COVER PAGE
(PART OF PROJECT NARRATIVE)

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

- The project title:
- Applicant/Institution:
- Street Address/City/State/Zip:
- Postal Address:
- Administrative Point of Contact name, telephone number, email:
- Lead PI name, telephone number, email:
- DOE National Laboratory Announcement Number: **LAB 16-1528**
- DOE/Office of Science Program Office: **Basic Energy Sciences**
- DOE/Office of Science Program Office Technical Contact: **James Davenport**
- PAMS Letter of Intent Tracking Number:

The lead applicant/awardee/recipient/organization must be the same as on the required LOI. **If an application is received for which the lead organization has changed since submission of the LOI, then the application will be deemed non-responsive and will be rejected without further review.** The Project Director should not be changed unless unavoidable and only minor edits should be made, if necessary, to the title. If necessary, the applicant may make changes to the other senior/key personnel and other participating institutions, although DOE discourages extensive changes.

On separate pages, as a supplement to the cover page, include the following personnel and summary budget information for all senior/key personnel and all partner institutions:

Table 1: Senior/key personnel on the application and institutional affiliations

Senior/Key Personnel			Institution
Last Name	First Name	Title	Institution Name

** Applicants are strongly encouraged to follow the exact format of the sample table above since the tabular information will be compiled across all applications. This includes the following elements:

- Include grid lines around each cell.
- Do not merge name or institution cells, even if individuals share the same institution.
- Do not change the order of the columns.

- Do not include any additional information (e.g. “PI”, “Co-PI”, or footnote symbols) under “Last Name” and “First Name”.
- Do not include departmental affiliations under Institutions.
- If an individual has a joint appointment, separate the institutions with a “/” (i.e. “Univ of X / National Lab Y”).

Table 2: Summary budget information for all partner institutions

Institution Name	Year 1 Budget	Year 2 Budget	Year 3 Budget	Year 4 Budget	Total Budget
Total Budget					

** Provide the total costs of the budget request in each year for each institution and totals for all rows and columns.

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). Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph. The font must not be smaller than Times New Roman 12 point. **Only the first 30 pages of the Project Narrative will be reviewed or considered.** This page limit does not apply to the Cover Page, any Table of Contents (optional, but if included should be limited to one page), Budget Page(s), Budget Justification, biographical material, publications and references, and appendices, each of which may have its own page limit. Headers/footers containing page numbers and project titles/logos may be inserted within the required one inch margins

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 contents of the Project Narrative are specified in order to ensure that the merit reviewers have the necessary information to conduct proper evaluations. Merit review criteria can be found in Section V. A.2 of this FOA. All Project Narratives must include the following sections:

I. Introduction and Background. This section should place the proposed project in the context of the scientific field in which it would operate by including the following:

- Briefly sketch the background leading to the application, 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 application and its potential scientific impact;
- Include any information that will help to establish the experience and competence of the 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, Project Director, and other senior/key personnel in research by teams of investigators.

II. 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 the plan and process that will be used to generate, validate, and utilize computational and experimental data;
- Describe how the software will be experimentally validated and the role of the experimental component of the proposed research;
- Describe how the proposed research will include development of software that will exploit the capabilities of today's petascale and tomorrow's exascale leadership computing facilities;

Describe how the proposed research embodies the scientific approaches detailed in the following reports: *Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science* (<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#CMSC>), *From Quanta to the Continuum: Opportunities for Mesoscale Science* (<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#OFMS>) and *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science* http://science.energy.gov/~media/bes/besac/pdf/Reports/CFME_rpt_print.pdf

- Describe the role and intellectual contribution of the Project Director, each co-Principal Investigator, and each other senior/key person in the application;

- 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;
- Relationship to other activities supported by BES or other federal agencies: As appropriate, briefly describe (less than one page) how the proposed research aligns with the core research activities and priorities within BES (<http://science.energy.gov/bes/mse/>, <http://science.energy.gov/bes/csgb/>); is clearly distinguishable from activities within the BES Energy Frontier Research Centers (<http://science.energy.gov/bes/efrc/>) and the Energy Innovations Hubs (<http://science.energy.gov/bes/research/doe-energy-innovation-hubs/>); and relates to other existing and planned research programs at the participating institutions.

III. 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 Project Director, co-principal investigators, and other senior/key personnel, including discussion of their potential involvement in other major projects;
- 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.

IV. Project Performance Site(s). Identify and describe the site(s) where the work will be performed. For research proposed by a team, 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 project director/principal investigator (PD/PI) and each senior/key person listed in Section A on the R&R Budget form.

- 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 should 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 12 point and must include:

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.

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

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

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

Personally Identifiable Information: Do not include sensitive personally identifiable information such as a Social Security Number, date of birth, or city of birth. Do not include information that a merit reviewer should not make use of.

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

Individual Commitment Statement: For the Lead Principal Investigator/Project Director, each Principal Investigator, and each additional senior/key person, provide a signed statement that reflects their commitment to this project, including their individual level of time commitment, for a minimum period of four years. Multiple personnel representing the same institution may sign the same letter of commitment, as applicable. Each letter of commitment is limited to one page (this page is not included in the two page limit for each biographical sketch).

Provide the Biographical Sketches 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 2: CURRENT AND PENDING SUPPORT

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

List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid.

For every activity, list the following items:

- The sponsor of the activity or the source of funding
- The award or other identifying number
- The title of the award or activity
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The person-months of effort per year being dedicated to the award or activity

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

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

APPENDIX 3: BIBLIOGRAPHY & REFERENCES CITED

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

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

APPENDIX 4: FACILITIES, EQUIPMENT & OTHER RESOURCES

This information is used to assess the capability of the organizational resources, including subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). List major items of equipment already available for this project and, if appropriate, identify location and pertinent capabilities. If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. For proposed investigations requiring access to experimental user facilities maintained by institutions other than the applicant, please provide a document from the facility manager confirming that the researchers will have access to the facility. Please provide the Facility and Other Resource information as an appendix to your project narrative.

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

APPENDIX 5: ADDITIONAL FUNDING

Discuss any additional funding and contributions-in-kind for the proposed project, including, but not limited to, optional cost sharing. If there is no additional funding, contributions-in-kind, or cost sharing, state “None.”

- 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 open, machine-readable, and digitally accessible to the public at the time of publication. This includes data that are displayed in charts, figures, images, etc. In addition, the underlying digital research data used to generate the displayed data should be made as accessible as possible to the public in accordance with the principles stated in the Office of Science Statement on Digital Data Management (<http://science.energy.gov/funding-opportunities/digital-data-management/>). This requirement could be met by including the data as supplementary information to the published article, or through other means. The published article should indicate how these data can be accessed.
3. DMPs should consult and reference available information about data management resources to be used in the course of the proposed research. In particular, DMPs that explicitly or implicitly commit data management resources at a facility beyond what is conventionally made available to approved users should be accompanied by written approval from that facility. In determining the resources available for data management at Office of Science User Facilities, researchers should consult the published description of data management resources and practices at that facility and reference it in the DMP. Information about other Office of Science facilities can be found in the additional guidance from the sponsoring program.
4. DMPs must protect confidentiality, personal privacy, Personally Identifiable Information, and U.S. national, homeland, and economic security; recognize proprietary interests, business confidential information, and intellectual property rights; avoid significant negative impact on innovation, and U.S. competitiveness; and otherwise be consistent with all applicable laws, and regulations. There is no requirement to share proprietary data.

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

- 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; and
- This appendix will not count in the Project Narrative page limitation.

APPENDIX 8: STATEMENT OF CONFLICT OF INTEREST

At the time of submission, the applicant shall include information identifying potential, apparent, or actual organizational and individual conflicts of interest and proposed mitigation. This shall include the applicant, their team members, and senior/key personnel named in the application. Negative responses are also required. Prior to award, DOE reserves the right to require the submission of a Conflict of Interest Management Plan describing the applicants approach to managing conflicts of interest.

- Do not attach a separate file; and
- This appendix will not count in the Project Narrative page limitation.

APPENDIX 9: ORGANIZATIONAL LETTERS OF COMMITMENT

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 and must be current, signed, and dated by a person authorized to commit the participating organization to a legally binding agreement for this project.

- Do not attach a separate file; and
- This appendix will not count in the Project Narrative page limitation.

APPENDIX 10: LIST OF COLLABORATORS AND POSSIBLE CONFLICTS OF INTEREST

In tabular form following the example below, provide a list of collaborators for all senior/key personnel, including co-authors over the past 48 months, graduate and postdoctoral advisors of the senior/key personnel, graduate students and postdoctoral associates that have been supervised by the senior/key personnel during the past 60 months, and any other current close associations of the senior/key personnel. The table should exclude all personnel at any of the institutions participating in this application.

Collaborator			Institution
Last Name	First Name	Title	Institution Name

** Applicants are strongly encouraged to follow the exact format of the sample table because the tabular information will be compiled across all applications. This includes the following elements:

- Include grid lines around each cell.
 - Do not merge name or institution cells, even if individuals share the same institution.
 - Do not change the order of the columns.
 - Do not include any additional information (e.g. “PI”, “Co-PI”, or footnote symbols) under “Last Name” and “First Name”.
 - Do not include departmental affiliations under Institutions.
 - If an individual has a joint appointment, separate the institutions with a “/” (i.e. “Univ of X / National Lab Y”).
-
- Do not attach a separate file; and
 - This appendix will not count in the Project Narrative page limitation.

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 application. Reviewers are not required to consider information in this appendix.

- Do not attach a separate file.
 - This appendix will not count in the project narrative page limitation.
-
- **Follow the above instructions to include the information as appendices to the project narrative file.**
 - **These appendices will not count toward the project narrative’s page limitation.**

3. Detailed Instructions for the Budget

Budgets are required for the entire project period. A budget form should be completed for each

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

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

Section A. Senior/Key Person (Required)

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

Section B. Other Personnel

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

Section C. Equipment Description

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

Section D. Travel

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

Section E. Participant/Trainee Support Costs:

If applicable, submit training support costs. Educational projects that intend to support trainees (precollege, college, graduate and post graduate) must list each trainee cost that includes stipend levels and amounts, cost of tuition for each trainee, cost of any travel (provide the same information as needed under the regular travel category), and costs for any related training

expenses. Participant costs are those costs associated with conferences, workshops, symposia or institutes and breakout items should indicate the number of participants, cost for each participant, purpose of the conference, dates and places of meetings and any related administrative expenses. In the budget justification, indicate whether trainee cost estimates are based upon past experience of support of similar number of trainees on similar projects; past experience of support of similar number of participants attending similar conferences/workshops/symposia; or something else (describe).

Section F. Other Direct Costs:

Enter Other Direct Costs information for each item listed.

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

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

Section G. Direct Costs

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

Section H. Other Indirect Costs

Enter the Indirect Cost information for each field. Only four general categories of indirect costs are allowed/requested on this form, so please consolidate if needed.

Section I. Total Direct and Indirect Costs

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

D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS

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

E. SUBMISSION DATES AND TIMES

1. Letter of Intent Due Date

March 7, 2016 at 5 PM Eastern Time

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

2. Pre-proposal Due Date

None

3. Proposal Due Date

April 25, 2016 at 5 PM Eastern Time.

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

4. Late Submissions

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

justifications include the following:

- Failure to begin submission process early enough.
- Failure to provide sufficient time to complete the process.
- Failure to understand the submission process.
- Failure to understand the deadlines for submissions.
- Failure to satisfy prerequisite registrations.
- Unavailability of administrative personnel.
- An upper respiratory infection (a “cold”) the week of the deadline.

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

Applicants must contact the Program Office/Manager listed in this 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.

Requests for late submission are only rarely approved.

F. FUNDING RESTRICTIONS

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

G. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS

1. Where to Submit

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

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

2. Registration Process

ONE-TIME REGISTRATION PROCESS

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

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

inquiries about this DOE National Laboratory Program Announcement should reference **LAB 16-1528**.

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 Program Announcement has been submitted; (3) all mandatory requirements are satisfied; (4) the proposed project is responsive to the objectives of the Program Announcement, and (5) the proposed project is not duplicative of programmatic work. Proposals that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

Be advised that proposals focused on structural, thermoelectric, and energy storage materials; structural properties; and synthesis of 2-d layered materials, assemblies of nanoparticles, isolated molecules, liquids (including ionic liquids), and homogeneous catalysts will be considered non-responsive. Research that emphasizes density functional methods as currently implemented or semi-empirical approaches, dynamical mean field theory, and classical and first principles molecular dynamic will be considered non-responsive.

2. Merit Review Criteria

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

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

The evaluation process will also include program policy factors such as the relevance of the proposed research to the terms of the DOE National Laboratory Announcement and the agency's programmatic needs, the balance of activities within the program, and the utility of the proposed activities to the broader scientific community. Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of a proposal constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

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

SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROPOSED RESEARCH

- Does the application present a balanced and comprehensive program of basic research that, as needed, supports experimental, theoretical, and computational efforts and development of new capabilities for predictive design of functional materials?
- Does the proposed research embody the scientific approaches detailed in the following reports: *Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science* (<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#CMSC>), *From Quanta to the Continuum: Opportunities for Mesoscale Science* (<http://science.energy.gov/bes/news-and-resources/reports/abstracts/#OFMS>) and *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science* (http://science.energy.gov/~media/bes/besac/pdf/Reports/CFME_rpt_print.pdf)
- Does the application contain clearly defined four-year scientific research, data, and software goals?
- Will the research develop software that takes advantage of current and future DOE leadership class computing resources?
- Do the scientific, software, and data goals of the project have sufficient programmatic focus?
- Is the proposed research program likely to meet the stated four-year scientific research, software, and data goals?
- Is the Data Management Plan suitable for the proposed research; to what extent does it make the data available and useful to the scientific community?
- Will the proposed research likely result in useful software and data that will accelerate the design, discovery, and development of new functional materials?

APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

- Are the strategy and the plan for the development and operation of the project including the need for an approach involving several senior/key personnel, the means for achieving an integrated Team, and plans for leadership and guidance for the scientific and technical direction, appropriate?
- Does the application present integrated research that embodies the “team science” approach in which the research challenges to be addressed are those that are likely to be overcome only by a centrally managed, multi-disciplinary team?
- Are the proposed scientific methods or approaches detailed in the proposal appropriate to achieve the stated scientific goals?
- Are the plans (if any) for external collaborations and partnerships reasonable and appropriate?
- Are the roles and intellectual contributions of the Project Director, Principal Investigator(s), and all other senior/key personnel adequately described and appropriate?
- Is the proposed approach for making a community code and the associated experimental and computational data available to general users from the research community,

including the Open Source Software Distribution Plan, likely to be effective? Is there a plan to get input from the community that will use the data and software?

COMPETENCY OF APPLICANT'S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES

- Do the applicant's senior/key personnel have a proven record of research in the disciplines needed for success in this project?
- Do the lead organization, the Director, and the other senior/key personnel have proven records of success in project, program, and personnel management of diverse teams of scientific and technical professionals for projects of comparable complexity and magnitude?
- Is the plan for recruiting any additional scientific and technical personnel including new senior staff, students and postdocs reasonable and appropriate?
- Is the proposed access to existing research space, instrumentation and facilities at the partner institutions likely to meet the needs of the proposed team?
- Is there adequate access to experimental and computational capabilities as needed to ensure successful completion of the proposed research, including access to research capabilities and resources outside of the Team?
- Will the Project Director and senior/key personnel be sufficiently available given their role particularly taking into account their potential involvement in other major projects?
- Does the team have expertise and capabilities required to support the development and maintenance of community research codes and data?

REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET

- Are the requested operating budget and the distribution of the funds among research tasks/themes, software development and partners reasonable for the program?
- Are the equipment needs adequately identified, and costs for needed new instrumentation or upgrades realistically estimated?
- Are the budgeted costs for preparing space for existing and new equipment and instrumentation appropriate and reasonable?
- Are all subawards, travel, student costs and other ancillary expenses adequately estimated and justified?

STRENGTH OF THE MANAGEMENT PLAN

- Is there a clear lead organization and a Project Director with qualifications to manage a large team?
- Does the applicant present a comprehensive management plan? What is the likelihood that the applicant can overcome key scientific challenges and shift research directions in response to promising developments? Has the application presented a clearly defined mechanism to evaluate success/failure and to reconfigure research thrusts as needed?
- If needed, is there a well-defined plan to the use of state-of-the-art technology and frequent virtual meetings to enable meaningful, efficient long distance collaboration?
- Does the applicant present an organizational structure that delineates the roles and responsibilities of senior/key personnel and describes the means of providing external oversight and guidance for scientific and technical direction of the research program?

- Is the role of an advisory committee (required) and any executive committee, program committee, or their equivalent adequately described and appropriate?
- Are environment, safety, health and quality assurance (ESH & QA) issues responsibly anticipated and addressed? Does the applicant have a work planning and control process which considers them?

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

- Does the application describe a well-integrated team based approach to addressing the scientific and software development goals?
- Is the proposed team of researchers likely to work together in a cohesive and integrated manner? Have they demonstrated their ability to do so in the past?
- Have the applicants defined scientific problems that are likely to be addressed only through close collaboration among the researchers on the application?
- Are the elements of the proposed research appropriately integrated, coordinated, and synergistic?

DEVELOPMENT AND UTILIZATION OF UNIQUE FACILITIES, CAPABILITIES OR APPROACHES

- Does the research plan include full utilization of current (petascale) and future (exascale) leadership class computing resources?
- Does the proposed research rely on the use of unique facilities at the applicants' home institutions or at US or international user facilities?
- Have the applicants proposed the development of unique facilities, capabilities, or approaches to achieve the stated scientific goals?

B. REVIEW AND SELECTION PROCESS

1. Merit Review

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

2. Selection

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

- Scientific and technical merit of the proposed activity as determined by merit review
- Availability of funds
- Relevance of the proposed activity to Basic Energy Science (BES) priorities
- Ensuring an appropriate balance of BES activities
- Previous performance
- 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
- Relationship of the proposed project to other research and development programs in DOE, 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
- Potential for developing synergies between the proposed project and other ongoing BES research activities

3. Discussions and Award

The Government may enter into discussions with a selected applicant for any reason deemed necessary. Failure to resolve satisfactorily the issues identified by the Government will preclude award to the applicant.

C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES

It is anticipated that the award selection will be completed by September 30, 2016. It is expected that awards will be made in Fiscal Year 2016.

DOE is interested in seeing projects supported under this FOA begin work by September 30, 2016.

Section VI - AWARD ADMINISTRATION INFORMATION

A. AWARD NOTICES

1. Notice of Selection

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

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

2. Notice of Award

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

B. REPORTING

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

Section VII - QUESTIONS/AGENCY CONTACTS

A. QUESTIONS

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

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

Section VIII - OTHER INFORMATION

A. MODIFICATIONS

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

B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE

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

C. COMMITMENT OF PUBLIC FUNDS

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

D. PROPRIETARY PROPOSAL INFORMATION

Patentable ideas, trade secrets, proprietary or confidential commercial or financial information, disclosure of which may harm the applicant, should be included in a proposal only when such information is necessary to convey an understanding of the proposed project. The use and disclosure of such data may be restricted, provided the applicant includes the following legend on the first page of the project narrative and specifies the pages of the proposal which are to be restricted:

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

To protect such data, each line or paragraph on the pages containing such data must be specifically identified and marked with a legend similar to the following:

“The following contains proprietary information that (name of applicant) requests not be released to persons outside the Government, except for purposes of review and evaluation.”

E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL

In conducting the merit review evaluation, the Government may seek the advice of qualified non-Federal personnel as reviewers. The Government may also use non-Federal personnel to conduct routine, nondiscretionary administrative activities. The applicant, by submitting its proposal, consents to the use of non-Federal reviewers/administrators. Non-Federal reviewers must sign conflict of interest and non-disclosure agreements prior to reviewing a proposal. Non-Federal personnel conducting administrative activities must sign a non-disclosure agreement.

F. AVAILABILITY OF FUNDS

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