DEPARTMENT OF ENERGY (DOE)
OFFICE OF SCIENCE (SC)
BASIC ENERGY SCIENCES (BES)

COMPUTATIONAL MATERIALS SCIENCE – EXPLORATORY RESEARCH AT THE EXASCALE

DOE NATIONAL LABORATORY PROGRAM ANNOUNCEMENT NUMBER: LAB 24-3290

ANNOUNCEMENT TYPE: AMENDMENT 000001

Amendment 000001 is issued to clarify the instructions on page 9.

Announcement Issue Date:	**January 11, 2024**
Submission Deadline for Letter of Intent:	**February 15, 2024 at 5:00 PM Eastern Time** **A Letter of Intent (LOI) is required for new and renewal proposals.** **Letters of Intent must be submitted by an authorized institutional representative**
Submission Deadline for Proposals:	**March 28, 2024 at 5:00 PM Eastern Time**

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UPDATES AND REMINDERS

RECOMMENDATION

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

PROMOTING INCLUSIVE AND EQUITABLE RESEARCH (PIER) PLAN

All new and renewal proposals must provide a Promoting Inclusive and Equitable Research (PIER) Plan as an appendix to the research narrative. Please read the instructions in Section IV and the associated review criteria in Section V.

INTERAGENCY FORMATS FOR CURRENT AND PENDING SUPPORT AND BIOGRAPHICAL SKETCHES

Interagency common instructions for preparing current and pending support and biographical sketches are being developed. The Science Experts Network Curriculum Vitae (SciENcv) system at https://www.ncbi.nlm.nih.gov/sciencv/ will be updated to support the forthcoming common instructions and formats. The fillable PDFs provided by the National Science Foundation at https://nsf.gov/bfa/dias/policy/nsfapprovedformats/ are no longer available. When interagency common formats and instructions are promulgated, their use will be required. SC strongly encourages all researchers to use the online SciENcv system to ensure that their documents are prepared in the appropriate format with the least inconvenience.

INDIVIDUALS WHO SHOULD NOT SERVE AS MERIT REVIEWERS

Follow the updated instructions in Section VIII and consider the use of the Collaborato Template available at https://science.osti.gov/grants/Policy-and-Guidance/Agreement-Forms. Do not include this list as part of the biographical sketch.

SC STATEMENT OF COMMITMENT

The DOE SC is fully and unconditionally committed to fostering safe, diverse, equitable, and inclusive work, research, and funding environments that value mutual respect and personal integrity. SC is committed to advancing belonging, accessibility, justice, equity, diversity, and inclusion across the portfolio of activities we sponsor. SC's effective stewardship and promotion of safe, accessible, diverse, and inclusive workplaces that value and celebrate the diversity of people, ideas, cultures, and educational backgrounds across the country and that foster a sense of belonging in our scientific community is foundational to delivering on our mission. We are committed to promoting people from all backgrounds, including individuals and communities that were historically underrepresented and minoritized in science, technology, engineering, and math (STEM) fields and the activities we sponsor in recognition of our responsibility to serve the public. We also recognize that harnessing a broad range of views, expertise, and experiences drives scientific and technological innovation and enables the SC community to push the frontiers of scientific knowledge for U.S. prosperity and security. Discrimination and harassment

undermine SC's ability to achieve its mission by reducing productivity, discouraging, or inhibiting talent retention and career advancement, and weakening the integrity of the SC enterprise overall. SC does not tolerate discrimination or harassment of any kind, including sexual or non-sexual harassment, bullying, intimidation, violence, threats of violence, retaliation, or other disruptive behavior at institutions receiving SC funding or other locations where activities funded by SC are carried out. All applicants and collaborators should familiarize themselves with the SC Statement of Commitment available at https://science.osti.gov/SW-DEI/SC-Statement-of-Commitment.

UPDATING YOUR PAMS PROFILE

All applicants are encouraged to update their profiles in the PAMS website at https://pamspublic.science.energy.gov regularly, at least annually, to ensure SC has your most up to date information. The PAMS profile now requires that individuals provide responses to the demographic related fields. SC strongly encourages personnel at applicant and awardee institutions, including Principal Investigators (PIs), Co-PIs, and other Key Personnel, to provide their demographic information. By providing your demographic information, you are assisting with SC's continued commitment to advancing diversity, equity, and inclusion in its business practices. Alternatively, for information you wish not to disclose, please select, "Do not wish to provide." Your individual demographic information will not be shared with peer reviewers and the information in your PAMS profile is protected by the requirements established in the Federal Privacy Act of 1974. Aggregate, anonymized demographic information may be shared with confidential review committees who are charged to evaluate the quality and efficacy of SC's business practices. For example, summary statistics of all applicants to or award selections from a particular SC FOA may be reviewed by a Committee of Visitors.

PDF GENERATION

The research narrative in a proposal must be one single machine-readable PDF file that contains the DOE Title Page, project narrative, all required appendices, and other attachments. This single PDF file may not be scanned from a printed document and must be uploaded in PAMS. This must be a plain PDF file consisting of text, numbers, and images without editable fields, signatures, passwords, redactions, or other advanced features available in some PDF-compatible software. The research narrative will be read by SC staff using the full version of Adobe Acrobat: Please ensure that the narrative is readable in Acrobat. If combining multiple files into one research narrative, ensure that a PDF portfolio or binder is not created. If creating PDF files using any software other than Adobe Acrobat, please use a "Print to PDF" or equivalent process to ensure that all content is visible in the research narrative. Once a research narrative has been assembled, please submit the combined research narrative file through a "Print to PDF" or equivalent process to ensure that all content is visible in one PDF file that can be viewed in Adobe Acrobat. Review your submission to ensure that blank pages are not present.

Checklist for Avoiding Common Errors:

Item	Issue
Proposals	Submitted in PAMS. Do not submit proposals in Grants.gov or FedConnect. Do not attempt to submit a proposal unless you are affiliated with a DOE/NNSA National Laboratory.
Letters of Intent (LOIs)	- Submit your LOI in PAMS. - Do not submit your LOI in Grants.gov. - Follow the instructions in Section IV for the preparation of an LOI.
Page Limits	Strictly followed throughout proposal, including particular attention to: - Research Narrative - Appendix 2 Narrative, if any - Biosketches - Data Management Plan(s) (DMPs) - Letter(s) of Recommendation, if any
Personally Identifiable Information	None present in the proposal
Research Narrative	Composed of one PDF file including all appendices
Project Summary / Abstract	Name(s) of applicant, PI(s), PI's institutional affiliation(s), Co-Investigator(s), Co-Investigator's institutional affiliation(s)
DOE Title Page	Follow instructions closely
Budget	Use current negotiated indirect cost and fringe benefit rates
Budget Justification (attached to budget)	Justify all requested costs
Biographical Sketches	Follow page limits strictly and do not include list of collaborators.
Current and Pending Support	Ensure complete listing of all activities, regardless of source of funding.
List of Individuals who Should not Serve as Merit Reviews	Provided as separate file in proposal
Data Management Plans (DMP)	- If referring to an experiment's DMP, describe the relationship to the proposed research - Include a DMP even if no experimental data is expected
Promoting Inclusive and Equitable Research (PIER) Plan	PIER Plans are a new requirement for new and renewal proposals.
Institutions capable of being funded through the DOE Field Work System	Do not create new institutions in the PAMS website for any DOE/NNSA National Laboratory or DOE Site. Submissions will be evaluated for technical

	merit, but any resulting funding, work, or awards will be made under the laboratory or site's contract with DOE. No separate financial assistance awards will be made. No administrative provisions of this Announcement will apply to the laboratory or any laboratory subcontractor.

GENERAL INQUIRIES ABOUT THIS ANNOUNCEMENT SHOULD BE DIRECTED TO:

Technical/Scientific Program Contacts:
Dr. Matthias Graf (matthias.graf@science.doe.gov) and Dr. Claudia Mewes (claudia.mewes@science.doe.gov). Please select Matthias Graf as program manager, when submitting in PAMS.

SUMMARY

The DOE SC program in Basic Energy Sciences (BES) hereby announces its interest in receiving new and renewal proposals in Computational Materials Sciences (CMS) with the aim of producing widely applicable, validated public-access community codes and associated databases to enable science-based predictive design and discovery of functional materials. Exploratory research at the exascale is expected. Proposals should leverage the exascale software stack and work done under the DOE Exascale Computing Project. They must utilize DOE's exascale Leadership Computing Facilities to study real-world materials that otherwise would be impractical or impossible to investigate due to their complexity. The research component should meet the priorities of the BES research program as determined by BES community planning documents (see references below) and peer review.

Targeted topics are described in the Supplementary Information section below. Proposals that do not identify and address one or more of these specific topics may be declined without review.

CMS supports integrated, multidisciplinary team awards that must focus on the creation of computational open-source community codes, including contributions to public-access databases, that are necessary for addressing basic energy sciences challenges. The teams combine skills and expertise in materials theory, modeling, computation, and artificial intelligence, that result in advances that will not be accomplished by those same researchers working separately. Furthermore, research should involve the development of new ab-initio methods in computational solid-state theory, where science-based predictions by those developed codes must be verified as well as experimentally validated by the team or through collaborations. See Additional Requirements in the Supplementary Information section for more information on topical and excluded research areas for this funding opportunity.

This effort is part of the DOE BES research related to the Artificial Intelligence for Science Initiative, the Materials Genome Initiative, as well as the Exascale Computing Initiative. BES has funded Computational Materials Sciences awards since 2015. Additional information on these awards can be found at the websites listed in the references.

SUPPLEMENTARY INFORMATION

Background

Major progress in building and unifying the Materials Innovation Infrastructure envisioned by the Materials Genome Initiative (MGI) [1] has helped to manage, integrate, and share knowledge to accelerate materials research and development. A combination of algorithm and hardware advances has led to a phenomenal increase in computational power over the past four decades. The culmination of these advances has made many real-world materials problems, which include defects, disorder, interfaces, and electronic correlations, tractable with the arrival of exascale computing hardware and software through the DOE Exascale Computing Project (ECP) [2, 3]. ECP's enhanced computational capabilities push the technology and predictive science to new frontiers in accuracy, system size, energy and time scales, especially when combining traditional ab-initio calculations, modeling, and simulations with algorithm development.

This rapid development has seen further acceleration through artificial intelligence/machine learning (AI/ML) techniques that have the potential to radically transform the materials research landscape, and the availability of high-quality materials data to realize this opportunity. The last few years have seen exponential growth in physics-aware AI/ML-enabled materials discovery, modeling, and simulation in support of the Artificial Intelligence for Science Initiative [4].

The goal of this Announcement is to leap beyond simple extensions of current theory and models of materials by transitioning predictive research into a post-exascale computing era, in which open hardware interfaces, open software interoperability and modularity will be a growing trend of the future. This paradigm shift will enable the usage of open-source, public-access computational software for the design, discovery, and development of new materials with unique properties. In turn, this will create new advanced and innovative technologies. Given the importance of materials to virtually all technologies, computational materials sciences are critical for American competitiveness, innovation, and the Nation's energy security.

Development of fundamentally new design principles could enable interoperable or modular research codes and integrated software packages to address correlations over long length and time scales for prediction of the total functionality of materials over a lifetime of use. Examples include, but are not limited to, the dynamics and correlated interactions of matter with atomic precision, conversion of solar energy to electricity, and superior electronic and magnetic properties for improved low-power electronics. Success will require extensive R&D with the goal of creating verified and experimentally validated, open-source, public-access community software that will enable functional materials innovation.

Exploratory research at the exascale and development of these computational codes require a fully integrated, multi-investigator team approach, combining the skills of experts in materials theory, modeling, computation, and artificial intelligence. The range of the research includes development of new ab initio theory, advanced materials modeling, physics-guided AI/ML, and mining data from databases, to confirm the predictions of the codes.

Many of the underlying phenomena require understanding the materials dynamics at ultrafast time scales or 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.

Computational exploratory research at the exascale should focus on discovery, design, and understanding of advanced materials with unique properties. The composition of teams should build on past successes, team synergy, and reflect any new directions. Diversity, equity, and inclusion should be considered in the team selection and is part of the evaluation.

For renewal proposals, the inclusion of new and exciting research directions evolving from the previous funding cycle is highly encouraged.

Topics and Additional Requirements

To be considered, a proposal must address the specific Eligibility requirements in Section III and the Review Criteria in Section V. In addition, proposals must focus on functional materials research and address at least one of the following two topics:

Topic A: Computational discovery and design of functional materials with unique physical properties (e.g., quantum and topological materials, transition metal oxides, perovskites, two-dimensional van-der-Waals materials, wide-bandgap semiconductors, and optoelectronic materials).

Topic B: Computational modeling of emergent and ordered magnetic, superconducting, and/or ferroelectric phases, including their dynamics.

Suitable types of software development will emphasize electronic correlations, relativistic effects, spin-orbit coupling, and coupling of electrons with phonons, magnons, plasmons, excitons, as well as electronic and optical properties or spectroscopies, and excited state dynamics.

Exclusions: Excluded are proposals that emphasize density functional theory approaches and first-principles methods as currently implemented. Furthermore, excluded are proposals on cold atoms, structural materials, molecules, ionic liquids, electrolytes, batteries, catalysts, and soft matter.

In addition, proposals must address:
- Open-source, public-access community software developed under this Announcement should have broad applicability, interoperability, and provide functionalities beyond current codes. Proposers must describe how the software will be distributed as open source in an Open-Source Software Distribution Plan. This plan describes the maintenance and long-term accessibility of the software, including a plan and mechanisms for research community input to software development and validation.
- Provide a Data Management Plan that addresses FAIR (Findable, Accessible, Interoperable, and Reusable) [5] principles and how they will apply to the anticipated datasets, software [6], and models [7] to be developed.
- Provide a detailed plan for the full utilization of today's midscale to petascale to exascale leadership computing facilities. The open-source software must be ready for or capable of exascale computing.

- Proposals must have integrated, multi-investigator teams combining expertise in materials theory, modeling, computation, and physics-guided AI/ML, supported by a clearly articulated management plan that ensures a coherent team science approach.
- Multiple national laboratories and other organizations proposing as a team must designate a lead organization. For limitations on LOIs and proposals see III.D. LIMITATIONS ON SUBMISSIONS. The designated lead organization must perform a greater percentage of the effort, as determined by the budget distribution by institution, than any other partner organization or subawardee.

Meetings

The selected awardees will be expected to attend one biennial PI meeting and participate in biennial coordination activities with other programs. Applicants should anticipate a need for travel to effectively communicate with other researchers and request appropriate funding in their budgets.

Open Science

SC is dedicated to promoting the values of openness in Federally-supported scientific research, including, but not limited to, ensuring that research may be reproduced and that the results of Federally-supported research are made available to other researchers. These objectives may be met through any number of mechanisms including, but not limited to, data access plans, data sharing agreements, the use of archives and repositories, and the use of various licensing schemes.
The use of the phrase "open-source" does not refer to any particular licensing arrangement but is to be understood as encompassing any arrangement that furthers the objective of openness.

References

[1] Materials Genome Initiative Strategic Plan. November 2021. https://www.mgi.gov/sites/default/files/documents/MGI-2021-Strategic-Plan.pdf
[2] https://www.exascaleproject.org/
[3] Transitioning ASCR after ECP. October 2020. https://science.osti.gov/-/media/ascr/ascac/pdf/meetings/202004/Transition_Report_202004-ASCAC.pdf
[4] https://science.osti.gov/Initiatives/AI
[5] Wilkinson, M. D. et al. The FAIR Guiding Principles for Scientific Data Management and Stewardship. Sci. Data 3, 160018, 2016. https://doi.org/10.1038/sdata.2016.18
[6] Hong, C., et al. FAIR Principles for Research Software version 1.0. (FAIR4RS Principles v1.0). Research Data Alliance (2022). https://doi.org/10.15497/RDA00068
[7] Ravi, N., et al. FAIR principles for AI models with a practical application for accelerated high energy diffraction microscopy. Sci Data 9, 657 (2022). https://doi.org/10.1038/s41597-022-01712-9

Below are additional informative references:
[8] Report of the Department of Energy Workshop on Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and

Science, July 2010. https://science.osti.gov/-/media/bes/pdf/reports/files/Computational_Materials_Science_and_Chemistry_rpt.pdf
[9] Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology, Report of the Office of Basic Energy Sciences Workshop on Quantum Materials. https://science.osti.gov/-/media/bes/pdf/reports/2016/BRN_Quantum_Materials_for-Energy_Relevant_Technology.pdf
[10] DOE's Computational Materials Sciences (CMS) webpage: https://science.osti.gov/bes/Research/Computational-Materials-and-Chemical-Sciences-CMS-CCS/Computational-Materials-Sciences

SC uses two different mechanisms to support teams of multiple institutions.

COLLABORATIVE PROPOSALS

Collaborative proposals will not be accepted under this Announcement.

SUBAWARDS

Multi-institutional teams must submit one proposal from a designated lead national laboratory with all other team members proposed as subawards.

Section II – AWARD INFORMATION

II.A. TYPE OF AWARD INSTRUMENT

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

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

II.B. ESTIMATED FUNDING

DOE anticipates, subject to the availability of future year appropriations, a total of up to $13 million will be available under this DOE National Laboratory Announcement in current and future fiscal year funds. Up to 4 national laboratory awards are expected. Proposers should request project support for two years. Following the first-year award, out-year support will be contingent on the availability of appropriated funds, progress of the research, and programmatic priorities. Awards are expected to begin in fiscal year 2024.

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.

II.C. MAXIMUM AND MINIMUM AWARD SIZE

(See B. Estimated Funding section above.)

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

The ceiling and floor described in this FOA represent the expected range of award sizes.

Ceiling

$2,000,000 per year

Applications requesting more than this amount of support may be declined without further review.

Floor

$1,000,000 per year

Applications requesting less than this amount of support may be declined without further review.

For renewal proposals, notwithstanding the "Floor" identified above, DOE may consider limited-

term renewal awards to allow for the completion of research projects and orderly closeout of CMS awards that do not merit long-term continued support. Annual funding for such awards could fall below the $1,000,000 floor.

II.D. EXPECTED NUMBER OF AWARDS

(See B. Estimated Funding Section above.)

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

II.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.

II.F. PERIOD OF PERFORMANCE

(See B. Estimated Funding section above.)

DOE anticipates making awards with a project period of two years.

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

II.G. TYPE OF PROPOSAL

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

Section III – ELIGIBILITY INFORMATION

III.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.

III.B. COST SHARING

Cost sharing is not required.

III.C. ELIGIBLE INDIVIDUALS

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

III.D. LIMITATIONS ON SUBMISSIONS

Applicant institutions are limited to no more than one Letter of Intent and one proposal as the lead institution. Should DOE receive submissions in excess of the applicable limits, DOE reserves the right, in its sole discretion, to request additional or clarifying information to ascertain the institution's intended submissions. Otherwise, DOE will consider the latest received submissions to be the institution's intended submission.

If more than one proposal is received from a National Laboratory, DOE will consider only the proposal that matches the qualified Letter of Intent (as described below in Section IV.B.2). The remaining proposals will be deemed non-responsive and rejected without further review. However, there is no limitation on the number of proposals in which a national laboratory may participate as a team member or subawardee.

LIMITATIONS ON PI

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

Section IV – PROPOSAL AND SUBMISSION INFORMATION

IV.A. ADDRESS TO REQUEST PROPOSAL PACKAGE

Proposal submission instructions are available in this Announcement on the DOE SC Portfolio Analysis and Management System (PAMS). Screenshots showing the steps in DOE National Laboratory proposal submission are available in the PAMS Help materials, accessible by navigating to https://pamspublic.science.energy.gov and clicking on the "PAMS Help" link.

Proposals submitted outside of PAMS will not be accepted.

IV.B. LETTER OF INTENT AND PRE-PROPOSAL

IV.B.1. Letter of Intent

LETTER OF INTENT DUE DATE

The LOI due date is printed on the cover of this Announcement.

A LOI is required and must be submitted by the date indicated on the cover of this FOA.

The LOI is to help in planning the review and the selection of potential reviewers for the proposal. The LOI must include, at the top of the first page, the following information:

Title of Planned Research Application
Lead Principal Investigator Name, Job Title
Lead National Laboratory
Lead PI Phone Number, Lead PI Email Address
Announcement Number: Include the Number indicated on the cover of this Announcement.
Primary Topic Area (Include only 1; select topic A or topic B described in Section I, Supplementary Information):
Secondary Topic Area (Optional; in case your planned research addresses both topics, list the second topic described in Section I, Supplementary Information):
Partner Institutions: If applicable, list all partner institutions.

The material listed here defines the required content of a cover page. Additional material is not allowed.

Immediately following the header information, the LOI should include the following table:

Table 1: Principal Investigator or Senior/Key Person		
Last (Family) Name	**First (Given) Name**	**Institution (Full Name)**

The cover page must be followed by a clear and concise description of the objectives and technical approach of the proposed research. The description of the proposed research may not exceed two pages, when printed using standard letter-size (8.5-inch x 11-inch) paper with 1-inch margins (top, bottom, left, and right). The font must not be smaller than 11 points. Figures and references, if included, must fit within the two-page limit.

The LOI must be machine-readable. Do not submit a scanned image of a printed document.

In addition, the LOI must include a listing of senior/key personnel and a listing of individuals who should not serve as merit reviewers of a subsequent proposal. Detailed instructions for how to craft such a listing are provided in Section VIII of this Announcement. **Note that the listing of individuals who should not serve as merit reviewers is rarely empty because the instructions contain mandatory inclusions requirements.** This listing will not count toward the LOI's page limit. The list of individuals must be included as an "Additional Attachment" to your LOI in PAMS, preferably in Excel format using the template provided in Section VIII.

LOI SUBMISSION

LOIs are created in the software system of your choice and must be submitted electronically through the DOE SC Portfolio Analysis and Management System (PAMS) website https://pamspublic.science.energy.gov/. You cannot draft or edit an LOI in PAMS. Do not submit an LOI through FedConnect or Grants.gov.

LOIs may only be submitted by a user at the Lead PI's institution with the "Submit to DOE" privilege in PAMS. A Lead PI may draft a LOI but will only be able to submit the LOI for institutional countersignature.

Applicants are strongly encouraged to inform their DOE Program Manager if teaming arrangements, proposed personnel, topics, or the anticipated title change between submitting the LOI and when a proposal is submitted, to ensure that their proposal is properly linked to their LOI and that reviewers are properly assigned to the proposal.

Detailed instructions about how to submit an LOI are in Section VIII of this Announcement.

IV.B.2. Pre-proposal

Not applicable.

IV.C. PROPOSAL SUBMISSION AND CONTENT

IV.C.1. Summary of Proposal Contents

Each DOE National Laboratory proposal will contain the following sections:

- A Cover Page, entered into PAMS as structured data using the on-screen form
- 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 Title Page
    - Table of Contents
    - Project Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel)
    - Appendix 1: Biographical Sketch(es)
    - Appendix 2: Current and Pending Support
    - Appendix 3: Bibliography and References Cited
    - Appendix 4: Facilities and Other Resources
    - Appendix 5: Equipment
    - Appendix 6: Data Management Plan
    - Appendix 7: Promoting Inclusive and Equitable Research (PIER) Plan
    - Appendix 8: Open-Source Software Distribution Plan
    - Appendix 9: Renewal Proposal Products (renewals only)
    - Appendix 10: Letter Of Commitment
    - Appendix 11: Other Attachments (optional)
- Collaborator Information

SUBMISSION INSTRUCTIONS

Completed proposals must be submitted into the DOE SC Portfolio Analysis and Management System (PAMS) at https://pamspublic.science.energy.gov.

Important Instructions to the Sponsored Research Office of Submitting Institutions: SC requires that you create one single machine-readable PDF file that contains the DOE Title Page, project narrative, biographical sketch, current and pending support, bibliography and references cited, facilities and other resources, equipment, data management plan, and other attachments. This single PDF file may not be scanned from a printed document and must be uploaded in PAMS. This must be a plain PDF file consisting of text, numbers, and images without editable fields, signatures, passwords, redactions, or other advanced features available in some PDF-compatible software. Do not use PDF portfolios or binders. The research narrative will be read by SC staff using the full version of Adobe Acrobat: Please ensure that the narrative is readable in Acrobat. If combining multiple files into one research narrative, ensure that a PDF portfolio or binder is not created. If creating PDF files using any software other than Adobe Acrobat, please use a "Print to PDF" or equivalent process to ensure that all content is visible in the research narrative. Once a research narrative has been assembled, please submit the combined research narrative file through a "Print to PDF" or equivalent process to ensure that all content is visible in one PDF file that can be viewed in Adobe Acrobat.

WARNING: The PAMS website at https://pampspublic.science.energy.gov will permit

you to edit a previously submitted proposal in the time between your submission and the deadline. If you choose to edit, doing so will remove your previously submitted version from consideration. If you are still editing at the time of the deadline, you will not have a valid submission. Please pay attention to the deadline.

PROPOSAL DUE DATE

The proposal due date is printed on the cover of this Announcement.

LETTERS

Letters from collaborators or from institutions providing access to data, models, software, equipment and/or facilities may be appended to your research narrative and are not considered part of the research narrative's page limit. Please ensure that letters from collaborators or from institutions providing access to data, models, software, equipment and/or facilities only describe the nature of the collaboration or the access to data, models, software, equipment and/or facilities. Letters of support or recommendation are not allowed in applications under this Announcement.

All letters may be addressed "To Whom It May Concern:".

Letters of collaboration for unfunded or funded collaborations should be placed in Appendix 11 (Other Attachments). Each letter of collaboration may contain two and only two sentences and must use the following format:

> Dear <Principal Investigator Name>:
>
> If your application entitled, "<Application Name>," is selected for funding under the Announcement Name, it is my intent to collaborate in this research by <Complete Sentence with a Very Short Description of What the Collaborator Offers to Do or Provide>.
>
> Thank you for the opportunity to participate.
>
> Sincerely,
>
> <Collaborator's Name and Signature Block>

IV.C.2. Abstract

The project summary/abstract is a summary of the proposed activity suitable for distribution to the public and sufficient to permit potential reviewers to identify conflicts of interest. It must be a self-contained document. The project summary/abstract must be comprised of
- A cover sheet containing the name of the applicant, the project title, the PI and the PI's institutional affiliation, and any coinvestigators and their institutional affiliations.
- This information must be followed by a statement of the project's objectives, a

description of the project, including methods to be employed, and the potential impact of the project (i.e., benefits, outcomes).

- The description of the proposed research may not exceed one page when printed using standard letter-size (8.5-inch x 11 -inch) paper with 1-inch margins (top, bottom, left, and right). The body text font must not be smaller than 11-point. Figures and references, if included, must fit within the one-page limit.

A sample is provided below:

Project Title
A. Smith, Lead Institution (Principal Investigator) A. Brown, Institution 2 (Co-Investigator) A. Jones, Institution 3 (Co-Investigator) Text of abstract (no more than one page, excluding Project Title and list of investigators)

The narrative portion of the project summary must not exceed one page when printed using standard letter-size (8.5-inch x 11-inch) paper with 1-inch margins (top, bottom, left and right) with body text font not smaller than 11-point. To attach a Project Summary/Abstract, click "Add Attachment."

If an application is recommended for award, the project summary will be used in preparing a public abstract about the award. Award abstracts and titles form a Government document that describes the project and justifies the expenditure of Federal funds in light of the DOE and SC mission statements at https://energy.gov/mission and https://science.osti.gov/about/.

- Do not include any proprietary or sensitive business information.
- DOE may use the abstract to prepare public reports about supported research.

IV.C.3. Budget and Justification

The budget must be submitted into PAMS using the PAMS budget form.

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. 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.

While subawards are listed in PAMS as "optional," that is because the presence of a subaward is optional. If a subaward exists, its budgetary information is required. The standard subaward budget form allows for a maximum of 10 subawards. If a proposal contains more than 10 subawards, please present the budgets for the eleventh and subsequent subawards in a tabular

format, followed by the appropriate budget justification, as a part of the lead applicant's budget justification.

IV.C.4. Proposal

DOE TITLE PAGE
(PART OF PROJECT NARRATIVE)

The following proposal title 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: Include the Number indicated on the cover of this Announcement
- DOE/SC Program Office: Basic Energy Sciences
- DOE/SC Program Office Technical Contact: Matthias Graf
- PAMS Letter of Intent tracking number:
- Primary Topic Area (Include only 1; select topic A or topic B described in Section I, Supplementary Information):
- Secondary Topic Area (Optional; in case your planned research addresses both topics, list the second topic described in Section I, Supplementary Information):
- Type of Proposal: (New or Renewal)
- Was the narrative machine generated (e.g. using generative AI)? (Yes or No)

Immediately following the header information, the application must include the following two tables, which will not count toward the page limit for the Project Narrative:

Table 1: Principal Investigator or Senior/Key Person		
Last (Family) Name	**First (Given) Name**	**Institution (Full Name)**

Table 2: Summary budget information for lead institution and all partner institutions			
Institution (Full Name)	**Year 1 Budget ($K)**	**Year 2 Budget ($K)**	**Total Budget ($K)**
Institution 1 (Lead National Laboratory)			**$0**
Institution 2			**$0**

			$0
			$0
Total Budget	$0	$0	$0

Include all partner institutions, including the lead institution. Include the total costs ($ in thousands) of the budget request in each year for each institution and totals for all rows and columns.

PROJECT NARRATIVE

The project narrative **must not exceed a page limit of 25 pages** of technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard letter-size (8.5-inch x 11-inch) paper with 1-inch margins (top, bottom, left, and right). The body text font of all main text must not be smaller than 11-point. Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph. This page limit does not apply to the Title Page, Budget Page(s), Budget Justification, biographical material, publications and references, and appendices, each of which may have its own page limit defined later in this Announcement.

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 Section VIII for instructions on how to mark proprietary proposal information.

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

The following organization of the Project Narrative is suggested:

- **Background/Introduction**: Explanation of the importance and relevance of the proposed work as well as a review of the relevant literature. Provide clear statements about which topic(s) described in Section I, Supplementary Information your proposed work addresses. If applicable make concise connections to the Materials Genome Initiative, the Exascale Computing Initiative, the Artificial Intelligence for Science Initiative, and/or the BES-sponsored workshop reports.
- **Project Objectives:** This section should provide a clear, concise statement of the specific objectives/aims of the proposed project. Objectives/Aims should address research, software, and community adaptation activities.
- **Progress Report (for Renewal Applications Only):** The Project Narrative of a renewal

application must include a separate section that includes a description of results of the work accomplished during the current project period (since the last new or renewal award), an analysis of how the results relate to the activities proposed to be undertaken during the renewal period, and a description of any changes that affected the overall direction of the research being performed. Include an estimate of any remaining funds from the current project period at its anticipated end. Please address specifically your software's readiness for or capability of exascale computing and its community adaption.

- **Proposed Research and Methods**: Identify the hypotheses to be tested (if any) or challenging scientific questions to be addressed and provide details of the methods to be used including the integration of theoretical and computational research efforts with software development activities. This section must include:
  - Provide a detailed description of how the proposed research leaps beyond simple extensions of current theory and models of materials, and how this will drive software development. Describe the role and intellectual contribution of the Lead PI, and as appropriate, other PIs in the proposal. Address the unique skill of your team in materials theory, modeling, computation, and/or AI/ML.
  - Address your software package's applicability and interoperability, why its functionalities are beyond current codes, and how it will be further developed. Provide a detailed plan for the full utilization of today's midscale to petascale to exascale leadership computing facilities. Provide evidence that your open-source software is ready for or capable of exascale computing.
  - Provide technical details to assess the proposed methodologies. Data driven approaches should address data availability. If applicable, provide details on the proposed physics-guided AI/ML approaches and how they are integrated in the overall workflow.
  - Provide a detailed research plan with timeline, and an assessment of the potential scientific impact of the research. Include risk assessment and mitigation strategies and describe how the research plan will attain the 2-year scientific goals.
  - Describe the verification and validation process for the developed software including the process that will be used to generate, verify, validate, and utilize computational data.
  - Briefly outline the resources available to your team (Appendix 4 should include detailed information about facilities, equipment, and capabilities available for the research). Describe plans for development and utilization of distinctive facilities, capabilities or approaches to address the scientific goals.

- **Management Plan**: Provide a clear, substantive overview of the vision, management, and organization of the proposed team. This section must include:
  - Describe the strategy and plan for project operations. Address how you will achieve an integrated research and development team.
  - Address the role of the Lead PI, and as appropriate, other PIs in the proposal regarding their leadership responsibilities for scientific and technical direction of the project. Delineates the roles and responsibilities of each senior/key personnel.
  - Describe the management processes for evaluation of research and software development progress, decision making across the team, handling of intellectual property, and fostering team synergy. Describe 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 **external advisory committee (required).**

- Include a brief (less than one page) overview of environmental, safety, health, and quality assurance (ES&H and QA) practices and oversight at each participating institution, including any required permits, licenses, and approvals that must be obtained.
- **Project Performance Site(s):** Required for teams involving more than one institution. Identify and describe the site(s) where the work will be performed. Work sites at all partner institutions should be briefly described. Appendix 4 should include detailed information about facilities, equipment, and capabilities available for the research. Costs for new construction (including new buildings or additions to existing buildings) will not be allowed in the award.

The Project Narrative is considered the intellectual work of the proposed researchers. Concurrent submission of the same or substantially similar narratives attributed to different researchers may constitute academic dishonesty or research misconduct. Submission of a research narrative that is not the work of the proposed researchers, including machine-generated research narratives, may constitute academic dishonesty or research misconduct.

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the PI and each senior/key person as an appendix to your technical narrative.
- 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.

Detailed instructions may be found in Section VIII of this Announcement.

> **WARNING**: These instructions have been significantly revised to require disclosure of a variety of potential conflicts of interest or commitment, including participation in foreign government-sponsored talent recruitment programs.
>
> The PI and each senior/key person at the prime applicant and any proposed subaward must provide a list of all sponsored activities, awards, and appointments, whether paid or unpaid; provided as a gift with terms or conditions or provided as a gift without terms or conditions; full-time, part-time, or voluntary; faculty, visiting, adjunct, or honorary; cash or in-kind; foreign or domestic; governmental or private-sector; directly supporting the individual's research or indirectly supporting the individual by supporting students, research staff, space, equipment, or other research expenses. All foreign government-sponsored talent recruitment programs must be identified in current and pending support.

APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support for the PI and senior/key personnel, including subawardees. Provide the Current and Pending Support as an appendix to your project narrative. Concurrent submission of a proposal to other organizations for simultaneous consideration will not prejudice its review.

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

Detailed instructions may be found in [Section VIII](#) of this Announcement.

APPENDIX 3: BIBLIOGRAPHY & REFERENCES CITED

Provide a bibliography of any references cited in the Project Narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. For research areas where there are routinely more than ten coauthors of archival publications, you may use an abbreviated style such as the *Physical Review Letters* (PRL) convention for citations (listing only the first author). For example, your paper may be listed as, "A Really Important New Result," A. Aardvark et. al. (MONGO Collaboration), PRL 999. Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal. Provide the Bibliography and References Cited information as an appendix to your project narrative.
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 4: FACILITIES & OTHER RESOURCES

This information is used to assess the capability of the organizational resources, including subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. For proposed investigations requiring access to experimental user facilities maintained by institutions other than the applicant, please provide a document from the facility manager confirming that the researchers will have access to the facility. Please provide the Facility and Other Resource information as an appendix to your project narrative.
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 5: EQUIPMENT

List major items of equipment already available for this project and, if appropriate identify location and pertinent capabilities. Provide the Equipment information as an appendix to your project narrative.
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 6: DATA MANAGEMENT PLAN

Provide a Data Management Plan (DMP) as an appendix to the research narrative.

- This appendix should not exceed a page limit of **3 pages** including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard letter-size (8.5-inch x 11-inch) paper with 1-inch margins (top, bottom, left, and right)
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

The standard requirements for a DMP may be found in Section VIII of this Announcement. In addition, the DMP must specifically address:

- How FAIR (Findable, Accessible, Interoperable, and Reusable)[1] principles will apply to the anticipated data sets, software[2], and models[3] to be developed.
- What developed software, data sets, and models will be made available using an "opensource" licensing arrangement, noting the Software Package Data Exchange (SPDX) identifier(s) (https://spdx.org/licenses/) when possible, and where deviation in this arrangement is expected from The Open Source Initiative's "Open Source Definition" (https://opensource.org/osd), a specific justification must be provided.
- How best practices in scientific software development will be applied to any development activities. For more information on best practices, see Better Scientific Software (https://bssw.io/).

APPENDIX 7: PROMOTING INCLUSIVE AND EQUITABLE RESEARCH (PIER) PLAN

All new and renewal proposals that are not for conference support must provide a Promoting Inclusive and Equitable Research (PIER) Plan as an appendix to the research narrative. The PIER plan should describe the activities and strategies of the applicant to promote equity and inclusion as an intrinsic element to advancing scientific excellence in the research project within the context of the proposing institution and any associated research group(s). Plans may include, but are not limited to: strategies of your institution (and collaborating institutions, if applicable) for enhanced recruitment of undergraduate students, graduate students, and early-stage investigators (postdoctoral researchers, and others), including individuals from diverse backgrounds and groups historically underrepresented in the research community; strategies for creating and sustaining a positive, inclusive, safe, and professional research and training environment that fosters a sense of belonging among all research personnel; and/or training, mentoring, and professional development opportunities.[4] Plans may incorporate or build upon

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[1] Wilkinson, M. D. et al. The FAIR Guiding Principles for Scientific Data Management and Stewardship. Sci. Data 3:160018, 2016. https://doi.org/10.1038/sdata.2016.18

[2] Chue Hong, N. P., Katz, D. S., Barker, M., Lamprecht, A-L, Martinez, C., Psomopoulos, F. E., Harrow, J., Castro, L. J., Gruenpeter, M., Martinez, P. A., Honeyman, T., et al. (2022). FAIR Principles for Research Software version 1.0. (FAIR4RS Principles v1.0). Research Data Alliance. https://doi.org/10.15497/RDA00068

[3] Ravi, N., Chaturvedi, P., Huerta, E.A. et al. FAIR principles for AI models with a practical application for accelerated high energy diffraction microscopy. Sci Data 9, 657 (2022). https://doi.org/10.1038/s41597-022-01712-9

[4] Please see additional information at https://science.osti.gov/SW-DEI/DOE-Diversity-Equity-and-Inclusion-Policies/Q-and-As#definitions.

existing diversity, equity, accessibility, and inclusion efforts of the project key personnel or applicant institution(s), but should not be a re-statement of standard institutional policies or broad principles. The complexity and detail of a PIER is expected to increase with the size of the research team and the number of personnel to be supported.

- Do not attach a separate file.
- This appendix should not exceed a page limit of 3 pages when printed using standard letter-size (8.5 -inch x 11-inch) paper with 1-inch margins (top, bottom, left, and right) This appendix will not count in the project narrative page limitation

APPENDIX 8: 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) https://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 software or the Announcement requires that the software or other information be shared or disseminated to others.
5. A plan of how your team plans to integrate community input and how success for community adaptation would look like. Renewal applications should clearly describe the current community usage of their code(s) and define specific goals to increase community usage.

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

- This appendix should not exceed a page limit of **3 pages** including charts, graphs, maps,

photographs, and other pictorial presentations, when printed using standard letter-size (8.5-inch x 11-inch) paper with 1-inch margins (top, bottom, left, and right)
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 9: RENEWAL PROPOSAL PRODUCTS

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

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

APPENDIX 10: LETTER OF COMMITMENT

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

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

APPENDIX 11: OTHER ATTACHMENT

If you need to elaborate on your responses to the PAMS Cover Page, please provide the Other Attachment information as an appendix to your project narrative. Information not easily accessible to a reviewer may be included in this appendix, but do not use this appendix to circumvent the page limitations of the proposal. Reviewers are not required to consider information in this appendix.
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

IV.C.5. Collaborator Information

Provide a listing of senior/key personnel at the applicant institution and any proposed subawards and a listing of individuals who should not serve as merit reviewers. You may also indicate

suggested merit reviewers. Detailed instructions for these listings may be found in [Section VIII](#) of this Announcement.

IV.D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS

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

IV.E. SUBMISSION DATES AND TIMES

IV.E.1. Letter of Intent Due Date

The LOI due date is printed on the cover of this Announcement.

You are encouraged to submit your Letter of Intent well before the deadline. LOIs may be submitted at any time between the publication of this Announcement and the stated deadline.

IV.E.2. Pre-proposal Due Date

Not applicable; a pre-proposal is not requested or required.

IV.E.3. Proposal Due Date

The proposal due date is printed on the cover of this Announcement.

You are encouraged to transmit your proposal well before the deadline. Proposals may be submitted at any time between the publication of this Announcement and the stated deadline.

IV.E.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.

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

Applicants must contact the Program Office/Manager listed in this Announcement to discuss

the option of a late submission. Contacting the Program Office/Manager after the deadline may reduce the likelihood that a request will be granted.

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

Section V - PROPOSAL REVIEW INFORMATION

V.A. CRITERIA

V.A.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.

V.A.2. Merit Review Criteria

Proposals will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria, the first five of which will be weighted more heavily than the final three. The first five criteria are of equal value. The final three criteria are of equal value.

- Scientific and/or Technical Merit of the Project
- Appropriateness of the Proposed Method or Approach
- Competency of Applicant's Personnel and Adequacy of Proposed Resources
- Reasonableness and Appropriateness of the Proposed Budget
- Quality and Efficacy of the Promoting Inclusive and Equitable Research (PIER) Plan
- Strength of the Management Plan
- Synergy Among the PIs, including Cohesion and Integration of the Research and Software Development Activities
- Development and Utilization of Distinctive 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

- What is the scientific innovation of the proposed research?
- What is the likelihood of achieving valuable results?
- How might the results of the proposed work impact the direction, progress, and thinking in

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relevant scientific fields of research?

- How does the proposed work compare with other efforts in its field, both in terms of scientific and/or technical merit and originality?
- For renewal proposals, comment on the progress and impact for the prior award period.
- Is the Data Management Plan suitable for the proposed research and software development? To what extent does it support the validation of results? To what extent will research products, including data and software packages, be made available and reusable to advance the field of research?
- To what extent does the Data Management Plan address the specific requirements for open-source, public-access community software development, including the FAIR data principles?

APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

- Does the proposed effort employ innovative concepts or methods and what are those?
- Comment on the balance between scientific research, software development, and community outreach for software dissemination.
- How logical and feasible are the approaches?
- How well are the conceptual framework, methods, and analyses justified, adequately developed, and likely to lead to scientifically valid conclusions?
- Describe and assess the plans for verification and validation of the proposed code package.
- How does the applicant recognize significant potential problems and consider alternative strategies?

COMPETENCY OF APPLICANT'S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES

- Assess the record of research accomplishments and computational/experimental skills of the Lead PI and team members (if appropriate).
- Comment on experience/expertise of the PIs and institutions in the development and maintenance of community research codes and data.
- Does the proposed work take advantage of unique facilities and capabilities?
- Are the environment and facilities adequate for performing the proposed effort?

REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET

- Are the proposed budget and staffing levels adequate to carry out the proposed work?
- Is the budget reasonable and appropriate for the scope?

QUALITY AND EFFICACY OF THE PROMOTING INCLUSIVE AND EQUITABLE RESEARCH PLAN

- Is the proposed Promoting Inclusive and Equitable Research (PIER) Plan suitable for the size and complexity of the proposed project and an integral component of the proposed project?
- To what extent is the PIER plan likely to lead to participation of individuals from diverse backgrounds, including individuals historically underrepresented in the research community?
- What aspects of the PIER plan are likely to contribute to the goal of creating and maintaining an equitable, inclusive, encouraging, and professional training and research environment and

supporting a sense of belonging among project personnel?
- How does the proposed plan include intentional mentorship and are the associated mentoring resources reasonable and appropriate?

STRENGTH OF THE MANAGEMENT PLAN

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

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

- Comment on how the applicant's approach addresses the scientific and software development goals in an integrated and coherent manner.
- Comment on the likelihood that the proposed team will work together in a cohesive and integrated manner.
- For renewal proposals comment on the synergy of the PIs through joint publications and other measurable joint activities.

DEVELOPMENT AND UTILIZATION OF DISTINCTIVE FACILITIES, CAPABILITIES, OR APPROACHES

- How will the team utilize today's midscale to petascale to exascale leadership computing facilities?
- Comment on the proposed software package's readiness for, or capability of, exascale computing.
- Assess the quality of the Open-Source Software Distribution Plan and the involvement of the researcher and developer communities.

V.B. REVIEW AND SELECTION PROCESS

V.B.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.

V.B.2. Program Policy Factors

The Selection Official may consider any of the following program policy factors in making the selection, listed in no order of significance:

- Availability of funds
- Relevance of the proposed activity to SC priorities
- Ensuring an appropriate balance of activities within SC programs
- Performance under current awards
- Commitment to sharing the results of research and managing open-source software for broad community access
- Delineation of the scope of the proposed research from other research activities in which the principal investigators are involved, particularly those supported by DOE and by other federal agencies
- Diversity of research activities that will address the scientific grand challenges and use-inspired basic research as articulated in the Basic Energy Sciences Advisory Committee (BESAC) and BES workshop reports
- Potential for developing synergies between the proposed project and other ongoing BES research activities
- Ensuring a distribution of supported researchers at various career stages
- Promoting the diversity of supported investigators

V.B.3. Selection

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

V.B.4. Review of Risk

In addition, DOE will conduct a review of any potential risks to the research, technology, or economic security of the United Staes. DOE may conduct a review, through Government resources, of any project personnel with a connection to a foreign country. This includes, but is not limited to, (1) performance of work in, (2) travel to, and (3) awardee personnel's higher education in a foreign Country, as well as (4) partnerships with international collaborators. DOE may make use of other publicly available information and the history of an applicant's performance under DOE or other Federal agency awards.

The result(s) of any review of risk may supersede the results of merit review, preventing DOE from authorizing work, requiring DOE to reverse an authorization, requiring the disengagement of specific personnel, the imposition of other requirements, or requiring that authorized work be stopped. The results of any review of risk are not appealable. Any decision to not authorize work, reverse an authorization, or require the disengagement of specific personnel before work is authorized will be made by the Selection Official or SC Program Official. Any decision to require the disengagement of specific personnel after work is authorized, the imposition of other requirements, or that authorized work be stopped will be made in consultation with the National Laboratory.

V.B.5. 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.

V.C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES

It is anticipated that the award selection will be completed by August 2024. It is expected that awards will be made in Fiscal Year 2024.

Section VI - AWARD ADMINISTRATION INFORMATION

VI.A. AWARD NOTICES

VI.A.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.

VI.A.2. Notice of Award

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

VI.B. ADMINISTRATIVE AND POLICY REQUIREMENTS

The following additional policy provisions are applicable to this Announcement. The full text of each provision is in Section VIII of this Announcement and may be accessed by navigating to the hyperlinks below:

VIII.B.1. Availability of Funds
VIII.B.2. Commitment of Public Funds
VIII.B.3. Environmental, Safety and Health (ES&H) Performance of Work at DOE Facilities
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VIII.B.6. Funding Restrictions
VIII.B.7. Government Right to Reject or Negotiate
VIII.B.8. Modification
VIII.B.9. Proprietary Proposal Information
VIII.B.10. Publications

VI.C. REPORTING

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

VII.A. QUESTIONS

For help with PAMS, click the "PAMS Help" 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 the Announcement number printed on the cover.
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.

VII.B. AGENCY CONTACTS

PAMS Customer Support	855-818-1846 (toll-free) 301-903-9610 sc.pams-helpdesk@science.doe.gov
Program Manager Scientific Contact	Matthias Graf, Ph.D. Matthias.graf@science.doe.gov

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

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

<u>**Section VIII – SUPPLEMENTARY MATERIAL**</u>

VIII.A. HOW-TO GUIDES

VIII.A.1. How Consortia May be Used

INCORPORATED CONSORTIA

Incorporated consortia are eligible to apply for funding as a prime recipient (lead organization) or subrecipient (team member).

Each incorporated consortium must have an internal governance structure and a written set of internal rules. Upon request, the consortium must provide a written description of its internal governance structure and its internal rules to the DOE contracting officer. There is no requirement that subawards be formalized into incorporated consortia.

UNINCORPORATED CONSORTIA

Unincorporated consortia (team arrangements) must designate one member of the consortium to serve as the prime recipient/consortium representative (lead organization). There is no requirement that subawards be formalized into unincorporated consortia.

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 proposal and results in one award with subawards to consortia members. Multi-institutional teams may, if permitted under this Announcement, submit collaborative proposals with each institution submitting its own proposal with an identical research narrative, resulting in multiple awards to the collaborating institutions.

VIII.A.2. How to Submit Letters of Intent

It is important that the LOI be a single file with extension .pdf, .docx, or .doc. The filename must not exceed 50 characters. The 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.**

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 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 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.

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

VIII.A.3. How to Submit a Pre-Proposal

It is important that the pre-proposal be a single file with extension .pdf, .docx, or .doc. The filename must not exceed 50 characters. The PI and anyone submitting on behalf of the PI must register for an account in PAMS before it will be possible to submit a pre-proposal. All PIs and those submitting pre-proposals on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays.

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

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

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

VIII.A.4. How to Prepare and Submit a Proposal

SUBMITTING A PROPOSAL

The following information is provided to help with proposal submission. Detailed instructions and screen shots can be found in the PAMS Help materials, accessible by clicking the "PAMS Help" link on the PAMS home page. Onscreen instructions are available within PAMS.

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

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

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

PROPOSAL PREPARATION

All files submitted a part of a proposal must be PDF files unless otherwise specified in this Announcement. Attached PDF files must be plain files consisting of text, numbers, and images without editable fields, signatures, passwords, redactions, or other advanced features available in some PDF-compatible software. Do not use PDF portfolios or binders.

Please note the following restrictions that apply to the names of all files attached to your proposal:
- Please limit file names to 50 or fewer characters
- Do not attach any documents with the same name. All attachments must have a unique name.
- Please use only the following characters when naming your attachments: A-Z, a-z, 0-9, underscore, hyphen, space, period, parenthesis, curly braces, square brackets, ampersand, tilde, exclamation point, comma, semi colon, apostrophe, at sign, number sign, dollar sign, percent sign, plus sign, and equal sign. Attachments that do not follow this rule may cause the entire proposal to be rejected or cause issues during processing.

RESUBMISSION OF PROPOSALS

Proposals submitted under this announcement may be withdrawn from consideration by using the PAMS website at https://pamspublic.science.energy.gov. Proposals may be withdrawn at any time between when the applicant submits the proposal and when DOE makes the proposal available to merit reviewers. Such withdrawals take effect immediately and cannot be reversed. Please exercise due caution. After the proposal is made available to merit reviewers, the applicant may contact the DOE program office identified in this Announcement to request that it be withdrawn.

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

IMPROPER CONTENTS OF PROPOSALS

Proposals submitted under this Announcement will be stored in controlled-access systems, but they may be made publicly available if an award is made. As such, it is critical that applicants follow these guidelines:
- Do not include information subject to any legal restriction on its open distribution, whether classified, export control, or unclassified controlled nuclear information.
- Do not include sensitive and protected personally identifiable information, including social security numbers, birthdates, citizenship, marital status, or home addresses. Pay particular attention to the content of biographical sketches and curriculum vitae.
- Do not include letters of support from Federal officials.
- Do not include letters of support on Federal letterhead. Letters that are not letters of support (such as letters confirming access to sites, facilities, equipment, or data; or letters from cognizant contracting officers) may be on Federal letterhead.
- Clearly mark all proprietary or trade-secret information.

VIII.A.5. How to Prepare a Biographical Sketch

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

SC requires the use of the format approved by the National Science Foundation (NSF), which may be generated by the Science Experts Network Curriculum Vitae (SciENcv), a cooperative venture maintained at https://www.ncbi.nlm.nih.gov/sciencv/. The fillable PDFs provided by the National Science Foundation at https://nsf.gov/bfa/dias/policy/nsfapprovedformats/ are no longer available. If an interagency common format for a biographical sketch has been promulgated, that format must be used in an application. The use of a format required by another agency is intended to reduce the administrative burden to researchers by promoting the use of common formats.

Requested information may be appended to a biographical sketch, whether produced from a

fillable PDF or in SciENcv.

SC strongly recommends the use of SciENcv to reduce administrative burden by allowing the use of digital persistent identifiers, including the Open Researcher and Contributer ID (ORCiD).

Do not attach a listing of individuals who should not be used as merit reviewers: This information is no longer collected as part of a biographical sketch.

VIII.A.6. How to Prepare a List of Individuals Who Should Not Serve as Reviewers

To assist in identifying individuals who should not serve as merit reviews, provide the following information for each and every senior/key person who is planned to be or is identified in Section A of the proposal budget for the applicant and any proposed subrecipients:
- Advisees (graduate students or postdocs) of the senior/key person
- Advisors of the senior/key person while a graduate student or a postdoc
- Close associates of the senior/key person over the past 48 months
- Co-authors of the senior/key person over the past 48 months
- Co-editors of the senior/key person over the past 48 months
- Co-investigators of the senior/key person over the past 48 months
- Collaborators of the senior/key person over the past 48 months

Do not identify any personnel at the applicant institution or any proposed subrecipient or team institution: Those personnel are prohibited from serving as merit reviewers.

Large collaborations of 10 or more researchers do not require that all collaborators be identified: rather, only list the researchers with whom the senior/key person actually collaborated.

For all identified individuals, provide the following information:
- The senior/key person to whom the individual was an advisee, advisor, close associate, co-author, co-editor, co-investigator, or collaborator, identified by first name and last name.
- The individual's first (given) name.
- The individual's last (family) name.
- The individual's Open Researcher and Contributor ID (ORCiD), if known.
- The individual's institutional affiliation spelling out acronyms (For joint appointments, separate each institution with a slash ("/"). Do not list departmental affiliations.).
- The reason for listing the individual (advisee, advisor, close associate, co-author, co-editor, co-investigator, collaborator).
- The year when the individual last was a close associate, co-author, co-editor, co-investigator, or collaborator.

You may also provide a list of all senior/key personnel who are planned to be or are identified in Section A of the proposal budget for the applicant and any proposed subrecipients.

The lists do not need to be sorted in any method.

The lists must be submitted in tabular format, preferably as Microsoft Excel (.xls or .xlsx) files.

For your convenience, a template is available at https://science.osti.gov/grants/Policy-and-Guidance/Agreement-Forms. If using the template:

- Do not add tabs to the spreadsheet.
- Do not merge the existing tabs.
- Do not remove headers.
- Fill out the requested headers on both tabs with the same information.
- Ensure that given and family names are presented in the correct columns.

VIII.A.7. How to Prepare Current and Pending Support

> **WARNING**: These instructions have been significantly revised to require disclosure of a variety of potential conflicts of interest or commitment, including participation in foreign government-sponsored talent recruitment programs.

Current and Pending support is intended to allow the identification of potential duplication, overcommitment, potential conflicts of interest or commitment, and all other sources of support. The PI and each senior/key person at the prime applicant and any proposed subaward must provide a list of all sponsored activities, awards, and appointments, whether paid or unpaid; provided as a gift with terms or conditions or provided as a gift without terms or conditions; full-time, part-time, or voluntary; faculty, visiting, adjunct, or honorary; cash or in-kind; foreign or domestic; governmental or private-sector; directly supporting the individual's research or indirectly supporting the individual by supporting students, research staff, space, equipment, or other research expenses. Include the current application and any application submitted to any source of funding in a list of current and pending support. All sources of support must be disclosed, but for work that is subject to government classification or enforceable non-disclosure agreements, the general area of the research should be described without disclosing sensitive details and the sponsor should be listed as "Government Agency" or "private sponsor." All foreign government-sponsored talent recruitment programs must be identified in current and pending support.

SC requires the use of the format approved by the National Science Foundation (NSF), which may be generated by the Science Experts Network Curriculum Vitae (SciENcv), a cooperative venture maintained at https://www.ncbi.nlm.nih.gov/sciencv/. The fillable PDFs provided by the National Science Foundation at https://nsf.gov/bfa/dias/policy/nsfapprovedformats/ are no longer available. If an interagency common format for current and pending support has been promulgated, that format must be used in an application. The use of a format required by another agency is intended to reduce the administrative burden to researchers by promoting the use of common formats.

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. If the title of the award or activity is not descriptive, add a brief description of the research being performed that would identify any overlaps or synergies with the proposed research.
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The award period (start date – end date).
- The person-months of effort per year being dedicated to the award or activity.

If required to identify overlap, duplication of effort, or synergistic efforts, append a description of the other award or activity to the current and pending support.

Requested information may be appended to current and pending support, whether produced from a fillable PDF or in SciENcv.

SC strongly recommends the use of SciENcv to reduce administrative burden by allowing the use of digital persistent identifiers, including the Open Researcher and Contributer ID (ORCiD).

Details of any obligations, contractual or otherwise, to any program, entity, or organization sponsored by a foreign government must be provided on request to either the applicant institution or DOE.

VIII.A.8. How to Prepare a Data Management Plan

In general, a DMP should address 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 (https://science.osti.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 at https://science.osti.gov/user-facilities/.

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 SC research proposal merit review process. Applicants are encouraged to consult the SC website for further information and suggestions for how to structure a DMP: https://science.osti.gov/funding-opportunities/digital-data-management

VIII.A.9. How to Prepare a Budget and Justification

The following advice will improve the accuracy of your budget request:
- Funds requested for personnel (senior, key, and other) must be justified as the product of their effort on the project and their institutional base salary.
- Funds requested for fringe benefits must be calculated as the product of the requested salary and, if present, the negotiated fringe benefit rate contained in an institution's negotiated indirect cost rate agreement.
- Funds requested for indirect costs must be calculated using the correct indirect cost base and the negotiated indirect cost rate.
- You are encouraged to include the rate agreement used in preparing a budget as a part of the budget justification.
- Do not prepare a budget justification using the expired DOE form F4260.1.

Budget Fields

Section A Senior/Key Person	For each Senior/Key Person, enter the requested information. List personnel, base salary, the number of months that person will be allocated to the project, requested salary, fringe benefits, and the total funds requested for each person. The requested salary must be the product of the base salary and the effort. Include a written narrative in the budget justification that justifies the need for requested personnel. Within the justification, explain the fringe benefit rate used if it is not the standard faculty rate.
Section B Other Personnel	List personnel, the number of months that person will be allocated to the project, requested salary fringe benefits, and the total funds requested for each person. Include a written narrative in the budget justification that fully justifies the need for requested personnel. Within the justification, provide the number of positions being filled in each category of other personnel.
Section C Equipment	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, unless a different threshold is specified in a negotiated Facilities and Administrative Cost Rate. (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. Do not aggregate items of equipment. Allowable items ordinarily will be limited to research equipment and apparatus not already available for the conduct of the work. General-purpose office equipment is not eligible for support unless primarily or exclusively used in the actual conduct of scientific research.
Section D Travel	For purposes of this section only, travel to Canada or to Mexico is considered domestic 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 the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). 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. Domestic travel is to be justified separately from foreign travel. Within the budget justification, detail the number of personnel planning to travel and the estimated per-traveler cost for each trip.
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. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).
Section F Other Direct Costs	**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. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). **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. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar

	items, or some other basis).
	• **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. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).
	• **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. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).
	• **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. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).
	• **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 through F). PAMS will automatically calculate this.
Section H Other Indirect Costs	Enter the Indirect Cost information, including the rates and bases being used, for each field. Only four general categories of indirect costs are allowed/requested on this form, so please consolidate if needed. Include the cognizant Federal agency and contact information if using a negotiated rate agreement. Within the budget justification, explain the use of multiple rates, if multiple rates are used.
Section I Total Direct and Indirect Costs	This is the total of Sections G and H. PAMS will automatically calculate this.

VIII.A.10. How to Register in PAMS

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

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.

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 to the "Having Trouble Logging In?" page. (If you have been an SC merit reviewer or if you have previously submitted a proposal, you may already be linked to an institution in PAMS. If this happens, you will be taken to the PAMS home page.)

REGISTER TO YOUR INSTITUTION:

1. 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.)
2. PAMS will take you to the "Register to Institution" page.
3. 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.)

4. 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.
5. 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.
6. 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.

For help with PAMS, click the "PAMS Help" 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 Announcement should reference the number printed on the cover page.

VIII.A.11. How to View Proposals in PAMS

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

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

VIII.B. POLICY PROVISIONS

VIII.B.1. 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.

VIII.B.2. 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.

VIII.B.3. Environmental, Safety and Health (ES&H) Performance of Work at DOE Facilities

With respect to the performance of any portion of the work under this award which is performed at a DOE-owned or controlled site, the recipient agrees to comply with all state and Federal

ES&H regulations, and with all other ES&H requirements of the operator of such site.

Prior to the performance on any work at a DOE-Owned or controlled site, the recipient shall contact the site facility manager for information on DOE and site specific ES&H requirements.

The recipient shall apply this provision to all subawardees at any tier.

VIII.B.4. 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 a conflict of interest and a certificate of confidentiality prior to reviewing a proposal. Non-Federal personnel conducting administrative activities must sign a non-disclosure agreement.

VIII.B.5. Federal, State, and Local Requirements

With respect to the performance of any portion of the work under this award, the recipient agrees to comply with all applicable local, state, and Federal ES&H regulations. The recipient shall apply this provision to all sub awardees at any tier.

VIII.B.6. 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.

VIII.B.7. 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.

VIII.B.8. Modification

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

VIII.B.9. 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 any document included in the proposal that contains such proprietary

information and specifies the pages of the document which are to be restricted:

"The data contained in pages _____ of this document have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes, provided that if this applicant receives an award as a result of or in connection with the submission of this proposal, DOE shall have the right to use or disclose the data herein to the extent provided in the award. This restriction does not limit the government's right to use or disclose data obtained without restriction from any source, including the applicant."

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."

VIII.B.10. Publications

Researchers are expected to publish or otherwise make publicly available the results of the work conducted under any authorization resulting from this Announcement. Publications and other methods of public communication describing any work based on or developed under an authorization resulting from this Announcement must contain an acknowledgment of SC support. The format for such acknowledgments is provided at https://science.osti.gov/funding-opportunities/acknowledgements/. The author's copy of any peer-reviewed manuscript accepted for funding must be announced to DOE's Office of Scientific and Technical Information (OSTI) and made publicly available in accordance with the instructions contained in the Reporting Requirements Checklist incorporated in all Assistance Agreements.