# DEPARTMENT OF ENERGY OFFICE OF SCIENCE



### EARLY CAREER RESEARCH PROGRAM

# DOE NATIONAL LABORATORY PROGRAM ANNOUNCEMENT NUMBER: LAB 20-2173

**ANNOUNCEMENT TYPE: INITIAL** 

# AMENDMENT 000001: This Amendment extends the deadline to accommodate disruptions from the COVID-19 outbreak

<b>Announcement Issue Date:</b>	November 21, 2019
<b>Submission Deadline for Letter of Intent:</b>	NA
Submission Deadline for Pre-Proposal:	January 7, 2020 at 5:00 PM Eastern Time
	A Pre-Proposal is required
Pre-Proposal Response Date:	January 30, 2020
<b>Submission Deadline for Proposals:</b>	March 30, 2020 at 5:00 PM Eastern Time

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### REGISTRATIONS

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

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

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

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

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

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

### 1. CREATE PAMS ACCOUNT:

To register, click the "Create New PAMS Account" link on the website <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>.

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

### 2. REGISTER TO YOUR INSTITUTION:

• Click the link labeled "Option 2: I know my institution and I am here to register to the institution." (Note: If you previously created a PAMS account but did not register to an

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

For help with PAMS, click the "External User Guide" link on the PAMS website, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submissions and inquiries about this DOE National Laboratory Announcement should reference **LAB 20-2173.** 

### <u>UPDATES AND REMINDERS</u>

#### 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, pre-proposals, and proposals well before the deadline.

### DATA MANAGEMENT PLAN

The Office of Science Statement on Digital Data Management, published at <a href="https://science.osti.gov/Funding-Opportunities/Digital-Data-Management">https://science.osti.gov/Funding-Opportunities/Digital-Data-Management</a>, governs proposals submitted under this Announcement. Compliance is detailed in Section IV of this Announcement.

### ACKNOWLEDGMENT OF FEDERAL SUPPORT

SC published guidance about how its support should be acknowledged at <a href="https://science.osti.gov/Funding-Opportunities/Acknowledgements">https://science.osti.gov/Funding-Opportunities/Acknowledgements</a>.

#### **AVOIDING ERRORS**

The following advice is compiled from actual experiences of applicants for SC awards.

- Please ensure that the research narrative is comprised of one and only one Portable Document Format (PDF) file, including all appendices, when it is uploaded.
- When using the PAMS website at <a href="https://pamspublic.science.energy.gov">https://pamspublic.science.energy.gov</a>, please avoid using the back-arrow button in your web browser to navigate.
- Please ensure that the proposal contains no personally identifiable information (PII).
- Please ensure that the budget is calculated using the applicable negotiated indirect cost and fringe benefit rates.

### Checklist for Common Errors:

Item	Issue
Page Limits	Strictly followed throughout proposal,
	including particular attention to:
	- Research Narrative
	- Appendix 2 Narrative, if any
	- Biosketches
	- DMP(s)
	- 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 PI, PI's institutional affiliation(s),
	Co-Investigator(s), Co-Investigator's
	institutional affiliation(s)
DOE Cover 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
Current and Pending Support	Ensure completeness, including brief abstract
	of scope of work for all items listed
Data Management Plans	- If referring to an experiment's DMP,
	describe the relationship to the proposed
	research
	- Include a DMP even if no experimental
	data is expected

### Section I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION

### GENERAL INQUIRIES ABOUT THIS ANNOUCNEMENT SHOULD BE DIRECTED TO:

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

Questions regarding the specific program areas/technical requirements can be directed to the program managers/technical contacts listed for each program within the funding announcement.

### Administrative Contact (questions about budgets and eligibility):

Questions about program rules should be sent to SC.Early@science.doe.gov

### **SUMMARY**

SC hereby invites national laboratory proposals for support under the Early Career Research Program in the following program areas: Advanced Scientific Computing Research (ASCR); Biological and Environmental Research (BER); Basic Energy Sciences (BES), Fusion Energy Sciences (FES); High Energy Physics (HEP), and Nuclear Physics (NP). The purpose of this program is to support the development of individual research programs of outstanding scientists early in their careers and to stimulate research careers in the areas supported by SC.

### SUPPLEMENTARY INFORMATION

SC's mission is to deliver the scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic, and national security of the United States. SC is the Nation's largest Federal sponsor of basic research in the physical sciences and the lead Federal agency supporting fundamental scientific research for our Nation's energy future.

SC accomplishes its mission and advances national goals by supporting:

- The frontiers of science—exploring nature's mysteries from the study of fundamental subatomic particles, atoms, and molecules that are the building blocks of the materials of our universe and everything in it to the DNA, proteins, and cells that are the building blocks of life. Each of the programs in SC supports research probing the most fundamental disciplinary questions.
- The 21st Century tools of science—providing the nation's researchers with 27 state-of-the-art national scientific user facilities the most advanced tools of modern science propelling the U.S. to the forefront of science, technology development and deployment through innovation.
- Science for energy and the environment—paving the knowledge foundation to spur discoveries and innovations for advancing the Department's mission in energy and environment. SC supports a wide range of funding modalities from single principal investigators to large team-based activities to engage in fundamental research on energy

production, conversion, storage, transmission, and use, and on our understanding of the earth systems.

Early Career Research Program opportunities exist in the following SC research programs. Additional details about each program, websites, and technical points of contacts are provided in the materials that follow.

- I. Advanced Scientific Computing Research (ASCR);
- II. Biological and Environmental Research (BER);
- III. Basic Energy Sciences (BES);
- IV. Fusion Energy Sciences (FES);
- V. High Energy Physics (HEP); and
- VI. Nuclear Physics (NP)

The topics for the FOA are indicated by letters under each Program Office name (ASCR, BER, BES, FES, HEP, or NP). For example, under ASCR, the first topic is "Adaptive Algorithms, Solvers, and Optimization for High Performance Computing."

### **Advanced Scientific Computing Research (ASCR)**

Program Website: <a href="https://www.energy.gov/science/ascr/advanced-scientific-computing-research">https://www.energy.gov/science/ascr/advanced-scientific-computing-research</a> or <a href="https://science.osti.gov/ascr">https://science.osti.gov/ascr</a>

ASCR's mission is to advance applied mathematics and computer science; deliver the most advanced computational scientific applications in partnership with disciplinary science; advance computing and networking capabilities; and develop future generations of computing hardware and software tools for science and engineering, in partnership with the research community, including U.S. industry. The ASCR program gives the science and technology community, including U.S. industry, access to world-class supercomputers and the tools to use them for science and engineering. ASCR accomplishes this by developing and maintaining world-class computing and network facilities for science; and advancing research in applied mathematics, computer science, and advanced networking.

The computing resources and high-speed networks required to meet the scientific needs of the future exceed the state-of- the-art by a significant margin. Furthermore, the algorithms, software tools, the software libraries and the distributed software environments needed to accelerate scientific discovery through modeling and simulation are beyond the realm of commercial interest. To establish and maintain DOE's modeling and simulation leadership in scientific areas that are important to its mission, ASCR operates Leadership Computing facilities, a high-performance production computing center, and a high-speed network, and implements a broad base research portfolio to solve complex problems on computational resources that are on a trajectory to reach well beyond hundreds and thousands of petaflops within a few years.

For the purposes of the Early Career Research Program, proposed research must be responsive to one of the specific topic areas below:

### **Applied Mathematics**

This program supports basic research leading to fundamental mathematical advances and

computational breakthroughs across DOE and SC missions. Applied Mathematics efforts span a range of research in scalable high-performance solvers, adaptive multiscale mathematical models, and coupled scientific data analysis, statistical methodologies, and algorithms. These research developments are the foundation for enabling predictive models, simulations, and analysis of DOE-relevant science and engineering applications. The specific topic areas of interest are:

# (a) Adaptive Algorithms, Solvers, and Optimization for High Performance Computing Technical Contact: William Spotz, 301-903-9938, William.Spotz@science.doe.gov

Basic research in the design, synthesis, analysis, and demonstration of algorithms that provide numerical solutions to mathematical models of systems with relevance to the DOE missions. Solver research opportunities include new classes of algorithms with one or more of the following characteristics: low-communication, asynchronous, mixed-precision, fault-tolerant, resilient, energy-efficient, randomized, or stochastic. A key research characteristic is that the results will also be useful for high-performance computing simulations.

# (b) Multiscale Mathematics for Coupled High Performance Scientific Simulations Technical Contact: Steven Lee, 301-903-5710, <a href="mailto:Steven-Lee@science.doe.gov">Steven-Lee@science.doe.gov</a>

Innovative mathematics research to improve the fidelity and predictability of continuous and/or distributed complex systems that accurately capture the physics and/or subcomponent interactions across vastly different time and length scales. Novel discretizations, multiphysics coupling approaches, scale bridging, uncertainty quantification, and sensitive analysis in such systems are of particular interest.

# (c) Research Foundations for Scalable Scientific Data Analysis and Algorithms Technical Contact: William Spotz, 301-903-9938, William.Spotz@science.doe.gov

Rigorous mathematical and computationally efficient approaches for analyzing and extracting information and insight from large-scale data relevant to the DOE missions. Of particular interest are computational approaches addressing the integration of observational data, experimental data, simulations and/or models using new statistical methodologies for large-scale data.

For Topics (a), (b), and (c) above, crosscutting research that enables greater adaptivity and automation in scientific computing capabilities is of particular interest. Such forward-looking and versatile capabilities can stem from research advances in artificial intelligence, machine learning, uncertainty quantification, sensitivity analysis, error estimation, and related areas.

For Applied Mathematics, topics and approaches that are out of scope include:

- Research where the mathematical challenges are not clearly articulated in the pre-proposal;
- Approaches for specific scientific or engineering problems that are not applicable to a broader class of problems;
- Approaches with primary emphasis on tailoring or implementation of existing numerical methods for specific scientific problems; or
- High-performance computing (HPC) implementation or "framework" for scientific or

engineering calculations that are primarily based on specific programming models or architectures.

• Research that primarily results in evolutionary improvements to the existing state of practice.

<u>Important note for encourage and discourage decisions</u>: Pre-proposals must clearly articulate the main scientific motivations and barriers to progress, the technical basis for overcoming those barriers, and the key insights or novel approaches for addressing the scientific and technical challenges. The lack of such details is sufficient for discouragement of the proposed research.

### **References:**

Report on Applied Mathematics Research for Exascale Computing https://science.osti.gov/-/media/ascr/pdf/research/am/docs/EMWGreport.pdf

Report on the Extreme Scale Solvers Workshop <a href="https://science.osti.gov/-/media/ascr/pdf/program-documents/docs/reportExtremeScaleSolvers2012.pdf">https://science.osti.gov/-/media/ascr/pdf/program-documents/docs/reportExtremeScaleSolvers2012.pdf</a>

DOE Workshop Report on Multiphysics Simulations

 $\frac{https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/MultiPhysics-Simulations-Report.pdf}{Report.pdf}$ 

Report on A Multifaceted Mathematical Approach for Complex Systems <a href="https://science.osti.gov/-/media/ascr/pdf/program-documents/docs/Multifaceted\_Mathematical\_Approach\_for\_Complex\_Systems.pdf">https://science.osti.gov/-/media/ascr/pdf/program-documents/docs/Multifaceted\_Mathematical\_Approach\_for\_Complex\_Systems.pdf</a>

Basic Research Needs for Scientific Machine Learning: Core Technologies for Artificial Intelligence

https://www.osti.gov/biblio/1478744-workshop-report-basic-research-needs-scientific-machine-learning-core-technologies-artificial-intelligence

### **Computer Science**

This program supports research that enables computing and networking at extreme scales and the understanding of extreme scale and complex data from both simulations and experiments. It aims to make high performance scientific computers and networks highly productive and efficient to solve scientific challenges while attempting to reduce domain science application complexity as much as possible.

Topics of interest for this FOA are focused on the following key core computer science research areas:

### (d) Systems

Technical Contact: Robinson Pino, 301-903-1263, Robinson.Pino@science.doe.gov

a. **Programming Models and Environments**: Innovative programming models for developing applications on next-generation platforms, exploiting unprecedented parallelism, heterogeneity of memory systems (e.g. Non-Uniform Memory Access [NUMA], non-coherent shared memory, hybrid memory cube, scratchpads), and

- heterogeneity of processing (e.g., Graphics Processing Units [GPUs], Field-Programmable Gate Arrays [FPGAs], other types of accelerators, big-small cores, processing in memory and near memory, etc.), with particular emphasis on making it easier to program at scale. Particularly welcome are proposals that infuse artificial intelligence/machine learning into the programming environment.
- b. **Operating and Runtime Systems**: System software that provides intelligent, adaptive resource management and support for workflow management systems, and that facilitates effective and efficient use of heterogeneous computing technologies, including diverse execution models, processors, accelerators, and memory and storage systems.
- c. **Performance Portability**: Algorithms and methods that support automated and semiautomated refinements from high-level specification of an application to low-level code, optimized at runtime to different HPC platforms. The focus is on enabling performance portability of applications developed for extreme-scale computing and beyond.

Proposals are not restricted to a single Systems topic above and may span all of them, provided the scope of work remains appropriate for the program.

### (e) Data Management, Visualization, and Analytics Technical Contact: Laura Biven, 301-903-9556, <u>Laura.Biven@science.doe.gov</u>

- a. **Data management** approaches for managing and analyzing large data from scientific instruments and simulation including methods for reducing the size and/or complexity of the data for further analysis, particularly in real time; in situ workflow management and techniques for carrying out data management and analysis in situ to meet research needs; and data management for preservation and archiving, to support collaboration and sharing, and to facilitate re-use.
- b. **Analytic Methods and Environments** to improve visual exploration and understanding of petabyte to exabyte multi-scale, multi-physics scientific data sets from simulations and/or experimental platforms; to support efficient analysis of data across federated resources; to support interactivity with simulation and/or real-time steering of experiments, including remote interactions; and to help answer scientifically relevant questions from the data about, for example, uncertainty, sensitivity analysis, causality, and the debugging of codes and methods. As appropriate, applicants are encouraged to consider evaluation methods for new visualization tools and techniques resulting from the proposed research.

### (f) Emerging Computing Technologies Technical Contact: Robinson Pino, 301-903-1263, <u>Robinson.Pino@science.doe.gov</u>

- a. **Machine Learning**: Scalable software, methods, and techniques that ensure algorithm scalability to extreme scales and applications that are generalizable to scientific computing applications and operation of HPC systems.
- b. **Neuromorphic Computing:** Specific to HPC-enabled modeling and simulation of computing architecture at extreme scales for generalizable applications of the proposed approach.
- c. **HPC Cybersecurity:** Investigate methods and techniques to achieve scientific integrity

through repeatable computing results whose process, origin, and data provenance are understood, whose correctness is understood, and for which uncertainty estimates are provided with associated metrics analytics and with specific emphasis to low system overhead approaches.

# (g) Applied Network Science for Complex Interconnected Engineered Systems Technical Contact: Thomas Ndousse-Fetter, 301-903-9960, Thomas.Ndousse-Fetter@science.doe.gov

The focus of this subtopic is on the application of network science for the characterization and understanding of the behavior of complex interconnected engineered systems such as wide area communication networks, large-scale supercomputing facilities, networked scientific instruments, regional unity grids, super-facilities, and hybrid systems. Potential topics of interest include but are not limited to the following: machine learning-based techniques, network interdependencies and cascading failures, networks of networks, network sampling and measurement, and cascading dynamics in quantum networks.

### Topics that are out of scope include:

- Pre-proposals and proposals that do not address the specific Computer Science topics described above.
- Pre-proposals and proposals that do not explain/describe their relevance to current and future high performance computing platforms and/or data-centric science as well as their relevance to the mission of SC and ASCR.
- Pre-proposals and proposals with primary emphasis on computer hardware design, fabrication, or integration; materials science; and computing devices and/or device/circuit design and/or manufacturing;
- Research primarily focused on advancing discipline-specific data analytics and informatics
  without a clear articulation of how the proposed research could be generalized to other SC
  priority mission areas;
- Research primarily focused on advancing Virtual Reality and Augmented Reality technologies;
- Research focused on the World Wide Web and/or Internet;
- Research that is only applicable to hand-held, tablets, laptops, portable, desktop, embedded or cloud computing;
- Research with a primary goal of developing hardware components for networks, including Intelligent Network Interface Cards, biological complex networks, social networks, or network acceleration hardware; and technologies that optimize wireless or other low-speed network infrastructures;
- Pre-proposals and proposals with a primary focus on development or deployment activities; or that suggest incremental upgrades to existing network architectures, protocols, tools, or services.
- Development and optimization of quantum algorithms; development of new candidate qubit systems; schemes based on qubits that have not yet demonstrated high-fidelity gates; schemes to improve the performance and functionality of qubits; quantum transduction; quantum communication, networking, and key distribution; cryptography and cryptanalysis;

research solely relevant to large-scale, high-fidelity, fault-tolerant machines; projects that are duplicative of or competitive with industry; software development other than what is required to maintain efficient operation of the laboratory.

### References

NITRD LSN Workshop Report on Complex Engineered Networks, <a href="https://www.nitrd.gov/pubs/nitrd\_lsn\_workshop\_report\_2012.pdf">https://www.nitrd.gov/pubs/nitrd\_lsn\_workshop\_report\_2012.pdf</a>

DOE Workshop report. DOE Network 2025: Network Research Problems and Challenges for DOE Scientists Workshop, February 2016. <a href="https://science.osti.gov/-media/ascr/pdf/programdocuments/docs/2017/DOE\_Network\_2025.pdf">https://science.osti.gov/-media/ascr/pdf/programdocuments/docs/2017/DOE\_Network\_2025.pdf</a>

DOE Workshop report. "Software Defined Networking for Extreme-Scale Science: Data, Computer, and Instrument Facilities," <a href="https://www.orau.gov/ionInfrastructure2014/intelligent-network-infrastructure-workshop-report.pdf">https://www.orau.gov/ionInfrastructure2014/intelligent-network-infrastructure-workshop-report.pdf</a>

DOE Workshop report. STREAM2016: Streaming Requirements, Experience, Applications, and Middleware workshop, March 2016. <a href="https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/2017/STREAM2016.pdf">https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/2017/STREAM2016.pdf</a>

DOE Workshop report: "Management, Analysis and Visualization of Experimental and Observational Data: The Convergence of Data and Computing," <a href="https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/2018/DOE-ExascaleReport-CrossCut.pdf">https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/2018/DOE-ExascaleReport-CrossCut.pdf</a>

DOE Workshop report: Crosscut Report: Exascale Requirements Reviews, March 2017. <a href="https://science.osti.gov/~/media/ascr/pdf/programdocuments/docs/2018/DOE-ExascaleReport-CrossCut.pdf">https://science.osti.gov/~/media/ascr/pdf/programdocuments/docs/2018/DOE-ExascaleReport-CrossCut.pdf</a>

DOE Workshop report: Neuromorphic Computing – Architectures, Models, and Applications, June 2016. <a href="https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/Post-Workshop Report 2016 Neuromorphic Computing.pdf">https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/Post-Workshop Report 2016 Neuromorphic Computing.pdf</a>

DOE Workshop report: Neuromorphic Computing – From Materials Research to Systems Architecture, <a href="https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/Neuromorphic-Computing-Report\_FNLBLP.pdf">https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/Neuromorphic-Computing-Report\_FNLBLP.pdf</a>

DOE Workshop report: ASCR Cybersecurity for Scientific Computing Integrity, January 2015 <a href="https://science.osti.gov/">https://science.osti.gov/</a>-

DOE Workshop report: The 2015 Cybersecurity For Scientific Computing Integrity – Research Pathways and Ideas, June 2015. <a href="https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/ASCR">https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/ASCR</a> Cybersecurity 20 Research Pathways and Ideas Workshop.pdf

DOE Workshop report: Machine Learning and Understanding For Intelligent Extreme Scale Scientific Computing and Discovery, <a href="https://science.osti.gov/-/media/ascr/pdf/program-documents/docs/Machine\_Learning\_DOE\_Workshop\_Report.pdf">https://science.osti.gov/-/media/ascr/pdf/program-documents/docs/Machine\_Learning\_DOE\_Workshop\_Report.pdf</a>

### **Research and Evaluation Prototypes**

The Research and Evaluation Prototypes (REP) activity addresses the challenges of next generation computing systems. By actively partnering with the research community, including industry and Federal agencies, on the development of technologies that enable next-generation machines, ASCR ensures that commercially available architectures serve the needs of the scientific community. The REP activity also prepares researchers to effectively use future generation of scientific computers, including novel technologies, and seeks to reduce risk for future major procurements.

### (h) Quantum Computing

Technical Contact: Claire Cramer, 301-903-9958, Claire.Cramer@science.doe.gov

Research to evaluate the suitability of specific quantum computing hardware architectures for science applications. Feedback and control systems for physical qubits in quantum processors. Compilation and optimization tools, including efficient mapping of algorithms to circuits in real-world hardware and research to develop more effective gates. Techniques for minimizing or mitigating error in real-world quantum processors.

Proposed research should focus on applications of quantum computing relevant to SC and on devices that are already available or that become available during the term of the award rather than large-scale, high-fidelity, fault-tolerant machines.

Topics that are out of scope include:

- Pre-proposals and proposals that do not address the specific REP topics described above;
- Development of quantum algorithms;
- Development of new candidate qubit systems or improvements to physical qubits;
- Quantum transduction;
- Quantum communication, networking, and key distribution;
- Cryptography and cryptanalysis;
- Error correction codes and implementation of error correction codes;
- Research solely relevant to large-scale, high-fidelity, fault-tolerant machines; and
- Projects that are duplicative of or competitive with industry.

### References

ASCR Report on Quantum Computing for Science, February 2015. https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/ASCRQuantumReport-final.pdf

ASCR Report on a Quantum Computing Testbed for Science, February 2017. https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/2017/QTSWReport.pdf

### **Biological and Environmental Research (BER)**

Program Website: <a href="https://www.energy.gov/science/ber/biological-and-environmental-research">https://www.energy.gov/science/ber/biological-and-environmental-research</a> or <a href="https://science.osti.gov/ber">https://science.osti.gov/ber</a>

BER's mission is to support transformative science and scientific user facilities to achieve a predictive understanding of complex biological, earth, and environmental systems for energy and infrastructure security and resilience.

### **Biological Systems Science**

The Biological Systems Science Division (BSSD) within BER supports fundamental systems biology research to advance understanding of microbes and multispecies communities in energy and the environment. Exploring the translation of organisms' genomes into catalytic and structural macro molecules, regulatory systems, and metabolic pathways can shed new light on the mechanistic basis of biological processes and how these processes change in response to biological community interactions and shifting environmental regimes. BSSD aims at achieving a predictive understanding of the relationships between systems biology properties of microbial communities and environmental processes, elucidating global biogeochemical cycles from molecular to ecosystem scales.

BER is seeking Biological Systems Science research only in the following area:

# (a) Fundamental systems biology-driven research on the roles of microbiomes in biogeochemical cycling processes

Technical Contact: Pablo Rabinowicz, 301-903-0379, pablo.rabinowicz@science.doe.gov

Proposals are requested for systems biology and 'omics driven basic research on the contribution of microbial communities to biogeochemical cycling in terrestrial soil environments. Proposals should focus on innovative approaches to understand regulatory, metabolic, and/or signaling networks of environmental microbes and microbiomes. Proposals focused on novel microbial processes or interactions with a significant impact on terrestrial soil environments are strongly encouraged. Proposed research may focus on natural microbial communities and/or model microbial consortia. Selected experimental systems may include the development of microbial community-scale metabolic and regulatory models that examine fundamental principles informative to understanding larger-scale biogeochemical processes. The development of genome-enabled techniques (e.g. metagenomics, metatranscriptomics, metaproteomics, community-scale metabolomics, etc.) is encouraged, as long as they are applied to understand ecosystem processes or to predict microbial responses to environmental change or stress.

NOTE: BER encourages the submission of innovative "high-risk/high-reward" research proposals that address critical knowledge gaps and have the potential for high impact. The probability of success and the risk-reward balance will be considered when making funding decisions.

The following topics are NOT within the scope of the BSSD research area: Proposals focusing on natural or model microbial consortia that are of limited relevance to understanding global-

and regional-scale biogeochemical cycle processes are not encouraged. Proposals primarily focused on agroecosystems or urban environments are not encouraged for this FOA. Proposals focused on bioremediation processes are not encouraged. Proposals primarily focused on metagenomic sequencing are not encouraged for this funding opportunity and should instead be directed to the DOE Joint Genome Institute's Community Science Program (<a href="https://jgi.doe.gov/user-programs/program-info/csp-overview/">https://jgi.doe.gov/user-programs/program-info/csp-overview/</a>). Proposals for research that would result in incremental advances in our current understanding or technology are not encouraged. Proposals that are solely focused on technology development are not encouraged. While macro-eukaryotes (insects, worms, etc.) are important members of the overall soil ecosystem, they should not be the primary focus of a proposal responding to this FOA.

DOE User Facilities and Other Specialized Resources: Applicants are encouraged to consider the use of resources provided by DOE Science User Facilities and Community Resources. These include the DOE Systems Biology Knowledgebase (KBase; <a href="http://www.kbase.us">http://www.kbase.us</a>), DOE Environmental Molecular Sciences Laboratory (EMSL; <a href="http://www.emsl.pnl.gov/emslweb">http://www.emsl.pnl.gov/emslweb</a>), National Energy Research Scientific Computing Center (NERSC; <a href="http://www.nersc.gov">http://www.nersc.gov</a>), DOE Structural Biology Resources (<a href="https://berstructuralbioportal.org">https://berstructuralbioportal.org</a>), and DOE Joint Genome Institute (JGI; <a href="http://jgi.doe.gov">https://jgi.doe.gov</a>). Awarded projects will receive prioritized consideration for use of JGI capabilities, subject to an assessment of technical feasibility by the facility. Annual Principal Investigator (PI) Meeting: if an award is made, at least one project participant will be required to attend an annual investigator meeting each year of funding. Reasonable travel expenses may be included as part of the project budget.

### **Earth and Environmental Systems Sciences**

The Earth and Environmental Systems Sciences (EESS) subprogram supports fundamental science and research capabilities that enable major scientific developments in earth systemrelevant atmospheric and ecosystem process and modeling research in support of DOE's mission goals for transformative science for energy and national security. There are five grand challenges that frame the subprogram and investments: (a) advancing the understanding of the integrated water cycle by studying relevant processes involving the atmospheric, terrestrial, oceanic, and human system components and their interactions and feedbacks across local, regional, and global scales, thereby improving the predictability of the water cycle and reducing associated uncertainties in response to short- and long-term perturbations; (b) advancing a robust, predictive understanding of coupled biogeochemical processes and cycles across spatial and temporal scales by investigating natural and anthropogenic interactions and feedbacks and their associated uncertainties within Earth and environmental systems; (c) understanding and quantifying the drivers, interactions, and feedbacks both among the high-latitude components and between the high latitudes and the global system to reduce uncertainties and improve predictive understanding of high-latitude systems and their global impacts; (d) advancing next-generation understanding of Earth system drivers and their effects on the integrated Earth-energy-human system; and (e) developing a broad range of interconnected infrastructure capabilities and tools that support the integration and management of models, experiments, and observations across a hierarchy of scales and complexity to address EESS scientific grand challenges.

BER is seeking Earth and Environmental Systems Sciences research in the following area:

## (b) Earth and Environmental Systems Modeling (EESM) Technical Contact: Renu Joseph, 301-903-9237, Renu.Joseph@science.doe.gov

The goal of the EESM portfolio within the EESS subprogram is to develop and demonstrate advanced modeling and simulation capabilities, in order to enhance the predictability of the Earth system over multiple temporal and spatial scales. EESM investments therefore focus on Earth system model development, regional and global model analysis, and understanding of multisector dynamics within the coupled human-Earth system. The vision for EESM is to provide DOE with the best possible information about the evolving Earth system to inform planning for energy assets and infrastructures. Key examples of critical EESM scientific information supporting the DOE mission include projections of water availability, drought incidence and persistence, temperature extremes such as prolonged heat stress, probability of storms, opening of the Arctic Ocean, and convolved sea-level and storm-surge interactions within coastal regions.

One element of the EESM activity is the Energy Exascale Earth System Model (E3SM) project. E3SM is a state-of-the-science Earth system model development and simulation project to investigate energy-relevant science using advanced software that has been optimized for DOE's advanced computers. In 2018, the first version (v1) of the E3SM model was publicly released and E3SM moved to an open development model. Data from all major campaign simulations by the E3SM project will also be made available to the scientific community. More information on E3SM is available at <a href="https://e3sm.org/">https://e3sm.org/</a>. Given that no single modeling approach can adequately represent all facets and behaviors of the Earth system, EESM also invests in the development and use of multi-model and hierarchical modeling approaches.

## As part of this solicitation, BER is seeking modeling research proposals that address grand challenges and science questions that focus on <u>coastal systems</u>:

Coastal systems are among the most complex and dynamic regions of the integrated Earth system. While comprising only a small fraction of the Earth's total area, this narrow band is where terrestrial, marine, atmospheric, and human processes interact. Tightly interconnected built and natural environments along coastlines make these hot spots for rapid transitions, driven in part by weather patterns and extremes (e.g., hurricanes), storm surge, sea level rise (SLR), hydrologic shifts, concentrated economic activity and infrastructure, global trade and shipping, transport and distribution (including energy), land and resource pressures, population shifts, and more. For purposes of this solicitation, the term "coast" is not limited to the precise delineation of water and land boundaries, but implies a geographic domain where broader interactions of terrestrial, atmospheric, and aquatic systems and processes occur.

EESM is interested in research around major, interacting, coastal system processes with a drive toward improving integrated modeling and analysis of the processes that govern coastal landscapes. A primary goal is to provide the scientific underpinning for predictive earth system modeling and analysis tools to inform coastal-region development pathways for energy and related sectors.

More specifically, and for this solicitation, EESM seeks proposals that respond to one or both of

the following two categories:

- 1) Regional and Global Model Analysis
- 2) Earth System Model Development

### Category 1: Regional and Global Model Analysis (RGMA):

The overarching goal of the RGMA component of EESM is to enhance predictive and process level understanding of variability and change in the Earth system by advancing capabilities to design, evaluate, diagnose, and analyze global and regional Earth system models informed by observations. The focus on this category should be to use a multi-model and a hierarchical modeling approach (which must include the use of E3SM simulations and existing output and/or the super-parametrized/variable resolution versions of the E3SM) to examine the role of sequential extreme and/or multivariate or multiple-compounding extreme events on natural components of the coastal system. Accordingly, the model analysis must include at least two extreme phenomena that are simultaneous or closely occurring in space and time, i.e., as sequential or compounding events that affect the natural system. This may include, e.g., simultaneously occurring extreme heat, wildfire, and/or drought in the same region that can impact future flooding; sequential hurricanes and flooding in the same region; repeating atmospheric rivers in the same region that can impact flood and/or other land processes; etc. For instance, some examples of questions are: How do compounding land-falling Tropical Cyclones and/or compounding Atmospheric Rivers (both are primarily atmospheric) affect terrestrial coastal processes such as storm surges, landslides, or flooding? How do droughts followed by floods affect sediment transport or other dimensions of natural terrestrial system? How might changes in the frequency, distribution, intensity of these compounding/sequential extreme events affect runoff?

### Proposals associated with RGMA must:

- Focus on the North American coastal system
- Use the E3SM
  - o This could be done in a hierarchical framework, or in the context of the use of multiple models
  - o Variable Resolution or Super-Parameterized versions of E3SM can also be used
- Develop a set of scientific questions and hypothesis driven analysis to motivate tasks
- Advance an understanding of the extreme events being studied
- Examine impacts of compounding and/or sequential or multivariate extreme events on other components of the natural Earth system
- Use observations, data, or reanalysis to evaluate the nature of the extreme events.

### Proposals for RGMA category are also encouraged to consider the following:

- Develop and/or use emulators to facilitate understanding
- Use machine learning to inform their understanding of processes in the relevant domains
- Develop metrics to evaluate the processes of interest in ESMs and contribute it to already existing packages like (<u>PCMDI Metrics Package</u>-PMP, <u>International Land Model</u> Benchmarking- ILAMB, Coupled Model Evaluation Capabilities- CMEC)
- In addition, investigators who develop new diagnostics methodologies to analyze the Earth system should consider contributing their tools to the Toolkit for Extreme Climate Analysis

(<u>TECA</u>) repository, if appropriate.

Proposals in the RGMA category should not:

- Focus on collecting observations. The use of appropriate pre-existing observations is encouraged

### Category 2: Earth System Model Development (ESMD):

The overarching goal of ESMD is to provide accurate and computationally advanced representations of the fully coupled and integrated Earth system, in order to address scientific grand challenges outlined in the <a href="Strategic Plan">Strategic Plan</a>. For this solicitation, proposals must emphasize model development activities that improve the ability of global coupled earth system models to produce useful and credible simulations and predictions of Earth system behavior appropriate for coastal systems.

### Proposals in the ESMD category must:

- Focus on development for the E3SM
- Focus on improving physical or biogeochemical aspects of the natural Earth system (e.g., atmospheric dynamics, clouds, atmospheric chemistry, ocean circulation, ocean biogeochemistry, land biogeochemistry, hydrology, sea-ice, or land-ice)
- Articulate why the proposed model development activities are important for improved predictability of coastal systems within E3SM
- Propose specific coastal science questions that will be addressed with the improved model
- Include a plan for evaluation and assessment of the model development activities based on existing observations
- While initial model development and validation efforts can focus on a single region or location, the full proposal must include a plan for illustrating how the model development is extensible to the global earth system.
- Use modern and sustainable software practices and workflows

### Proposals in the ESMD category may include:

- Improvements to existing parameterizations or development of new parameterizations
- Improvements to coupling between major systems and components reflected in E3SM
- Development and incorporation of new diagnostic methods or tools
- Development of novel model initialization methods
- Development of regional refinement in a new region (relative to previous E3SM project configurations or simulations)

### Proposals in the ESMD category are encouraged to:

- Focus on interactions, interfaces, and interdependencies among components in the coupled system
- Consider the North American coastal system as a priority region for model validation and coastal science questions

Pre-proposals and proposals to the Coastal System Science sub-topic must state which of the two major sub-areas their proposal will address (proposals may address both sub-areas) and must

provide enough technical information to assess whether they are addressing all of the required elements in the given sub-area.

If an award is made, at least one project participant will be required to attend an annual investigator meeting for each year of funding. Reasonable travel expenses may be included as part of the project budget.

### **Basic Energy Sciences (BES)**

Program Website: <a href="https://www.energy.gov/science/bes/basic-energy-sciences">https://www.energy.gov/science/bes/basic-energy-sciences</a> or <a href="https://science.osti.gov/bes/">https://science.osti.gov/bes/</a>

BES's mission is to support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security. The portfolio supports work in the natural sciences by emphasizing fundamental research in materials sciences, chemistry, geosciences, and biosciences. BES-supported scientific facilities provide specialized instrumentation and expertise that enable scientists to carry out experiments not possible at individual laboratories.

More detailed information about BES sponsored research can be found at the BES website listed above. There you will find BES-sponsored workshop reports that address the current status and possible future directions of some important research areas. Also, Principal Investigators' Meetings Reports contain abstracts of BES supported research in topical areas associated with Division-sponsored technical conferences. Finally, the websites of individual BES Divisions may also be helpful. The following web pages are listed for convenience:

### BES Workshop Reports:

http://science.osti.gov/bes/community-resources/reports/

Materials Sciences and Engineering Division Principal Investigators' Meetings: <a href="http://science.osti.gov/bes/mse/principal-investigators-meetings/">http://science.osti.gov/bes/mse/principal-investigators-meetings/</a>

Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings: <a href="http://science.osti.gov/bes/csgb/principal-investigators-meetings/">http://science.osti.gov/bes/csgb/principal-investigators-meetings/</a>

Scientific User Facilities Division web page: http://science.osti.gov/bes/suf/

Many of the core research areas limit early career proposals to a subset of topics within their regular research programs. In those cases, the intention is to rotate topics on an annual basis. Proposed research must be responsive to a supported topic in one of the core research areas listed below. In addition, proposals that use modern data science approaches (artificial intelligence, machine learning, graph theory, uncertainty quantification, etc.) to accelerate discovery in chemical and materials sciences would be within the scope of all topical areas.

### (a) Materials Chemistry

Technical Contacts: Michael Sennett, 301-903-6051, <u>Michael Sennett@science.doe.gov</u> (select Michael Sennett in PAMS) and Craig Henderson, 301-903-0805, <u>Craig.Henderson@science.doe.gov</u>

This program supports scientific research on materials with a focus on the *chemical synthesis*, *chemical control*, *and chemical dynamics* of material composition and structure across the range of length scales from atomic to mesoscopic, with a view to elucidating fundamental aspects of materials' structure-property relationships. The major programmatic focus is on the discovery, design and synthesis of novel, energy-relevant materials with an emphasis on the *chemistry* and *chemical* control of composition, structure, and function across the range of length scales from atomic to mesoscopic, and consequent materials properties.

Recent BES Basic Research Needs (and other) workshops and reports have articulated those areas of the materials sciences that are most relevant to energy. All of the reports variously identify the overarching goal of fundamental materials chemistry research as providing the *knowledge* needed to *design and produce* new materials with *tailored properties from first principles*. This program will therefore emphasize research on the chemistry-based discovery, synthesis and transformations of materials and/or morphologies with the goal of providing fundamental knowledge with the potential to enable the development of next generation energy technologies.

For the early career program, the topic for proposals this year is strictly limited. The program will accept hypothesis-driven proposals ONLY in the following topical area:

• Chemical synthesis of metastable materials with novel compositions, structures, phases, and/or functions via <u>understanding and control</u> of non-equilibrium reaction pathways and conditions

Applicants should emphasize the impactful fundamental science aspects of their proposed project and the project should be focused on hypothesis-driven fundamental research that is transformative in nature. Note that the proposed use of non-equilibrium synthesis conditions alone (e.g., extremes of temperature, pressure, rapid quenching, pulsed energy input, etc.,) and/or the isolation of meta-stable products from such synthesis will not be considered responsive to this topic without concurrent elucidation and control of the non-equilibrium reaction pathway(s).

The program will NOT consider proposals this year on any other topic than the one listed above. Future Early Career Research Program competitions in Materials Chemistry will call for proposals in a different limited topical area or areas, to be determined by programmatic needs and priorities at the time of the announcement.

The program will NOT accept proposals describing the following categories of research activity: *Optimization* of material properties for any technology, *nanoparticle synthesis* or synthesis of *small molecules* as a primary goal, studies of *energetic materials* (i.e. propellants and explosives), *device fabrication and testing* as a primary goal, and *developing materials* for specific technologies.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant. Further, the proposed research must be technically delineated from other research.

### (b) Biomolecular Materials

Technical Contact: Michael Markowitz, 301-903-6779, <a href="mike.markowitz@science.doe.gov">mike.markowitz@science.doe.gov</a>

This activity supports basic research in the discovery, design and synthesis of functional materials and complex structures based on principles and concepts of biology. Since biology provides a blueprint for translating atomic and nanoscale phenomena into mesoscale materials that display complex yet well-coordinated collective behavior, the major programmatic focus is on the hypothesis-driven creation of energy-relevant versions of these materials optimized for harsher, non-biological environments.

Recent BES Basic Research Needs (and other) workshops and reports have clearly identified mastering the capabilities of living systems as a Grand Challenge that could provide the knowledge base to discover, design, and synthesize new materials with totally new properties for next-generation energy technologies. Biomolecular Materials research activity seeks to advance the ability for materials that can coherently manage collective chemical, optical, electronic, magnetic, mechanical, and thermal signals and processes; self-repair; regulate, clean, and sequester impurities; and tolerate abuse.

For the early career program, two separate topics (A and B shown below) are planned for alternate fiscal years. Based on programmatic priorities, science-driven research for assembly that incorporates defect-managing mechanisms will be emphasized for both topics. For this announcement, only proposals focused on Topic B will be considered.

- Topic A (Alternate years): The specific focus will be on research to design and create future next-generation materials for energy conversion and storage with programmable selectivity and transport based on biological gating and pumping functions.
- Topic B (This year): The focus should be creation of multicomponent, resilient, self-regulating materials that can reconfigure function and/or energy transfer, transport, and communication pathways; repair and rebuild structure without external input; or self-replicate.

For both of these topics, science-driven coupling of theory and experiment to achieve synthesis of materials with predetermined functions, assembly management attributes noted above, and morphology are encouraged. Bio-centric research **will be de-emphasized**, including activities focused on understanding of underlying biological synthetic or assembly processes, biologically-driven synthesis of monodisperse polymers, or creation of bio-hybrid materials. The program **will not** support projects that do not have a clear focus on materials science or are aimed at optimization of materials properties for any applications, device fabrication, sensor development, tissue engineering, and biological, or biomedical research.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

### (c) Synthesis and Processing Science Technical Contact: Bonnie Gersten, 301-903-0002, <u>bonnie.gersten@science.doe.gov</u>

This program supports basic scientific research on materials to understand the physical principles that underpin materials synthesis including diffusion, nucleation, and phase transitions, often using *in situ* diagnostics, and developing new techniques to synthesize materials. An important element of this activity is the development of real-time monitoring tools that probe the dynamic environment and the progression of structure and properties as a material is formed. This information is essential to the physical understanding of the underlying mechanisms that help gain atomic level control in materials synthesis and processing.

Recent BES Basic Research Needs (and other) workshops and reports, particularly the report on *Synthesis Science*, have identified the needs and challenges in synthesis and processing that are most relevant to next-generation energy technologies.

This year's Early Career Research Program invites applicants to submit hypothesis driven proposals that present novel understanding and creative approaches elucidating the physical mechanisms underlying the synthesis and processing of three-dimensional bulk materials. Proposals that integrate a creative experimental methodology with a theoretical-based approach to accelerate progress in understanding unifying principles for synthesis and/or processing are of particular interest. The focus of this activity on materials discovery and design by physical means is complementary to the BES Materials Chemistry and Biomolecular Materials research activities, which emphasize chemical and bio-inspired approaches.

The program **will not** support projects that involve biological materials or that are aimed at *optimization* of material properties for specific applications. In addition, the program **will not** support projects with a primary goal of device fabrication, nanoparticle synthesis, tribology, fluid dynamics, manufacturing or engineering scale-up/development. For this year, projects involving the synthesis or processing of two-dimensional, thin film, and stacked materials **will not** be supported.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

### (d) Experimental Condensed Matter Physics Technical Contact: Michael Pechan, 301-903-0540, Michael.Pechan@science.doe.gov

The Experimental Condensed Matter Physics (ECMP) program supports research that will advance our fundamental understanding of the relationships between intrinsic electronic structure and the properties of complex materials.

This year the Early Career call in ECMP will focus on nanostructured and low dimensional quantum materials wherein electronic, structural, charge and magnetic states are controlled to

produce novel functionality. Next year's call is anticipated to focus on bulk quantum materials.

The ECMP Program does not support proposals on electrochemistry, thermoelectric materials or photovoltaic materials; nor does it support projects aimed at materials optimization or device development. In addition, the ECMP Early Career Program will not accept proposals on topics in the following areas: conventional semiconductors, heavy fermion superconductivity, quantum Hall physics in compound semiconductor materials, cuprate superconductivity, and cold atom physics.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

### (e) Theoretical Condensed Matter Physics Technical Contact: Matthias Graf, 301-903-0874, <u>matthias.graf@science.doe.gov</u>

This program supports research in theoretical condensed matter physics with an emphasis on quantum materials, quantum computing, materials discovery, systems out of equilibrium (including transport and ultrafast response), and fundamental research in materials related to energy technologies. Examples of current research include strongly correlated electron systems, quantum phase transitions, magnetism, superconductivity, wide bandgap semiconductor physics, computational and data driven materials design, thermoelectric materials, optical response, and neutron and photon scattering. Novel, physics-based computational techniques are supported for quantum many-body problems.

This year, proposals are only sought in targeted areas of quantum materials, quantum computing, and systems out of equilibrium, including ultrafast response. Next year, the plan is to invite proposals in the areas of high-throughput computations, data-driven materials discovery, and materials theory/modeling solely related to energy technologies.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

### (f) Physical Behavior of Materials Technical Contact: Refik Kortan, 301-903-3308, <u>refik.kortan@science.doe.gov</u>

This program supports fundamental research on the physical behavior of materials. This year, the program invites early career proposals in the areas of spin-related properties of materials including magnetocaloric and multiferroic materials, and light-matter interactions in the areas of excitonics and plasmonics. The program will also consider proposals relevant to the field of Quantum Information Science for research on the creation and control of quantum coherent phenomena for transduction of quantum coherent states between different physical systems with high fidelity. The applicants should heavily emphasize the impactful and fundamental science aspects of their projects and these projects should be centered around hypothesis driven fundamental research that is potentially transformative in nature. This program also supports theory, modeling, and simulation activities, especially in combination with experimental research.

The program **will not** support projects aimed at optimization of materials properties for any applications, device fabrication, or sensor development.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

### (g) Mechanical Behavior and Radiation Effects Technical Contact: John Vetrano, 301-903-5976, john.vetrano@science.doe.gov

This activity supports hypothesis-driven basic research to understand defects in materials and their effects on the properties of strength, structure, deformation, and failure. Defect formation, growth, migration, and propagation are examined by coordinated experimental and modeling efforts over a wide range of spatial and temporal scales. Topics include fundamental studies of deformation of nanostructured materials and intelligent microstructural design for increased strength, formability, and fracture resistance in energy relevant materials. The goals are to develop the scientific underpinning for predictive design of materials having superior mechanical properties.

This year the emphasis is on mechanical behavior of materials, with the plan to alternate this topic with an emphasis on radiation effects annually. Research opportunities that can be realized by the application of mechanical behavior fundamentals to the general areas of self-assembly, physical behavior, and behavior under extreme environments (temperature, stress, strain, corrosion) of structural materials will be emphasized. In addition to traditional structural materials, there is an emphasis on understanding deformation and failure of other materials used in energy systems (e.g., polymers, membranes, coating materials, electrodes), although the focus should still be on gaining fundamental understanding of new/unique mechanisms. Proposals taking advantage of advanced synthesis methods to create tailored structures in order to better isolate mechanisms, and those utilizing advanced characterization techniques such as neutron or x-ray scattering, are of particular interest. The topics of wear, bioinspired materials, and high-strain rate deformation will not be explored in this program at this time. Proposals emphasizing mechanics of materials, rather than materials science, will not be considered responsive.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

### (h) X-ray Scattering

Technical Contact: Lane Wilson, 301-903-5877, <a href="mailto:lane.wilson@science.doe.gov">lane.wilson@science.doe.gov</a>

This activity supports basic research on the fundamental interactions of photons with matter to achieve an understanding of atomic, electronic, and magnetic structures and excitations and their relationships to materials properties. The main emphasis is on x-ray scattering, spectroscopy, and imaging research, primarily at major BES-supported user facilities. Instrumentation development and experimental research directed at the study of ultrafast physical phenomena in materials is an integral part of the portfolio. Based on programmatic priorities, this activity **will not** support

ultra-fast source development, but will focus on the application of ultra-fast probe interactions with materials and the resulting connection to materials dynamics.

Advances in x-ray scattering and ultrafast sciences will continue to be driven by scientific opportunities presented by improved source performance and optimized instrumentation. The x-ray scattering activity will continue to fully develop the capabilities at the DOE facilities by providing support for instrumentation, technique development and research. A continuing theme in the scattering program will be the integration and support of materials preparation (especially when coupled to *in situ* investigation of materials processing) as this is a core competency that is vital to careful structural measurements related to materials properties. New investments in ultrafast science will focus on research that uses radiation sources associated with BES facilities and beam lines. New pump schemes to manipulate dynamic states of quantum materials will be supported, especially those which can be adapted to XFEL and UED probe environments.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

### (i) Neutron Scattering

Technical Contact: P. Thiyagarajan (Thiyaga), 301-903-9706, p.thiyagarajan@science.doe.gov

This activity supports basic research on the fundamental interactions of neutrons with matter to achieve an understanding of the atomic, electronic, and magnetic structures and excitations of materials and their relationship to macroscopic properties. The main emphasis is on transformative research on materials and phenomena using neutron scattering, coupled with the advancement of neutron scattering techniques, primarily at the BES user facilities. A continuing theme of this program is that integrating neutron scattering measurements on high quality samples with theory and computational modeling is vital for an in-depth understanding of the relationship between structure, dynamics, and macroscopic properties.

The focus for this year's Early Career Research Program is on fundamental science on materials that exhibit novel emergent phenomena or unique properties useful for energy applications. Characterizing and controlling the emergent behavior are keys to optimizing and exploiting a wide range of materials' performance and functionality. *In situ* studies can measure structure and dynamics of materials in the appropriate environment and operational conditions, yielding direct data for comparison to predictions. The program will develop novel approaches that will exploit the unique aspects of neutron scattering to investigate novel materials over a wide range of length and time scales.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

### (j) Electron and Scanning Probe Microscopies Technical Contact: Jane Zhu, 301-903-3811, jane.zhu@science.doe.gov

This activity supports basic research in materials sciences using microscopy and spectroscopy techniques. The research includes experiments and theory to understand the atomic, electronic, and magnetic structures and properties of materials. This activity also supports the development of new instrumentation and techniques, including ultrafast diffraction and imaging techniques, to advance basic science and materials characterizations for energy applications. The goal is to develop a fundamental understanding of materials through advanced microscopy and spectroscopy.

The focus for this year's Early Career Research Program is on basic science based on the priority research directions in "Basic Needs Workshop on Quantum Materials for Energy Relevant Technology." New methods and approaches could provide an array of opportunities for groundbreaking science. These include understanding and controlling nano- or meso-scale inhomogeneity as well as the interplay between charge, orbital, spin and lattice degrees of freedom. Other areas of emphasis are imaging the functionality of materials; investigating the electronic structure, spin dynamics, magnetism, phase transitions and transport properties from atomistic to mesoscopic scales; and developing advanced *in situ* analysis capabilities or combination of multiple probes for study of quantum materials.

Based on programmatic priorities, projects aimed at technique development without science goals will not be considered.

For DOE national laboratory applicants, the proposed research must fit within the BES Materials Sciences and Engineering (MSE) Division funded programs at the laboratory of the applicant.

# (k) Atomic, Molecular, and Optical Sciences (AMOS) Technical Contact: Tom Settersten, 301-903-8428, <a href="mailto:thomas.settersten@science.doe.gov">thomas.settersten@science.doe.gov</a>

This program supports basic experimental and theoretical research aimed at understanding the structural and dynamical properties of atomic and molecular systems. The research emphasizes fundamental interactions of photons and electrons with atomic and molecular systems to characterize and control their behavior. The goal is to develop accurate quantum-mechanical descriptions of dynamical processes such as chemical bond breaking and forming, interactions in strong fields, and electron correlation. Topics of interest include the development and use of novel, ultrafast optical probes of matter; the interactions of atoms and molecules with intense electromagnetic fields; and quantum control of atomic and molecular systems. Projects involving technical development of sources or instrumentation must include a well-integrated scientific research focus.

The AMOS activity will continue to support science that advances DOE and BES mission priorities. Closely related experimental and theoretical efforts will be encouraged. AMOS will continue to have a prominent role at BES facilities in understanding and controlling the interaction of intense, ultrafast x-ray pulses with matter. Key targets for greater investment

include attosecond science, ultrafast x-ray science, and ultrafast electron diffraction from molecular systems.

The program emphasizes ultrafast, strong-field, short-wavelength science, and studies of correlated dynamics in atoms and molecules. Examples include ultrafast x-ray science at the Linac Coherent Light Source (LCLS-II) and the use of high-harmonic generation or its variants as soft x-ray sources for probing ultrafast dynamics. Applications of these light sources include ultrafast imaging of chemical reactions, diffraction and harmonic generation from aligned molecules, and inner-shell photoionization of atoms and molecules. Coherent control of nonlinear optical processes and tailoring of quantum-mechanical wave functions with lasers will continue to be of interest, particularly in molecular systems.

The AMOS program **is not** accepting proposals in the areas of nanoscience, bioscience, and ultracold science.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

## (l) Gas Phase Chemical Physics (GPCP) Technical Contact: Wade Sisk, 301-903-5692, wade.sisk@science.doe.gov

The Gas Phase Chemical Physics (GPCP) Program supports research on gas-phase chemical processes important in energy applications. The overall goal of this program is to understand energy flow and reaction mechanisms in complex, non-equilibrium, gas-phase environments in which the coupling of chemical and transport processes is poorly understood.

The program may be divided into four basic science research thrusts described below.

- 1. *Light-Matter Interactions*. This thrust consists of research in molecular spectroscopy and diagnostics development to probe molecular structure, dynamics and interactions in complex gas-phase systems. This research is expected to provide approaches for chemical and physical analysis of heterogeneous and dynamic gas-phase environments. (OPEN)
- 2. Chemical Reactivity. This thrust includes chemical kinetics and mechanisms, chemical dynamics, collisional energy transfer, and construction of, and calculations on, molecular potential energy surfaces. This research is expected to develop fundamental understanding of energy flows and chemical reactions, which is the basis for determining accurate rate constants and predictive chemical mechanisms, and to develop and validate new theoretical methods to improve accuracy of theoretical chemical kinetics. (OPEN)
- 3. Chemistry-Transport Interactions. Research in this area focuses on gaining a better understanding of how non-equilibrium and/or non-uniform environments impact kinetics and mechanisms. Efforts include both experimental and theoretical studies probing mechanistic processes and how they change in complex environments. This research can lead to development of multiplexed diagnostics that measure many variables simultaneously to overcome irreproducibility associated with non-uniform and dynamic environments such as those in turbulent reacting flows. (CLOSED)

4. *Gas-Particle Interconversions*. This thrust consists of research on the formation, growth and evaporation of small particulates and aerosols and the transition to supercritical fluids at high pressures. This research is expected to lead to the development of mechanistic models of particle formation and growth, as well as a better understanding of particle evaporation. (CLOSED)

Research proposals will be accepted from only two of the selected four research thrusts each year, with the remaining thrusts offered in alternate years. For this announcement, only proposals focused on thrusts 1 and 2 will be considered. Research proposals for thrusts 3 and 4 will not be considered this year, but considered in alternate years.

The GPCP program **does** *not* support research in the following areas: non-reacting fluid dynamics and spray dynamics, data-sharing software development, end-use combustion device development, and characterization or optimization of end-use combustion devices.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

# (m) Computational and Theoretical Chemistry Technical Contact: Jeffrey L. Krause, 301-903-5827, <a href="mailto:Jeff.Krause@science.doe.gov">Jeff.Krause@science.doe.gov</a>

Computational and Theoretical Chemistry emphasizes sustained development and integration of new and existing theoretical and massively parallel computational approaches for the deterministic, accurate and efficient prediction of chemical processes and mechanisms relevant to the BES mission. Part of the focus is on simulation of processes that are so complex that efficient computational implementation must be accomplished in concert with development of new theories and algorithms. Efforts should be tightly integrated with the research and goals of BES and should provide computational tools to advance the fundamental science that underpins the development of new processes for the generation, storage, and use of energy. Efforts should include applications to real molecular and nanoscale systems. Proposals may include the development or improvement of modular computational tools that enhance interpretation and analysis of advanced experimental measurements, including those acquired at DOE user facilities, or efforts aimed at enhancing the accuracy, precision, applicability and scalability of quantum-mechanical simulation methods. Also included are development of spatial and temporal multiscale methodologies that allow for time-dependent simulations of resonant, non-resonant and dissipative processes as well as rare events. Development of capabilities for simulation of light-matter interactions, conversion of light to chemical energy or electricity, and the ability to model and control externally driven electronic and spin-dependent processes in real environments are encouraged. These phenomena may be modeled using a variety of timeindependent and time-dependent simulation approaches. Examples include:

- Practical predictive methods for excited-state phenomena in complex molecular systems.
- Nontraditional or novel basis sets, meshes and approaches for quantum simulation.
- Simulation and coupling of all interactions/scales in a system including: electronic, vibrational and atomistic structure, dissipative interactions, interactions between matter,

radiation, fields and environment, spin-dependent and magnetic effects and the role of polarization, solvation and weak interactions.

Emphasis is given to (i) advancing the accuracy and affordability of electronic structure methods and (ii) developing simulation approaches that enable efficient use of accurate electronic structure approaches. The program does not support (i) projects based exclusively on the use of standard, off-the-shelf computational packages, or (ii) the development of phenomenological models and empirical parameterization of models.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

# (n) Condensed Phase and Interfacial Molecular Science (CPIMS) Technical Contact: Gregory Fiechtner, 301-903-5809, gregory.fiechtner@science.doe.gov

The CPIMS program emphasizes basic research at the boundary of chemistry and physics, pursuing a molecular-level understanding of chemical, physical, and electron- and photon-driven processes in liquids and at interfaces. With its foundation in chemical physics, the impact of this crosscutting program on DOE missions is far reaching, including energy utilization, catalytic and separation processes, energy storage, chemical synthesis, and subsurface chemical and transport processes. Experimental and theoretical investigations in the gas phase, condensed phase, and at interfaces aim at elucidating the molecular-scale chemical and physical properties and interactions that govern chemical reactivity, solute/solvent structure and transport. Studies of reaction dynamics at well-characterized surfaces and clusters lead to the development of theories on the molecular origins of surface-mediated catalysis and heterogeneous chemistry. Studies of model condensed-phase systems target first-principles understanding of molecular reactivity and dynamical processes in solution and at interfaces, including complex interfaces. Fundamental studies of reactive processes driven by radiolysis in condensed phases and at interfaces provide improved understanding of radiation-driven chemistry in nuclear fuel and waste environments.

Basic research is also supported to develop new experimental and theoretical tools that push the horizon of spatial and temporal resolution needed to probe chemical behavior selectively at interfaces and in solution, enabling studies of composition, structure, bonding and reactivity at the molecular level. The transition from molecular-scale chemistry to collective phenomena in complex systems is also of interest, allowing knowledge gained at the molecular level to be exploited through the dynamics and kinetics of collective interactions. In this manner, the desired evolution is toward predictive capabilities that span the microscopic to mesoscale domains, enabling the computation of individual molecular interactions as well as their role in complex, collective behavior at continuum scales.

The CPIMS program has recently added research projects that (1) explore quantum entanglement to drive and sense reactions and reaction dynamics remotely in solution and at interfaces, and studies of quantum entanglement in molecular systems and their interaction with light, including entanglement preservation at interfaces, (2) perform theoretical and computational studies of catalytic reactions at amorphous oxide surfaces, (3) examine rare electrochemical events (such as

nucleation and self-assembly) using machine learning and advanced sampling techniques of large data sets, and (4) study hydrogen bonding and solvation of ions in liquid electrolytes (including in conventional dipolar solvents, ionic liquids and deep eutectic solvents). The program has also added projects such as (1) studies of ion solvation and charge transfer at electrochemical interfaces using nonlinear soft x-ray spectroscopy; (2) research that pushes accurate quantum simulations toward large mesoscale systems; and (3) explorations of multidimensional infrared microscopy for visualizing chemical dynamics in heterogeneous environments. Descriptions of earlier awards are found in Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings under "Condensed-Phase and Interfacial Molecular Science". A more extensive description of program evolution can be found at the link: <a href="https://science.osti.gov/bes/csgb/Research-Areas/Condensed-Phase-and-Interfacial-Molecular-Sciences">https://science.osti.gov/bes/csgb/Research-Areas/Condensed-Phase-and-Interfacial-Molecular-Sciences</a>.

The CPIMS program **does not** fund research in continuum fluid mechanics or fluid dynamics, technological applications and device development, and research that is of principle importance to medical sciences and applications.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

### (o) Catalysis Science

Technical Contact: Viviane Schwartz, 301-903-0448, <u>viviane.schwartz@science.doe.gov</u> and Chris Bradley, 301-903-2047, <u>chris.bradley@science.doe.gov</u>

This program supports basic research pursuing novel catalyst design and quantum- and molecular-level control of chemical transformations relevant to the sustainable conversion of energy resources. Emphasis is on the understanding of reaction mechanisms, enabling precise identification and manipulation of catalytic active sites, their environments, and reaction conditions for optimized efficiency and selectivity. Elucidation of *catalytic reaction mechanisms in diverse chemical environments* and *the structure-reactivity relationships of solid and molecular catalysts* comprise the central component of the program. This year's Early Career Research Program invites applicants to submit hypothesis-driven proposals in the following areas of emphasis:

- Thermal or electro-catalysis mediated by Earth-abundant metals;
- Examination of the dynamics of catalyst and electronic structures occurring during catalytic cycles and deactivation;
- Investigation of emerging approaches to direct catalytic transformations in multicomponent mixtures, multiple reactions, and integrated processes, such as cascade and tandem processes;
- Advanced theory, modeling, and data-science approaches to mechanism identification, catalyst discovery and development, and efforts leading to benchmarks for catalytic properties;
- Strategies that explore catalysts and mechanisms associated with circular processing, including upcycling of synthetic polymers and *a priori* functional design for feedstock

recyclability.

Other topics not mentioned above will also be considered, but at a lower priority this year. This program does not support: (1) the study of transformations appropriate for pharmaceutical synthesis; (2) studies where the primary focus is photochemistry or photophysics; (3) non-catalytic stoichiometric reactions; (4) whole cell or organismal catalysis; (5) process or reactor design and optimization; or (6) device development or optimization.

Examples of research funded in catalysis can be found in Catalysis Science Program Meeting Reports at the link 'Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings' (search for "catalysis" in the title), and in the BES Research Summaries (<a href="https://science.osti.gov/bes/csgb/Research-Areas/Catalysis-Science">https://science.osti.gov/bes/csgb/Research-Areas/Catalysis-Science</a>). A 2017 BESAC-sponsored workshop, Basic Research Needs for Catalysis Science, outlining the current challenges and needs in this field, can also be found on the 'Basic Research Needs Reports' webpage. A 2019 BES roundtable report on Chemical Upcycling of Polymers, discussing the challenges of polymer deconstruction and redesign, will appear in the same webpage.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

### (p) Separation Science (SEP)

Technical Contact: Daniel Matuszak, 301-903-1411, Daniel.Matuszak@science.doe.gov

This program supports fundamental, hypothesis-based, separation science to advance the understanding of de-mixing transitions of complex mixtures or multi-phase systems caused by physical or chemical driving forces. This includes but is not limited to the capture or removal of constituents from a system and transfer into another system with designed stability. The program goal is to predict and ultimately control separation processes through the manipulation of molecular, atomic, and electronic factors.

In support of this aim, advancing the understanding of basic chemical and physical principles at the molecular-, nano-, and meso-scales is relevant to strengthening the foundation for novel separation processes. Research on separation systems that utilize new modes of action, multimodal mechanisms, and energy- and atom-efficient methods are supported. Investigations of novel structures for separations are appropriate, such as complex interfaces, functionalized surfaces, macromolecular architectures, and multiscalar or hybrid systems designed specifically for separations research. Other relevant topics are accepted, such as transport and reactivity, aqueous environments, and prediction and control of the atomic and molecular interactions and energy exchanges that determine the efficiency of chemical separations

A 2019 National Academies consensus report, "A Research Agenda for Transforming Separation Science" (https://www.nap.edu/catalog/25421/a-research-agenda-for-transforming-separation-science), highlights relevant key challenges that are broadly grouped into topics associated with selectivity, capacity and throughput; as well as topics associated with how separation systems change over time in operating environments; its aim is to impact the understanding and design of

advanced separation systems. In addition, relevant BES reports include but are not limited to the 2015 "Basic Research Needs for Environmental Management" and the 2010 "Basic Research Needs for Carbon Capture: Beyond 2020". Research funded in this program in the recent past can be found in the Chemical Sciences, Geosciences, & Biosciences Division Principal Investigators' Meetings Reports.

Based on programmatic priorities, the Separation Science program does not support applied research, engineering or scale up of processes, devices or sensors, microfluidics or medical applications. The program will not consider proposals on chemical analysis, though proposals that contain analytical aspects that inform chemical separation research may be considered.

For DOE national laboratory applicants, the proposed research must fit within the BES CSGB Division funded programs at the laboratory of the applicant.

### (q) Heavy Element Chemistry (HEC) Technical Contact: Philip Wilk, 301-903-4537, <a href="mailto:philip.wilk@science.doe.gov">philip.wilk@science.doe.gov</a>

This activity supports basic research on the fundamental chemistry of the actinide and transactinide elements with the goal to understand the underlying chemical and physical principles that determine their chemical behavior. The unique molecular bonding of the heavy elements is explored using theory and experiment to elucidate electronic and molecular structure as well as reaction thermodynamics. Emphasis is placed on the chemical and physical properties of the transuranic elements to determine their bonding and reactivity, the fundamental transactinide chemical properties, and the overarching goal of resolving the *f*-electron challenge. The *f*-electron challenge refers to the inadequacy of current electronic structure methods to accurately describe the behavior of *f*-electrons, in particular strong correlation, spin-orbit coupling, multiplet complexity, and associated relativistic effects. While the majority of the research supported by this activity is experimental, theoretical proposals are considered that integrate closely with existing experimental research.

The role of 5f electrons in bond formation remains the fundamental topic in actinide chemistry and is an overarching emphasis for this program. Theory and experiment show that 5f orbitals participate significantly in molecular actinide compounds. Resolving the role of the f-electrons is one of the three grand challenges identified in the Basic Research Needs for Advanced Nuclear Energy Systems (ANES) report of the Basic Energy Sciences Workshop (2006) and echoed in the report from the Basic Energy Sciences Advisory Committee: Science for Energy Technology: Strengthening the Link between Basic Research and Industry (2010). The ANES report describes in depth specific challenges that continue to underlie contemporary actinide science, and the recent Basic Research Needs for Future Nuclear Energy report (2017) expands upon some of these chemical challenges, focusing on understanding and mastering the chemistry and reactivity of actinides in multi-component, multi-phase systems under extreme conditions.

Proposals should be hypothesis-based. Based on programmatic priorities, the HEC program does not fund research on: the processes affecting the transport of subsurface contaminants, the form and mobility of contaminants including wasteforms, projects focused on the use of heavy-element surrogates, projects aimed at optimization of materials properties including radiation

damage, device fabrication, or biological systems; which are all more appropriately supported through other DOE programs. Research that is focused primarily on separations and does not address the unique properties of the heavy elements would be better aligned with the BES Separation Science program, which is described in section (p). More information about this activity can be found at <a href="https://science.osti.gov/bes/csgb/Research-Areas/Heavy-Element-Chemistry">https://science.osti.gov/bes/csgb/Research-Areas/Heavy-Element-Chemistry</a>.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

### (r) Geosciences (GEO)

Technical Contact: Jim Rustad, 301-903-1717, <u>james.rustad@science.doe.gov</u>

This research area supports fundamental geoscience research, with emphasis on the molecular-level origins of geochemical and geophysical processes. This year's geosciences early career call is aimed at earth science problems involving topics on Chemistry at Complex Interfaces; Charge Transport and Reactivity; Reaction Pathways in Diverse Environments; Chemistry in Aqueous Environments; and Ultrafast Chemistry. To be considered for funding for the FY20 Early Career Program, proposal ideas must focus on the molecular scale and make strong connections to one or more of these topics. Particular priority will be given to proposals that put together compelling strategies for understanding geochemical reaction mechanisms. Proposals that do not focus on the molecular scale and convincingly connect with at least one of the thematic areas above will not be considered. Purely theoretical/computational investigations will not be considered unless they make well-defined connections to particular experiments.

For information about the relationship of the Geosciences program to the main research themes of the Chemical Sciences, Geosciences, and Biosciences (CSGB) Division see <a href="https://science.osti.gov/bes/csgb/">https://science.osti.gov/bes/csgb/</a>.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

### (s) Solar Photochemistry

Technical Contact: Chris Fecko, 301-903-1303, <a href="mailto:christopher.fecko@science.doe.gov">christopher.fecko@science.doe.gov</a>

This activity supports fundamental, molecular-level research on solar energy capture and conversion in the condensed phase and at interfaces. These investigations of solar photochemical energy conversion focus on the elementary steps of light absorption, charge separation, and charge transport within a number of chemical systems, including those with significant nanostructured composition. Although the long-term mission of this Program is an understanding of the science behind solar-driven production of fuels and electricity, it is recognized that fundamental research in the interaction of light, matter and electrons in these systems is essential to the achievement of Program goals.

Supported research areas include organic and inorganic photochemistry, catalysis and photocatalysis, photoinduced electron and energy transfer in the condensed phase and across interfaces, photoelectrochemistry, photodriven generation or manipulation of quantum coherence in artificial molecular systems, and artificial assemblies for charge separation and transport that mimic natural photosynthetic systems. An enhanced theory and modeling effort is needed to improve current understanding of many photochemical phenomena.

Among the challenges for catalytic fuels production, knowledge gained in charge separation and electron transfer needs to be applied in a meaningful way to activation of small molecules including, among others,  $CO_2$  in its reduction to fuels and  $H_2O$  in its oxidation or reduction via transformative catalytic cycles. This spans the range from dark catalytic reactions to those driven by the energy of an absorbed photon and in both homogeneous and heterogeneous environments. The major scientific challenge for photoelectrochemical energy conversion for fuel generation is that small band gap semiconductors capable of absorbing solar photons are susceptible to oxidative degradation, whereas wide band gap semiconductors, which are resistant to oxidative degradation in aqueous media, absorb too little of the solar spectrum. Also of interest is research on the principles of hybrid systems that feature molecular catalysis at solid surfaces and of new nanoscale structures for the photochemical generation of fuels.

Research areas concerned with separation of charge that might result in electricity include molecular semiconductors, photosensitized nanoparticulate solids, and the study of the mechanism of multiple exciton generation within nanoparticles. There are also challenges in fundamental understanding of photoconversion processes, including energy transfer and the generation, separation, and recombination of charge carriers.

Another regime of chemistry initiated through creation of high energy excited states is highly ionizing radiation, as can be produced through electron pulse radiolysis, to investigate reaction dynamics, structure, and energetics of short-lived transient intermediates in the condensed phase. Among many topics, fundamental research is of interest in areas that have a long term impact upon the understanding of radiolytic degradation of nuclear tank waste, the reactivity of solid surfaces in reactor coolant systems, and the chemistry of reagents used in separations processes in nuclear cycles.

Solar Photochemistry does not fund research on device development or optimization.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

### (t) Photosynthetic Systems

Technical Contact: Stephen Herbert, 301-903-0383, stephen.herbert@science.doe.gov

This activity supports basic research on the capture and conversion of solar energy to chemically stored forms of energy in plants, algae, and photosynthetic microbes. Topics of study in natural photosynthesis include, but are not limited to, light harvesting, quantum coherent energy transfer,

proton and electron transport, reduction of carbon dioxide into organic compounds, and the self-assembly, dynamics, and self-repair of photosynthetic proteins, complexes and membranes. The goal of the program is to foster greater knowledge of the structure and function of the diverse photosynthetic systems found in nature. Projects funded by the program combine biochemistry, biophysics, molecular biology, computational chemistry, and other approaches to understand the biological capture of sunlight and its conversion to and storage as chemical energy at a fundamental level.

All submitted proposals must clearly state the energy relevance of the proposed basic research. Photosynthetic Systems does not fund: 1) development or optimization of devices or processes; 2) development or optimization of microbial strains or plant varieties for biofuel or biomass production; 3) phenotype analyses that do not test specific hypotheses relevant to the program; 4) genomic or other "omic" data acquisition that does not test specific hypotheses relevant to the program; and 5) projects that are primarily computational in nature.

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

### (u) Physical Biosciences

Technical Contact: Robert Stack, 301-903-5652, <a href="mailto:robert.stack@science.doe.gov">robert.stack@science.doe.gov</a>

This activity supports basic research that combines physical science techniques with biochemical, chemical, and molecular biological approaches to discover the underlying physical and chemical principles that govern how plants and non-medical microbes capture, convert, and store energy. Fundamental research supported by the program includes studies that will provide a better understanding of the structure/function, mechanistic and electrochemical properties of enzymes that catalyze complex multielectron redox reactions (especially those involved in the interconversion of CO<sub>2</sub>/CH<sub>4</sub>, N<sub>2</sub>/NH<sub>3</sub>, and H<sup>+</sup>/H<sub>2</sub>), determine how the complex metallocofactors at the active sites of these enzymes are synthesized, and understand how the potential of these cofactors can be "tuned" using ligand coordination to reduce overpotential and better enable catalysis using earth-abundant metals. The program also funds mechanistic studies on electron bifurcation and catalytic bias in enzyme systems, and identifies the factors that direct and regulate the flow of electrons through energy-relevant metabolic pathways on larger spatial and temporal scales.

Physical Biosciences **does not** fund research in: 1) animal systems; 2) prokaryotic systems related to human/animal health or disease; 3) development and/or optimization of devices and/or processes; 4) development and/or optimization of microbial strains or plant varieties for biofuel/biomass production; 5) cell wall breakdown or deconstruction; 6) transcriptional or translational regulatory mechanisms and/or processes; and 7) environmental remediation and/or identification of environmental hazards. Projects should ideally be hypothesis-driven; projects that develop or rely primarily on high-throughput screening approaches **will not** be supported nor will projects that are primarily computational in nature.

All submitted proposals must clearly state the energy relevance of the proposed research: How will the knowledge gained from the proposed project better our understanding of the structure, function, and/or mechanistic aspects of energy-relevant biological redox reactions at the molecular level?

For DOE national laboratory applicants, the proposed research must fit within the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division funded programs at the laboratory of the applicant.

## (v) Nanoscale Science Research Centers Technical Contact: George Maracas, 301-903-1264, george.maracas@science.doe.gov

This research area supports work that advances the instruments, techniques, and capabilities of the existing BES Scientific User Facilities and/or contributes to capabilities of future facilities in this area. Research topics that develop and exploit the unique potential of co-located facilities within and across the BES scientific user facilities are encouraged. We do not intend to support proposals to establish new, unrelated types of facilities or to develop techniques that do not relate to the missions of the Nanoscale Science Research Centers.

Five Nanoscale Science Research Centers (NSRCs) support the synthesis, fabrication, characterization, and analysis of materials and structures at the nanoscale (https://science.osti.gov/bes/suf/user-facilities/nanoscale-science-research-centers/). These centers are Department of Energy's premier user facilities for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools for synthesis, fabrication, characterization, and new computing approaches and capabilities. As such, research is supported across the spectrum of scientific and engineering disciplines to understand and exploit phenomena exhibited by materials and structures at the nanoscale. Areas include energy conversion and storage, structured materials derived from or inspired by nature, directed assembly of nanostructures, hard and crystalline materials (including the structure of macromolecules), magnetic and soft materials (including polymers and ordered structures in fluids), quantum structures for future computers, and integration from nano to meso scales. Tools for probing nanomaterials and phenomena are increasingly multi-modal, to enable synthesis and characterization of electrical, optical, and/or magnetic properties simultaneously in real time with high resolution over a range of length scales. The ability to characterize functional nanoscale materials in situ, under operating conditions (operando), is also increasingly important, from, for example, battery electrode charging/discharging, to catalysts at high pressures and temperatures, to biologically-inspired, soft, and/or hybrid materials behavior in liquid environments.

New approaches to probe at the nanoscale, notably leveraging complementary modalities at the co-located x-ray, neutron and other facilities are of particular interest. Closely coupling theory and modeling with experiment to accelerate understanding nanoscale phenomena and their resulting innovations is encouraged.

The electron-beam micro-characterization area focuses on developing next generation electron-beam instrumentation and on conducting corresponding research. Electron scattering techniques have key attributes making them complementary to x-ray and neutron beam techniques. They

have unsurpassed spatial resolution and can simultaneously obtain structural, chemical, and other types of information from sub-nanometer regions. This enables the study of the fundamental mechanisms of catalysis, energy conversion, corrosion, charge transfer, magnetic behavior, and many other processes dynamically and at short time scales. Key is acquiring fundamental understanding to develop new and to improve existing materials and structures for energy and security applications.

Allowed topics for instrumentation and technique development efforts are limited to scanning, transmission, and scanning transmission electron microscopes, atom probes and related field ion instruments, surface characterization apparatus, and scanning probe microscopes. Instrumentation that advances multi-modal, in situ, and operando studies of materials and chemical processes is preferred.

#### See the Relevant BES Reports

- Challenges at the Frontier of Matter and Energy report: Transformative Opportunities for Discovery Science
- Future of Electron Scattering and Diffraction
- Quantum Materials for Energy Relevant Technology
- From Quanta to the Continuum: Opportunities for Mesoscale Science

For DOE national laboratory applicants, the proposed research must fit within the BES Scientific User Facilities (SUF) Division funded programs at the laboratory of the applicant.

### (w) Accelerator and Detector Research Technical Contact: Eliane Lessner, 301-903-9365, eliane.lessner@science.doe.gov

This program supports work that advances the instruments, techniques, and capabilities of the existing and/or future BES Scientific User Facilities. We do not intend to support proposals to establish new, unrelated types of facilities or to develop techniques that do not relate to the missions of the light sources and neutron scattering centers.

In the accelerator and detector research program, the objective is to improve the output and capabilities of light sources and neutron scattering facilities that are the most advanced of their kind in the world. Two major components are required for the advancement of light sources: the production of photon beams with increased average flux and brightness, and the detection tools capable of responding to the high photon-beam intensity. The first component requires higher repetition-rate photocathode guns and radiofrequency (RF) systems, and photon beams of enhanced temporal coherence, such as produced by improved seeding techniques or x-ray oscillators in the case of free electron lasers. Secondly, detectors require higher computational capabilities per pixel, improved readout rates, radiation hardness, and better energy and temporal resolutions. Additionally, research and development (R&D) is required to produce ultrafast beam instrumentation capable of measuring accurately femto- and atto-second bunch lengths. Higher neutron-flux capabilities at the Spallation Neutron Source will demand high-

intensity H currents, requiring tight control of beam losses, and detectors designed for advanced neutron imaging with very high throughput. Particle accelerators are complicated

interconnected machines and ideal for applications of artificial intelligence and machine learning algorithms.

An excellent reference for accelerator physics needs for light sources can be found in *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Volume 618, Issues 1-3.* A detailed discussion of opportunities and needs for future electron sources and neutron and photon detector development at the existing and future BES facilities can be found in the Future Electron Sources Workshop report and in the Neutron and Photon Detector Workshop.

This program strongly interacts with BES programmatic research that uses synchrotron radiation and neutron sources.

For DOE national laboratory applicants, the proposed research must fit within the BES Scientific User Facilities (SUF) Division funded programs at the laboratory of the applicant.

### (x) X-ray Instrumentation and Technique Development Technical Contact: Peter Lee, 301-903-8484, Peter.Lee@science.doe.gov

This program supports work that advances the instruments, techniques, and capabilities of the existing and/or contributes to capabilities of future BES supported light source facilities. This program **will not** support proposals to establish new, unrelated types of facilities or to develop techniques not applicable to BES x-ray light source facilities.

The unique properties of the light source facilities include, for storage-ring based synchrotron sources, a continuous spectrum, high flux, and brightness and, for the Linac Coherent Light Source (LCLS), ultra-short pulses, high peak power, and high coherence, making them indispensable tools for the exploration of matter. The wide range of emitted photon wavelengths provide incisive probes for advanced research. The three broad categories of experimental measurement techniques performed at the light sources - spectroscopy, scattering, and imaging - probe the fundamental parameters by which we perceive the physical world (energy, momentum, position, and time). By exploiting the short pulse lengths of these light sources, especially the LCLS, each technique can also be performed in a timing fashion.

In order to fully exploit the wide range of capabilities of these x-ray light source facilities, this program encourages the development of imaginative concepts for new types of x-ray instruments as well as innovative uses of existing instruments, especially in the area of novel techniques for new experimental capabilities, advanced x-ray optics<sup>1</sup> development, and novel approaches to data visualization and analysis.

For DOE national laboratory applicants, the proposed research must fit within the BES Scientific User Facilities (SUF) Division funded programs at the laboratory of the applicant.

<sup>&</sup>lt;sup>1</sup> Report for the X-ray Optics for BES Light Source Facilities Workshop

## (y) Neutron Scattering Instrumentation and Technique Development Technical Contact: Pappannan Thiyagarajan, 301-903-9706,\_ P.Thiyagarajan@science.doe.gov

This program supports research that advances instrumentation and technique capabilities of the existing and/or future BES supported neutron scattering facilities.

Thermal neutron scattering is a unique and effective tool for probing many aspects of the atomic structure and dynamics of materials. It is particularly well-suited for determining the atomic positions of both light and heavy atoms in solid or soft matter systems. In addition, the neutrons are scattered by magnetic moments in the material, thus providing information on the magnetic structure. The neutron energy is well-matched to that of elementary atomic and magnetic excitations (spin waves and phonons) in a material and, via inelastic neutron scattering, can provide data crucial for understanding dynamics in a variety of materials.

In order to fully exploit the wide range of capabilities of the BES neutron scattering facilities, this program will encourage the development of innovative concepts for new types of scattering instruments as well as innovative uses of existing instruments, advanced optics, sample environments, and novel approaches to data visualization and analysis.

Note: This program **will not** support proposals to establish new, unrelated types of facilities or to develop techniques not applicable to BES neutron scattering facilities.

For DOE national laboratory applicants, the proposed research must fit within the BES Scientific User Facilities (SUF) Division funded programs at the laboratory of the applicant.

### **Fusion Energy Sciences (FES)**

Program Website: <a href="https://www.energy.gov/science/fes/fusion-energy-sciences">https://science.osti.gov/fes</a> or <a href="https://science.osti.gov/fes">https://science.osti.gov/fes</a>

FES's mission is to expand the fundamental understanding of matter at very high temperatures and densities and to build the scientific foundation needed to develop a fusion energy source. This is accomplished through the study of plasma, the fourth state of matter, and how it interacts with its surroundings.

One of the next frontiers for the FES program is the study of the burning plasma state, in which the fusion process itself provides the dominant heat source for sustaining the plasma temperature (i.e., self-heating). Production of strongly self-heated fusion plasma will allow the discovery and study of a number of new scientific phenomena. To achieve these research goals, FES invests in flexible U.S. experimental facilities of various scales, international partnerships leveraging U.S. expertise, large-scale numerical simulations based on experimentally validated theoretical models, development of advanced fusion-relevant materials, and invention of new measurement techniques.

FES also supports discovery plasma science, which is focused on research at the frontiers of basic and low temperature plasma science and high-energy-density laboratory plasmas.

FES research is guided by the priorities in the "Fusion Energy Sciences, a Ten-Year Perspective (2015-2025)", the research opportunities identified in a series of recently held community engagement workshops (<a href="https://science.osti.gov/fes/Community-Resources/Workshop-Reports">https://science.osti.gov/fes/Community-Resources/Workshop-Reports</a>), and reports from the Fusion Energy Sciences Advisory Committee (FESAC) such as the recent 2018 report on "Transformative Enabling Capabilities for Efficient Advance Toward Fusion Energy".

To address the strategic goals and the high-priority plasma science issues identified by the workshops and other community input, the Fusion Energy Sciences program supports research on the specific topics below:

## (a) Advanced Tokamak Experimental Research Technical Contact: Matthew Lanctot, 301-903-1972, matthew.lanctot@science.doe.gov

The Advanced Tokamak Experimental Research program seeks to utilize tokamak research facilities with conventional aspect ratios to develop the physics knowledge needed to advance the FES energy mission. The effort involves the operation of a set of experimental tokamak facilities, ranging from smaller-scale university experiments to large national facilities. The extensive plasma diagnostic and technology systems operating on these facilities provide the experimental data required to study fusion science, basic plasma physics, and fusion energy production. Validation and verification of plasma theory and simulations are primary pursuits of the effort, leading ultimately to a predictive understanding of plasma properties, their dynamics, and interactions with surrounding materials. Operation of major facilities will be focused on science issues relevant to: (i) the design, operation, and research plan of the ITER program and other high-performance tokamaks; (ii) burning plasma physics, (iii) magnetic confinement, and (iv) other high priority plasma physics issues identified by the community in research needs workshops.

Proposals to this area must have a primary focus on experimental research, and address critical issues that may affect the advanced tokamak concept (e.g. plasma disruptions, impulsive heat loads, confinement and transport, and operational maintenance and complexity), or investigate topics common to all fusion power plant concepts (e.g. interactions between plasma and material surfaces). Innovative proposals of transformational approaches and technologies such as machine learning, advanced manufacturing, and engineered materials are strongly encouraged.

Scientists from the U.S. may also participate in leading experiments on fusion facilities abroad and conduct comparative studies to supplement the scientific understanding they can obtain from domestic facilities.

#### (b) Spherical Tokamak Research

Technical Contact: Josh King, 301-903-9707, josh.king@science.doe.gov

The Spherical Tokamak Research program seeks to utilize spherical tokamak research facilities with low aspect ratios to develop the physics knowledge needed to advance the FES energy mission. An improved understanding of the spherical tokamak magnetic confinement configuration is needed to establish the physics basis for next-step spherical tokamak facilities, broaden the scientific understanding of plasma confinement for ITER, and maintain U.S. world leadership in spherical tokamak research capabilities. Operation at higher magnetic field, reduced collisionality, and with controllable fully-non-inductive current-drive are necessary next steps for assessing the spherical tokamak as a potentially cost-effective path to fusion energy. The program includes both domestic and international facilities. However, the largest domestic facility (i.e., NSTX-U) is currently down for an extended outage and new experimental data will not be immediately available to support research efforts. The operation of smaller-scale domestic facilities will be focused on research relevant to community needs workshops and recommendations from the National Academy of Sciences Report on a Strategic Plan for U.S. Burning Plasma Research (https://www.nap.edu/catalog/25331/final-report-of-the-committee-on-a-strategic-plan-for-usburning-plasma-research).

A variety of important research topics that broadly support the foundational science for burning plasmas are uniquely possible through the study of spherical tokamak plasmas. Specifically, spherical tokamaks have demonstrated much higher normalized plasma pressure than conventional aspect ratio tokamaks. Also, spherical tokamaks provide access to unique plasma turbulence, energetic particle instabilities, and edge plasma regimes.

Proposals to this area must focus on experimental research and/or model validation pertaining to spherical tokamak plasmas. While proposals involving NSTX-U will not be considered in this solicitation, all topics examined must be relevant to the NSTX-U mission, such that the knowledge gained will be wholly transferable to the domestic program. Proposals addressing high impact studies involving low recycling walls, or non-inductive plasma startup are also encouraged.

## (c) Stellarator Research in Magnetic Fusion Energy Sciences Technical Contact: Samuel Barish, 301-903-2917, <a href="mailto:samuelbarish@science.doe.gov">sam.barish@science.doe.gov</a>

This program supports stellarator research on small-, medium-, and large-scale facilities, thereby enhancing the understanding of magnetically-confined plasmas. The stellarator offers attractive solutions to critical challenges to achieve fusion energy by providing a steady-state, disruption-free fusion reactor concept with minimal power requirements for plasma sustainment. Key issues include, but are not limited to, understanding and (if possible) reducing the level of turbulent transport, and improving the understanding of 3-D shaping in an integrated manner in plasmas with higher levels of performance.

Also of interest is stellarator research aimed at resolving magnetic-confinement fusion plasma science issues that will be faced in the next generation of machines, including ITER, and addressing new and unique scientific regimes that can be achieved with long-pulse superconducting international stellarators.

## (d) Magnetic Fusion Energy Science Theory and Simulation Technical Contact: John Mandrekas, 301-903-0552, <u>john.mandrekas@science.doe.gov</u>

The Magnetic Fusion Theory and Simulation program focuses on advancing the scientific understanding of the fundamental physical processes governing the behavior of magnetically confined plasmas and contributes to the FES goal of developing the predictive capability needed for a sustainable fusion energy source. Specific areas of interest include:

- Macroscopic stability and dynamics of fusion plasmas, with a strong focus on the prediction, avoidance, control, and mitigation of deleterious or performance-limiting instabilities, such as plasma disruptions and other transient or off-normal events;
- Understanding and control of the multiscale, collisional and turbulent physical mechanisms responsible for the loss of heat, momentum, and particles from the confining region;
- Interaction of externally launched radiofrequency waves designed to heat the plasma and drive current, with the background plasma and surrounding structures;
- Nonlinear interaction between background plasma, various instabilities, and energetic particle populations, including the alpha particles generated by the fusion reactions, and its impact on the confinement of these particles and the overall plasma performance; and,
- The effect of multiscale and multiphysics processes at the plasma boundary, including the pedestal and scrape-off layer regions, on the plasma performance and on the interaction and interface of the hot plasma boundary with the material walls.

The efforts supported by this program provide the foundations for integrated whole-device modeling simulations of fusion systems and range from analytical work to the development and application of advanced simulation codes capable of exploiting the potential of current and next-generation high performance computers. Proposals focused on transformative approaches such as fusion-relevant computing aspects of quantum information science (QIS) and artificial intelligence / machine learning are also encouraged.

#### (e) Measurement Innovation

Technical Contact: Curt Bolton, 301-903-4914, <a href="mailto:curt.bolton@science.doe.gov">curt.bolton@science.doe.gov</a>

This program element supports the development of innovative diagnostics to make detailed measurements of the behavior of plasmas. Advances are sought in diagnostic systems to achieve higher resolution or higher reliability, reduce complexity, and improve the ability to function in a burning plasma environment or provide access to previously unmeasured parameters. The proposed measurement innovations should seek to enable breakthroughs in scientific understanding, the linking of theory/computation with experiments, or active control of plasma properties to optimize device operation and plasma performance in a variety of device configurations.

## (f) High-Energy-Density Plasma Science

Technical Contact: Kramer Akli, 301-903-2943, kramer.akli@science.doe.gov

High-energy-density laboratory plasmas (HEDLP) physics is the study of ionized matter at extremely high density and temperature, specifically when matter is heated and compressed to a

point that the stored energy in the matter reaches approximately 100 billion Joules per cubic meter (the energy density of a hydrogen molecule). This corresponds to a pressure of approximately 1 million atmospheres or 1Mbar. Systems in which free electrons play a significant role in the dynamics and for which the underlying assumptions and methods of traditional ideal-plasma theory and standard condensed matter theory do not apply (e.g., Warm Dense Matter at temperatures of a few eV) can have pressures as low as 0.1 Mbar and are also considered high-energy-density (HED) plasmas. Discovery-driven scientific explorations of HED states of matter are being supported in this program. Topical examples being emphasized include (1) high-energy-density hydrodynamics, (2) radiation-dominated dynamics and material properties, (3) magnetized HED plasmas, (4) nonlinear optics of plasmas and laser-plasma interactions, (5) relativistic HED plasmas and intense beam physics, and (6) warm dense matter. Proposals focusing on developing high energy density materials relevant to QIS are strongly encouraged. Proposals focusing on inertial fusion energy sciences are also encouraged.

# (g) General Plasma Science Experiment and Theory Technical Contact: Nirmol Podder, 301-903-9536, <u>nirmol.podder@science.doe.gov</u>

The General Plasma Science (GPS) program is focused on research at the frontiers of basic and low temperature plasma science. Focus areas include: (1) dynamical processes in laboratory plasmas, magnetospheric, solar, and astrophysical plasmas, such as magnetic reconnection, particle energization, plasma dynamo, turbulence and transport, energetic particles, flows, collisional and collisionless shocks; (2) understanding the behavior of dusty plasmas, nonneutral, single-component matter and/or anti-matter plasmas, and ultra-cold neutral plasmas; and (3) understanding plasma processes and/or plasma chemistry in low temperature plasmas, interfacial plasma, plasma-surface interaction, interaction of plasma with materials and/or biomaterials, microplasmas, synthesis of nanomaterials, and microelectronics processing.

For more information, please see the 2016 report of the panel on frontiers of plasma science.

(h) Fusion Nuclear Science, Materials Research and Enabling R&D Programs for Fusion Technical Contact for Fusion Nuclear Science and Enabling R&D: Guinevere Shaw, 301-903-9113, <a href="mailto:guinevere.shaw@science.doe.gov">guinevere.shaw@science.doe.gov</a>

Technical Contact for Materials Research: Daniel Clark, 301-903-4883, <a href="mailto:dank@science.doe.gov">daniel.clark@science.doe.gov</a>

The Fusion Nuclear Science, Materials Research and Enabling R&D programs support the advancement of fusion science for both the near and long-term by carrying out research on topics that: (1) enable domestic experiments to achieve their full performance potential and scientific research goals; (2) permit scientific exploitation of the performance gains being sought from physics concept improvements; (3) allow the U.S. to enter into international collaborations, thus gaining access to experimental conditions not available domestically; (4) develop the technology and materials required for future fusion facilities, and (5) explore the science underlying these technological advances. Due to the harshness of the fusion environment and the significant challenge to overcome it, one of the four major goals of the FES program is to support the development of the scientific understanding required to design and deploy the materials and technology needed to support a sustained burning plasma environment. Given this goal, these

programs are interested in fundamental research focused on the following topical areas:

- Development of plasma-facing materials and components
- Development of advanced structural and functional materials
- Development of breeder blanket concepts
- Development of tritium fuel cycle technologies
- Development of superconducting magnet technologies

For more information, please see the 2012 Fusion Energy Sciences Advisory Committee (FESAC) report titled *Opportunities for Fusion Materials Science and Technology Research Now and During the ITER Era* (<a href="https://science.osti.gov/-/media/fes/pdf/workshop-reports/20120309/FESAC-Materials-Science-final-report.pdf">https://science.osti.gov/-/media/fes/pdf/workshop-reports/2015</a> workshop Report on Science Challenges and Research Opportunities in Plasma Materials Interactions <a href="https://science.osti.gov/-/media/fes/pdf/workshop-reports/2016/PMI\_fullreport\_21Aug2015.pdf">https://science.osti.gov/-/media/fes/pdf/workshop-reports/2016/PMI\_fullreport\_21Aug2015.pdf</a>, and most recently, the 2018 FESAC report on Transformative Enabling Capabilities for Efficient Advance Towards Fusion Energy:

https://science.osti.gov/-/media/fes/fesac/pdf/2018/TEC\_Report\_15Feb2018.pdf.

## **High Energy Physics (HEP)**

Program Website: <a href="https://science.osti.gov/hep/Research">https://science.osti.gov/hep/Research</a>

HEP's mission is to understand how the universe works at its most fundamental level by discovering the elementary constituents of matter and energy, probing the interactions between them, and exploring the basic nature of space and time.

The scientific objectives and priorities for the field recommended by the High Energy Physics Advisory Panel (HEPAP) are detailed in its recent long-range strategic Particle Physics Project Prioritization Plan (P5), available at: <a href="https://science.osti.gov/-/media/hep/hepap/pdf/May-2014/FINAL\_P5\_Report\_Interactive\_060214.pdf">https://science.osti.gov/-/media/hep/hepap/pdf/May-2014/FINAL\_P5\_Report\_Interactive\_060214.pdf</a>.

The HEP program focuses on three experimental scientific frontiers:

The Energy Frontier, where powerful accelerators are used to create new particles, reveal their interactions, and investigate fundamental forces;

The Intensity Frontier, where intense particle beams from accelerators and reactors are studied using highly sensitive detectors to investigate fundamental forces and particle interactions that occur rarely in nature, and to provide precision measurements of these phenomena; and

*The Cosmic Frontier*, where non-accelerator-based experiments observe the cosmos and detect cosmic particles, making measurements of natural phenomena that can provide information about the nature of dark matter, dark energy, and other fundamental properties of the universe that impact our understanding of matter and energy.

Together, these three interrelated and complementary discovery frontiers offer the opportunity to

answer some of the most basic questions about the world around us. Also integral to the mission of HEP are three cross-cutting research areas that enable new scientific opportunities by developing the necessary tools and methods for discoveries:

Theoretical High Energy Physics, where the vision and mathematical framework for understanding and extending the knowledge of particles, forces, space-time, and the universe are developed;

Accelerator Science and Technology Research and Development, where the technologies and basic science needed to design, build, and operate the accelerator facilities essential for making new discoveries are developed; and

*Detector Research and Development*, where the basic science and technologies needed to design and build the High Energy Physics detectors essential for making new discoveries are developed.

The three frontiers and the three cross-cutting research areas are collectively the six research subprograms supported by HEP. Proposed research should address specific research goals in one or more of the six research subprograms, and explain how the research or technology development supports the broad scientific objectives and mission of the HEP program. Principal investigators should submit their proposals to the HEP subprogram that they consider to be the best "fit" to the preponderance of their research effort. Proposals for support of generic detector R&D efforts should be directed to the Detector Research and Development research area described below. However, applicants proposing physics studies and pre-conceptual R&D efforts directed towards a specific experiment within an experimental frontier should submit their proposal to the relevant HEP scientific frontier research area. Experimental HEP proposals that include an R&D component within the overall research scope are specifically encouraged.

Proposals should not attempt to bolster the case for facilities not currently approved for funding or not expected to be available during the course of the work.

## (a) Experimental Research at the Energy Frontier in High Energy Physics Technical Contact: Abid Patwa, 301-903-0408, Abid.Patwa@science.doe.gov

This research area seeks to support studies of fundamental particles and their interactions using proton-proton collisions at the highest possible energies. This is accomplished through direct detection of new phenomena or through sensitive measurements that probe the Standard Model and new physics beyond it. In particular, proposals are sought for physics research utilizing data being collected at the Large Hadron Collider (LHC) by the ATLAS (A Toroidal LHC ApparatuS) and CMS (Compact Muon Solenoid) experiments. This research area also provides graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities. Proposals addressing physics studies and pre-conceptual R&D directed towards specific future Energy Frontier experiments are also accepted. Support for Heavy Ion Physics research is <u>not</u> provided under this research area.

## (b) Experimental Research at the Intensity Frontier in High Energy Physics

## Technical Contact: Glen Crawford, 301-903-9458, Glen.Crawford@science.doe.gov

This research area seeks to support precision studies that are sensitive to new physical processes at very high energy scales, beyond what can be directly probed with energy frontier colliders, and that often require intense particle beams. This research area includes studies of the fundamental properties of neutrinos produced by a variety of sources, including accelerators and nuclear reactors; studies of rare processes or precision measurements probing new physics processes as described above with either high intensity stored beams or beams incident on fixed targets; and studies of high intensity electron-positron collisions. In addition, this research area includes searches for proton decay. Graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities are also provided. Proposals addressing physics studies and pre-conceptual R&D directed towards specific future Intensity Frontier experiments are also accepted. Support for Large Hadron Collider beauty experiment (LHCb) research or studies of neutrinoless double beta decay is <u>not</u> provided under this research area.

## (c) Experimental Research at the Cosmic Frontier in High Energy Physics Technical Contact: Kathy Turner, 301-903-1759, Kathy. Turner@science.doe.gov

This research area seeks to support precision studies using observations of the cosmos and naturally occurring cosmic particles to understand the properties of fundamental particles and fields. Priorities include studies of the nature of dark energy, direct-detection searches for dark matter particles and research efforts towards planning the next generation of ground-based cosmic microwave background experiments to explore the inflationary epoch, the nature of dark energy and place constraints on neutrino masses. Measurements using high-energy cosmic rays, gamma rays and other phenomena are included, but at a lower priority. Proposals are sought for physics research efforts in support of current experiments in the Cosmic Frontier, as well as physics studies and pre-conceptual planning directed towards specific future experiments being considered for the program. This research area also provides graduate and postdoctoral research training for the next generation of scientists, and equipment and computational support for physics research activities.

Research efforts aimed at developing techniques or understanding experimental data within the context of theoretical models that are expressly for or as part of an experimental research collaboration are included in this area. General theoretical or computational research proposals not specifically carried out as part of a particular Cosmic Frontier experimental collaboration should be directed to the Theoretical Research subprogram. Studies of gravitational physics (other than for cosmic acceleration), classical astrophysics phenomena, fundamental symmetries, or planning for future cosmic ray or gamma ray experiments are <u>not</u> included in this research area.

## (d) Theoretical Research in High Energy Physics Technical Contact: William Kilgore, 301-903-3711, <u>William.Kilgore@science.doe.gov</u>

This research area seeks to support theoretical activities that provide the vision and the mathematical framework for understanding and extending our knowledge of particles, forces,

space-time, and the universe. Theoretical research is essential to support current experiments at the Energy, Intensity and Cosmic Frontiers, to identify new directions for High Energy Physics and to provide a deeper understanding of nature. Topics studied in theoretical high energy physics research include but are not limited to: phenomenological studies that seek to interpret experimental data, suggest searches for new physics at existing facilities and develop a research program for future facilities; precision calculations of experimental observables to test our current theories at the level of quantum corrections; the development of new models of physical interactions to describe unexplained phenomena or to unify seemingly distinct concepts; progress in quantum field theory, quantum gravity and other possible frameworks to develop a deeper understanding of nature; and the development of analytical and numerical computational techniques to facilitate studies in these areas. This research area also provides graduate and postdoctoral research training for the next generation of scientists and the computational resources needed for theoretical calculations. Activities that rely on experimental data, performed expressly for or with an experimental research collaboration, are <u>not</u> included in this research area.

## (e) Accelerator Science and Technology Research & Development in High Energy Physics Technical Contact: L.K. Len, 301-903-3233, <u>Lk.Len@science.doe.gov</u>

The accelerator technology R&D subprogram develops the next generation of particle accelerators and related technologies that are essential for discoveries in HEP. This research area supports world-leading research in the physics of particle beams and long-range, exploratory research aimed at developing new concepts. This research area also provides graduate and postdoctoral research training, equipment for experiments and related computational efforts.

Topics studied in the accelerator science and technology R&D subprogram include, but are not limited to: accelerator and beam physics, including analytic and computational techniques for modeling particle beams and simulation of accelerator systems; novel acceleration concepts; the science of high gradients in accelerating cavities and structures; high-power radio-frequency sources; high-brightness beam sources; and beam instrumentation. Also of interest are superconducting materials and conductor development; innovative magnet design and development of high-field superconducting magnets; as well as associated testing and cryogenic systems. R&D proposals, which are focused on accelerator applications outside of high-energy physics, are now coordinated through the Accelerator Stewardship program and are outside the scope of this particular FOA.

## (f) Detector Research and Development in High Energy Physics Technical Contact: Helmut Marsiske, 301-903-6989, <u>Helmut.Marsiske@science.doe.gov</u>

The detector R&D subprogram develops the next generation of instrumentation for HEP. It supports research leading to fundamental advances in the science of particle and radiation detection, and the development of new experimental techniques. This is typically long-term, "generic" R&D that is high-risk, but has the potential for wide applicability and/or high-impact.

Topics studied in the detector R&D research area include, but are not limited to: low-mass, high channel density charged particle tracking detectors; high resolution, fast-readout calorimeters and

particle identification detectors; techniques for improving the radiation tolerance and fast-timing capabilities of particle detectors; detectors for photons from ultraviolet to infrared wavelengths; detectors for cosmic microwave background radiation; detectors and experimental techniques for ultralow-background experiments; and advanced electronics and data acquisition systems. Support for graduate and postdoctoral research training, engineering and other technical efforts, and equipment and computational efforts required for experimental detector R&D and fabrication *is* included in this research area.

**Nuclear Physics (NP)** 

Program Website: <a href="https://www.energy.gov/science/np/nuclear-physics">https://www.energy.gov/science/np/nuclear-physics</a> or <a href="https://science.osti.gov/np">https://science.osti.gov/np</a>

NP's mission is to discover, explore, and understand all forms of nuclear matter. Although the fundamental particles that compose nuclear matter—quarks and gluons—are themselves relatively well understood, exactly how they interact and combine to form the different types of matter observed in the universe today and during its evolution remains largely unknown. It is one of the enduring mysteries of the universe: What, really, is matter? What are the units that matter is made of, and how do they fit together to give matter the properties we observe? To solve this mystery, the NP program supports experimental and theoretical research—along with the development and operation of particle accelerators and advanced technologies—to create, detect, and describe the different forms and complexities of nuclear matter that can exist, including those that are no longer commonly found in our universe.

In executing this mission, nuclear physics focuses on three broad yet tightly interrelated areas of inquiry: 1) Quantum Chromodynamics, 2) Nuclei and Nuclear Astrophysics, and 3) Fundamental Symmetries and Neutrinos. These areas are described in detail in *Reaching for the Horizon* <a href="https://science.osti.gov/np/nsac/">https://science.osti.gov/np/nsac/</a>, a long-range plan for nuclear science released in 2015 by the Nuclear Science Advisory Committee (NSAC). Specific questions within these areas are addressed by the research activities of subprograms supported by NP as described below. In addition, the DOE Isotope Program, managed by NP, produces and/or distributes stable and radioactive isotopes that are critical for the Nation and supports research into production techniques for such isotopes.

The NP program supports the development of the tools and capabilities that make fundamental research possible, including accelerator research and development for current and future nuclear physics facilities. It also supports applications of nuclear science and technology to help bridge the gap between basic nuclear physics research and applied science, and an initiative on advanced detector technology research and development. Research, development and fabrication of equipment directed toward research in any NP subprogram may be proposed, but proposals including extensive projects requiring detailed review of scope, budget and schedule beyond the procedures for this announcement will not be considered. Proposals should not attempt to bolster the case for facilities or major items of equipment not currently approved for funding or not expected to be available during the course of the work. Under this FOA, NP does not support investigations into the development of nuclear reactors for purposes outside the scope of the NP subprograms described below.

Proposals are solicited for research in any of the NP subprograms:

- (a) Medium Energy Nuclear Physics
- (b) Heavy Ion Nuclear Physics
- (c) Low Energy Nuclear Physics Nuclear Structure and Nuclear Astrophysics
- (d) Low Energy Nuclear Physics Fundamental Symmetries
- (e) Nuclear Theory
- (f) Nuclear Data and Nuclear Theory Computing
- (g) Accelerator Research and Development for Current and Future Nuclear Physics Facilities
- (h) Isotope Development and Production for Research and Applications
- (i) Quantum Information Science and Technology for Nuclear Physics

Artificial Intelligence and Machine Learning (AI/ML) have been identified as important crosscutting topics, with potential impact across all SC mission areas. NP also encourages submission of innovative research ideas to address AI/ML in any of its subprograms.

## (a) Medium Energy Nuclear Physics

Technical Contact: Gulshan Rai, 301-903-4702, gulshan.rai@science.doe.gov

The Medium Energy subprogram of NP focuses primarily on questions having to do with the first area of Nuclear Physics, Quantum Chromodynamics (QCD), especially regarding the spectrum of excited mesons and baryons, and the behavior of quarks inside the nucleons (neutrons and protons). Specific questions that are being addressed include: What does QCD predict for the properties of excited mesons and baryons? What governs the transition of quarks and gluons into pions and nucleons? What is the role of gluons and gluon self-interactions in nucleons and nuclei? What is the internal landscape of the nucleons? Experimental research is primarily carried out at the Thomas Jefferson National Accelerator Facility (TJNAF), the Relativistic Heavy Ion Collider (RHIC), the High Intensity Gamma-Ray Source (HIGS), and on a smaller scale at other international facilities. Two major goals of the research program at TJNAF are the discovery of "exotic mesons" which carry gluonic excitations, and the experimental study of the substructure of the nucleons using high-energy electron beams. At RHIC, the goals are to elucidate how much the spin of gluons contributes to the proton's spin and study the spin-flavor structure of sea quarks in polarized proton-proton collisions. This subprogram also supports investigations of some aspects of the second and third areas, Nuclei and Nuclear Astrophysics, and Fundamental Symmetries and Neutrinos.

## (b) Heavy Ion Nuclear Physics

Technical Contact: Richard Witt, 301-903-9731, richard.witt@science.doe.gov

The Heavy Ion Nuclear Physics subprogram focuses on studies of condensed quark-gluon matter at extremely high densities and temperatures characteristic of the infant universe. In the aftermath of collisions at RHIC and at the LHC, researchers have seen signs of the same quark-gluon plasma that is believed to have existed shortly after the Big Bang. The goal is to explore and understand unique manifestations of QCD in this many-body environment and their influence on the universe's evolution. Important avenues of investigation are directed at

resolving properties of the quark gluon plasma at different length scales and learning more about its physical characteristics including exploring the energy loss mechanism for quarks and gluons traversing the plasma, determining the speed of sound in the plasma, and locating the critical point for the transition between the plasma and normal matter. Experimental research is carried out primarily using the U.S. RHIC facility and the LHC at the European Organization for Nuclear Research (CERN).

## (c) Low Energy Nuclear Physics - Nuclear Structure and Nuclear Astrophysics Technical Contact: Sharon Stephenson, 301-903-1963, <a href="mailto:sharon.stephenson@science.doe.gov">sharon.stephenson@science.doe.gov</a>

The Low Energy Nuclear Structure and Nuclear Astrophysics subprogram is second area of identified by NSAC. Relevant questions include: What is the nature of the nucleonic matter? What is the origin of simple patterns in complex nuclei? What is the nature of neutron stars and dense nuclear matter? What is the origin of the elements in the cosmos? What are the nuclear reactions that drive stars and stellar explosions? This subprogram oversees developing a comprehensive description of nuclei across the entire nuclear chart. The scope of the subprogram also includes utilizing rare isotope beams to reveal new nuclear phenomena and structures beyond those derived from studies using stable ion beams. The Nuclear Astrophysics portion of the subprogram leads efforts into measuring the specific cross sections of nuclear reactions that power stars and spectacular stellar explosions. These nuclear reactions are responsible for the synthesis of the elements.

## (d) Low Energy Nuclear Physics – Fundamental Symmetries Technical Contact: Paul Sorensen, 301-903-1952, paul.sorensen@science.doe.gov

The Low Energy Fundamental Symmetries subprogram investigates aspects of the third area identified by NSAC - Fundamental Symmetries and Neutrinos. Questions addressed in this area include: What is the nature of the neutrinos, what are their masses, and how have they shaped the evolution of the universe? Why is there now more matter than antimatter in the universe? What are the unseen forces that were present at the dawn of the universe but disappeared from view as the universe evolved? The subprogram supports measurements addressing these questions via techniques and experiments that rely on capabilities unique to nuclear science. Examples include experiments to measure, or set a limit on the neutrino mass, and to determine if the neutrino is its own antiparticle. Experiments with cold neutrons also investigate the dominance of matter over antimatter in the universe, as well as other aspects of Fundamental Symmetries and Interactions.

## (e) Nuclear Theory

Technical Contact: George Fai, 301-903-8954, george.fai@science.doe.gov

The Nuclear Theory subprogram supports theoretical research at universities and DOE national laboratories with the goal of improving our fundamental understanding of nuclear physics, interpreting the results of experiments, and identifying and exploring important new areas of research. This subprogram addresses all of the field's scientific thrusts described in NSAC's long-range plan, as well as the specific questions listed for the experimental subprograms above. Theoretical research on QCD (the fundamental theory of quarks and gluons) addresses the

questions of how the properties of the nuclei, hadrons, and nuclear matter observed experimentally arise from this theory, how the phenomenon of quark confinement arises, and what phases of nuclear matter occur at high densities and temperatures. In Nuclei and Nuclear Astrophysics, theorists investigate a broad range of topics, including calculations of the properties of stable and unstable nuclear species, the limits of nuclear stability, the various types of nuclear transitions and decays, how nuclei arise from the forces between nucleons, and how nuclei are formed in cataclysmic astronomical events such as supernovae and neutron star mergers. In Fundamental Symmetries and Neutrinos, nucleons and nuclei are used to test the Standard Model, which describes the interactions of elementary particles at the most fundamental level. Theoretical research in this area is concerned with determining how various (beyond) Standard Model aspects can be explored through nuclear physics experiments, including the interactions of neutrinos, unusual nuclear transitions, rare decays, and high-precision studies of cold neutrons.

### (f) Nuclear Data and Nuclear Theory Computing Technical Contact: George Fai, 301-903-8954, <a href="mailto:george.fai@science.doe.gov">george.fai@science.doe.gov</a>

This subarea includes the National "Nuclear Data" effort, as well as several activities that facilitate the application of high performance computing to Nuclear Physics. The US Nuclear Data Program (USNDP) collects, evaluates, and disseminates nuclear physics data for basic and applied nuclear research, maintains open databases of scientific information gathered over the past 100+ years of research in nuclear physics, and addresses gaps in the data through targeted experimental studies and the use of theoretical models. "Nuclear Theory Computing" includes the NP component of the ASCR program Scientific Discovery through Advanced Computing (SciDAC), which promotes the use of supercomputers to solve computationally challenging problems of great current interest. Recent topics in computational nuclear physics investigated under SciDAC include the theory of quarks and gluons on a lattice (LQCD), studies of a wide range of applications of models of nuclei and nuclear matter, including nuclear astrophysics, and the development of theoretical techniques for incorporating LQCD results in traditional manybody nuclear physics calculations. Early Career proposals in this subarea might include for example highly computational research programs in nuclear theory, or experimental studies of relevance to the national nuclear data program.

## (g) Accelerator Research and Development for Current and Future Nuclear Physics Facilities

Technical Contact: Manouchehr Farkhondeh, 301-903-4398, manouchehr.farkhondeh@science.doe.gov

This NP program supports a broad range of activities aimed at research and development related to the science, engineering, and technology of heavy-ion, electron, and proton accelerators and associated systems. Areas of interest include the R&D technologies of the Brookhaven National Laboratory's (BNL) RHIC, with heavy ion and polarized proton beams; linear accelerators such as the Continuous Electron Beam Accelerator Facility (CEBAF) at TJNAF; and development of devices and/or methods that would be useful in the generation of intense rare isotope beams for the next generation rare isotope beam accelerator facility, the Facility for Rare Isotope Beams (FRIB) currently under construction at Michigan State University and in the generation of stable

isotope beams at the Argonne National Laboratory's Argonne Tandem Linac Accelerator System (ATLAS). Also of interest is R&D in accelerator science and technology in support of next generation Nuclear Physics accelerator facilities such as an electron-ion collider (EIC). The current status of accelerator R&D, the present design concepts and a list of R&D priorities for EIC are described in the February 2017 Report of the Community Review of EIC Accelerator R&D for the Office of Nuclear Physics. This report may be accessed at <a href="https://science.osti.gov/np/Community-Resources/Reports">https://science.osti.gov/np/Community-Resources/Reports</a>. NP interests also include R&D in emerging technologies in Machine Learning and Artificial Intelligence with focus on increasing cost savings and operational efficiencies of NP accelerator user facilities and their experimental programs.

# (h) Isotope Development and Production for Research and Applications Technical Contact: Ethan Balkin, 301-903-1861, <a href="mailto:ethan.balkin@science.doe.gov">ethan.balkin@science.doe.gov</a>

The mission of the Isotope Development and Production for Research and Applications subprogram (DOE Isotope Program) is to support isotope production and research into novel or improved technologies for production of isotopes to assure the availability of critical isotopes that are in short supply to address the needs of the Nation. The program provides facilities and capabilities for the production and/or distribution of research and commercial stable and radioactive isotopes. The scientific and technical staff associated with general isotope production and isotope production research are also supported. Isotopes are made available by using unique facilities stewarded by the Isotope Program at Brookhaven National Laboratory, Los Alamos National Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory. The Program also coordinates and supports isotope production at a suite of university, national laboratory, and other federal accelerator and reactor facilities throughout the Nation to promote a reliable domestic supply of isotopes. Topics of interest are focused on the development of advanced, cost-effective and efficient technologies for producing, processing, recycling and distributing isotopes in short supply. This includes technologies for production of radioisotopes using existing reactor and accelerator facilities and new technologies for enriching stable isotopes. Excluded from this call are proposals related to the production of molybdenum-99 (Mo-99), as this isotope is under the purview of the National Nuclear Security Administration (NNSA) Office of Materials Management and Minimization. A primary document currently guiding Isotope Program priorities is entitled "Meeting Isotope Needs and Capturing Opportunities for the Future: The 2015 Long Range Plan for the DOE-NP Isotope Program." This document may be accessed at https://science.osti.gov/-/media/np/nsac/pdf/docs/2015/2015 NSACI Report to NSAC Final.pdf. Additional information about the Isotope Program may be found at https://science.osti.gov/np/Research/IDPRA.

## (i) Quantum Information Science and Technology for Nuclear Physics Technical Contact: Gulshan Rai, 301-903-4702, <a href="mailto:gulshan.rai@science.doe.gov">gulshan.rai@science.doe.gov</a>

This interdisciplinary program supports research on Quantum Computing (QC) and Quantum Information Science and Technology (QIST) with a clear line of sight to enable discoveries to explore and understand all forms of nuclear matter. The program emphasizes a science-first approach and supports efforts with the potential to have a transformative impact on the NP

mission area and/or to advance QIS development uniquely enabled by NP-supported science, technologies, and laboratory infrastructure. Likewise, QIS technologies offer the ability to discover and probe the fundamental structure and behavior of Nature with unprecedented sensitivity and accuracy. While recognizing the interdisciplinary and crosscutting nature of QIS, this program focuses on areas consistent with the unique role and relevance of NP in this rapidly developing field. Topics include quantum computation, quantum simulations and simulators, quantum sensing, nuclear physics detectors, nuclear many-body problem, 'squeezed' quantum states, entanglement at collider energies, and lattice gauge theories as well as novel areas of basic research.

#### **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.

#### Section II – AWARD INFORMATION

#### A. TYPE OF AWARD INSTRUMENT

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

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

#### B. ESTIMATED FUNDING

It is anticipated that approximately \$18,000,000 per year will be available under this DOE National Laboratory Announcement, contingent on satisfactory peer review and the availability of appropriated funds. Applicants should request project support for five years. Following the first year award, out-year support will be contingent on the availability of appropriated funds, progress of the research, and programmatic needs. Awards are expected to begin in fiscal year 2020.

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

#### C. MAXIMUM AND MINIMUM AWARD SIZE

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

#### Ceiling

There is no ceiling for these awards; the request should reflect the research to be performed and must support at least 50% of the PI's salary. However, historically, awards have typically been \$2,500,000 over five years, or an average of \$500,000 per year.

#### Floor

The proposal must request 50% of the PI's salary plus the additional funding needed to support the proposed research. The minimum award is approximately \$2,500,000 over 5 years

#### D. EXPECTED NUMBER OF AWARDS

The exact number of awards will depend on the number of meritorious proposals and the availability of appropriated funds. Historically, there have been an average of approximately 22 national laboratory awards each year; for this announcement, up to 35 national laboratory awards are anticipated.

#### E. ANTICIPATED AWARD SIZE

(See C. Minimum and Maximum Award Size above.) The size of a national laboratory award is commensurate with the requirement to charge twelve-month annual salaries (compared with professors, who are partially paid by academic institutions). A minimum of 50% and up to 100% of the Principal Investigator's salary should be proposed.

#### F. PERIOD OF PERFORMANCE

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

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

#### G. TYPE OF PROPOSAL

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

#### Section III – ELIGIBILITY INFORMATION

#### A. ELIGIBLE APPLICANTS AND TOPICS

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

Proposals must be submitted through a DOE national laboratory. A companion Funding Opportunity Announcement (DE-FOA-0002173) describes the Early Career Research Program opportunity for tenure-track untenured assistant professors and tenure-track untenured associate professors at U.S. academic institutions. An employee with a joint appointment between a university and a DOE national laboratory must apply through the institution that pays his or her salary and provides his or her benefits; the eligibility criteria (see C. Eligible Individuals and D. Limitations on Submissions) below must also be met.

The cover page for each pre-proposal and full proposal must be signed by the national laboratory director confirming that the proposed research idea fits within the scope of Office-of-Science-funded programs at the national laboratory. Proposing research that falls within this category ensures that investigators have the opportunity to belong to or join, at the laboratory's discretion, funded research groups. Investigators funded under this program must charge at least 50 % of their time to the award, allowing time to develop or maintain funded collaborations within the lab over the course of the award. Making sure that investigators have potential connections with Office-of-Science funded programs encourages the laboratory to actively plan to address funding transition issues that may arise when an award ends.

Proposals from DOE National Laboratories should not (a) attempt to revive previously terminated research areas within the laboratory or (b) topically isolate investigators.

Eligibility exemptions will not be granted.

#### **B. COST SHARING**

Cost sharing is not required.

#### C. ELIGIBLE INDIVIDUALS

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

The Principal Investigator must be a full-time, permanent, non-postdoctoral national laboratory employee as of the deadline for the proposal. No more than ten (10) years can have passed between the year the Principal Investigator's Ph.D. was awarded and 2019. For the present competition, those who received doctorates no earlier than 2009 are eligible. If a Principal

Investigator has multiple doctorates, the discipline of the one they have earned within the 10-year eligibility window should be relevant to the proposed research.

Extensions to eligibility will be considered for individuals who have had a major life event requiring an extended absence (3 months or longer) from the workplace, including but not limited to active military service, an absence due to personal disability, or an absence covered by the Family Medical Leave Act. A letter signed by the laboratory's human resources lead (or the laboratory's organizational equivalent) stating that the applicant had an approved absence from their national laboratory position, and the length of this absence, must be included with the preproposal. The request for an eligibility extension will be evaluated as part of the pre-proposal assessment.

There is NOT a U.S. citizenship requirement for the Principal Investigator or any project participants.

There can be no co-Principal Investigators.

Principal Investigators who have received awards previously under the SC Early Career Research Program are not eligible. Principal Investigators of early career awards funded by other agencies or entities are eligible, but the proposed research must have a scope different from that already funded by the other organization.

Eligibility exemptions will not be granted.

#### D. LIMITATIONS ON SUBMISSIONS

While there is no limit on the number of preproposals from a DOE national laboratory in a given year, each laboratory is responsible for ensuring that the research ideas submitted in its preproposals fit within the scope of Office-of-Science-funded programs at the national laboratory.

Each Principal Investigator may only submit one Office of Science Early Career Research Program proposal per annual competition. Additionally, a Principal Investigator may not participate in more than three Office of Science Early Career Research Program competitions.

Participation in the competition is defined as submission of a full proposal that completed the review/decision process. In rare cases, it is necessary to withdraw a proposal; a proposal withdrawn prior to it being officially declined will not count as a submission. Likewise, a proposal declined without merit review by the DOE SC will not count as a submission.

The act of submitting a proposal implies that the submitting institution has checked, confirmed, and certifies that the Principal Investigator is eligible. No additional certifying documentation is required.

Letters of recommendation are not allowed. Proposals that include recommendation letters will be subject to elimination from consideration during DOE's initial review.

#### Section IV – PROPOSAL AND SUBMISSION INFORMATION

### A. ADDRESS TO REQUEST PROPOSAL PACKAGE

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

Proposals submitted outside of PAMS will not be accepted.

#### B. LETTER OF INTENT AND PRE-PROPOSAL

#### 1. Letter of Intent

Not applicable.

#### 2. Pre-proposal

PRE-PROPOSAL DUE DATE

### January 7, 2020 at 5:00 PM Eastern Time

ENCOURAGE/DISCOURAGE DATE

#### **January 30, 2020**

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

Pre-proposals will be reviewed as outlined below. DOE will send a response by email to each applicant encouraging or discouraging the submission of a proposal by the date listed above Applicants who have not received a response regarding the status of their pre-proposal by this date are responsible for contacting the program to confirm this status. **Only those applicants that receive notification from DOE encouraging a proposal may submit proposals.** No other proposals will be considered.

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

Title of Pre-proposal Principal Investigator Name, Job Title Institution PI Phone Number, PI Email Address

Year Doctorate Awarded: XXXX Eligibility Extension Requested: (Yes/No – see below\*)

Number of Times Previously Applied†:

Topic Area\*\*:

Lab Announcement Number: LAB 20-2173 Signature of the Laboratory Director:\*\*\* Typed Name of the Laboratory Director

\*Extensions to eligibility will be considered for individuals who have had a major life event requiring an extended absence (3 months or longer) from the workplace, including but not limited to active military service, an absence due to personal disability, or an absence covered by the Family Medical Leave Act. A letter signed by the laboratory's human resources lead (or the laboratory's organizational equivalent) stating that the applicant had an approved absence from their national laboratory position, and the length of this absence, must be included with the preproposal. The request for an eligibility extension will be evaluated as part of the pre-proposal assessment.

† Indicate how many times the PI has previously submitted a full proposal in the SC Early Career Research Program. The program has been offered in ten previous years, FY 2010 – FY 2019. Participation in the competition is defined as submission of a full, formal proposal that was not withdrawn prior to official declination of the proposal. A PI who has participated in three past SC Early Career Research Program competitions is not eligible.

\*\*The topic area descriptions can be found in Part I, Supplementary Information, of this FOA. For example, the topic area might be *Synthesis and Processing Science* or *Magnetic Fusion Energy Science Theory and Simulation*. Please select from the list in Part I.

\*\*\* The signature of the Laboratory Director confirms that the proposed research idea fits within the scope of Office-of-Science-funded programs at the national laboratory.

This information must be followed by a clear and concise description of the objectives and technical approach of the proposed research. The pre-proposal may not exceed three pages, with a minimum text font size of 11 point and margins no smaller than one inch on all sides. Figures and references, if included, must fit within the three-page limit. If the pre-proposal narrative exceeds three-pages, only the first three pages will be evaluated in the review of the document.

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

Collaborators and Co-editors: List, in alphabetical order, all persons, including their current

organizational affiliations, who are, or who have been, collaborators or co-authors with the Principal Investigator on a research project, book or book article, report, abstract, or paper during the 48 months preceding the closing date of this announcement. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the Principal Investigator interacted on a regular basis while the research was being done. Also, list any individuals who are currently or have been in the past co-editors with the Principal Investigator on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the closing date of this announcement. If there are no collaborators or co-editors to report, state "None."

Since SC will never use individuals from your institution as reviewers, you may omit them from the pre-proposal list to save space. Listing collaborators on your pre-proposal is to help us identify reviewers; the content of the list does not affect the decision to encourage or discourage submission of a formal proposal – however, failure to include the list will result in the pre-proposal being discouraged from submitting a full proposal.

Graduate and Postdoctoral Advisors and Advisees: List the names of the Principal Investigator's own graduate advisor(s) and principal postdoctoral sponsor(s) and their current organizational affiliations. Also list the names of the Principal Investigator's graduate students and postdoctoral associates during the past five years and their current organizational affiliations.

#### PRE-PROPOSAL REVIEW

All complete pre-proposals will be reviewed to determine their responsiveness to the objectives of the funding announcement. In addition, if a scientific topic receives a large number of pre-proposals, federal Program Managers may evaluate the pre-proposals to determine their competitiveness within the scientific topic, based on the following criteria:

- 1. Responsiveness to the objectives of the funding announcement.
- 2. Scientific and technical merit.
- 3. Appropriateness of the proposed research approaches.
- 4. Likelihood of scientific impact.
- 5. Ensuring a diverse pool of applicants.

Pre-proposal comparative reviews will compare pre-proposals within a topical field with priority given to scientifically innovative and forward-looking basic research with the highest likelihood of success as a full proposal. These reviews will be conducted by no less than three federal program managers chosen for their topical knowledge and diversity of perspective. The results of the review will be documented.

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

The ratio of encourage/discourage results will differ between topical subjects. DOE is committed to ensuring that a sufficient number of applicants will be encouraged to submit proposals to foster a competitive merit review of full proposals. The intent in discouraging submission of certain pre-proposals is to benefit applicants who otherwise would have prepared and submitted

proposals with a negligible likelihood of success; noting that the failed proposal would also then "count" towards the PI's three allowed proposals to the SC Early Career Research program.

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

#### PRE-PROPOSAL SUBMISSION

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

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

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

#### **Submit Your Pre-Proposal:**

- Create your pre-proposal (called a preproposal in PAMS) outside the system and save it as a file with extension .docx, .doc, or .pdf. Make a note of the location of the file on your computer so you can browse for it later from within PAMS.
- Log into PAMS and click the Proposals tab. Click the "View / View / Respond to DOE National Laboratory Announcements" link and find the current announcement in the list. Click the "Actions/Views" link in the Options column next to this announcement to obtain a dropdown menu. Select "Submit Preproposal" from the dropdown.
- On the Submit Preproposal page, select the institution from which you are submitting this preproposal from the Institution dropdown. If you are associated with only one institution in the system, there will only be one institution in the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per preproposal; to do so, click the "Select PI" button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the "Actions" link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose "Select PI."
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the "Invite PI" link at the top left of the "Select PI" screen. You can enter an optional personal message to the PI in the

"Comments" box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the preproposal. Save the preproposal for later work by clicking the "Save" button at the bottom of the screen. It will be stored in "My Preproposals" for later editing.

- Enter a title for your preproposal.
- Select the appropriate technical contact from the Program Manager dropdown.
- To upload the preproposal file into PAMS, click the "Attach File" button at the far right side of the screen. Click the "Browse" (or "Choose File" depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the "Upload" button to upload the file.
- At the bottom of the screen, click the "Submit to DOE" button to save and submit the preproposal to DOE.
- Upon submission, the PI will receive an email from the PAMS system <<u>PAMS.Autoreply@science.doe.gov</u>> 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 <a href="https://pampspublic.science.energy.gov">https://pampspublic.science.energy.gov</a> will permit you to edit a previously submitted preproposal in the time between your submission and the deadline. If you choose to edit, doing so will remove your previously submitted version from consideration. If you are still editing at the time of the deadline, you will not have a valid submission. Please pay attention to the deadline.

For help with PAMS, click the "External User Guide" link on the PAMS website, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, email: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submission and inquiries about this Program Announcement should reference LAB 20-2173.

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

#### C. CONTENT AND PROPOSAL FORMS

PROPOSAL DUE DATE

### March 30, 2020 at 5:00 PM Eastern Time.

Files that are attached to the forms must be PDF files unless otherwise specified in this announcement. Attached PDF files must be plain files consisting of text, numbers, and images without editable fields, signatures, passwords, redactions, or other advanced features available in some PDF-compatible software. Do not attach PDF portfolios.

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

#### RESUBMISSION OF PROPOSALS

Proposals submitted under this Announcement may be withdrawn from consideration by using SC's PAMS website at <a href="https://pamspublic.science.energy.gov">https://pamspublic.science.energy.gov</a>. Proposals may be withdrawn at any time between when the Laboratory submits the proposal and when DOE makes the proposal available to merit reviewers. Such withdrawals take effect immediately and cannot be reversed.

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

SC will usually consider the last submission, according to its timestamp, to be the intended version. Please consult with your program manager to resolve any confusion about which version of a proposal should be considered.

#### IMPROPER CONTENTS OF PROPOSALS

Proposals submitted under this Announcement will be stored in controlled-access systems, but they may be made publicly available if an award is made, and they will be made available to merit reviewers. As such, it is critical that Laboratories follow these guidelines:

- Do not include information subject to any legal restriction on its open distribution, whether classified, export control, or unclassified controlled nuclear information.
- Do not include sensitive and protected personally identifiable information, including social security numbers, birthdates, citizenship, marital status, or home addresses. Pay particular attention to the content of biographical sketches and curriculum vitae.
- Do not include letters of support from Federal officials.
- Do not include letters of support on Federal letterhead. Letters that are not letters of support (such as letters confirming access to sites, facilities, equipment, or data; or letters from cognizant contracting officers) may be on Federal letterhead.
- Clearly mark all proprietary or trade-secret information.

#### LETTERS

Letters of recommendation are not allowed. A department chair letter is not required and should not be included. Proposals that include recommendation letters or department chair letters will be subject to elimination from consideration during DOE's initial review.

Optional letters of collaboration for unfunded or funded collaborations may be placed in Appendix 7 (Other Attachments). Letters of collaboration should state the intention to participate, but they must not be written as recommendation or endorsement letters, which are not allowed.

Each optional letter of collaboration may contain two and only two sentences and must use the following format:

Dear < Principal Investigator Name>:

If your proposal entitled, "<Proposal Name>," is selected for funding under the DOE SC Early Career Research Program, 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>

#### 1. Summary of Proposal Contents and Information about PAMS

Each DOE National Laboratory proposal will contain the following sections:

- Budget, entered into PAMS as structured data using the PAMS budget form
- Abstract (one page), entered into PAMS as a separate pdf
- Budget justification, entered into PAMS as a separate pdf
- Proposal, combined into a single pdf containing the following information:
  - o Proposal Cover Page
  - o 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)
  - o Appendix 1: Biographical Sketch(es)
  - o Appendix 2: Current and Pending Support
  - o Appendix 3: Bibliography and References Cited
  - o Appendix 4: Facilities and Other Resources
  - o Appendix 5: Equipment
  - o Appendix 6: Data Management Plan
  - o Appendix 7: Other Attachments (optional)

#### SUBMISSION INSTRUCTIONS

Completed proposals must be submitted into the DOE SC Portfolio Analysis and Management System (PAMS). For help with PAMS, click the "External User Guide" link on the PAMS website, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free number) or (301) 903-9610, Email: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submissions and inquiries about this Program Announcement should reference LAB 20-2173. Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than the date shown in Section IV, Section C, Proposal Due Date.

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

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

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

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

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

For help with PAMS, click the "External User Guide" link on the PAMS website, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free number) or (301) 903-9610, Email: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submissions and inquiries about this Program Announcement should reference LAB 20-2173.

#### 2. Detailed Contents of the Proposal

BUDGET AND BUDGET EXPLANATION

The budget must be submitted into PAMS using the PAMS budget form. Research proposed under this announcement should have five annual budget periods. Please enter the following budget period start and end dates into PAMS for proposals submitted to this announcement:

- Budget Period 1: 09/01/2020 08/31/2021
- Budget Period 2: 09/01/2021 08/31/2022
- Budget Period 3: 09/01/2022 08/31/2023
- Budget Period 4: 09/01/2023 08/31/2024
- Budget Period 5: 09/01/2024 08/31/2025

PAMS will calculate the cumulative budget totals for you.

A written justification of each budget item is to follow the budget pages. The budget justification must be placed in a separate, single pdf document and attached on the appropriate screen in

PAMS. Further instructions regarding the budget and justification are given below and in the PAMS software.

PROJECT SUMMARY/ABSTRACT (NO MORE THAN ONE PAGE)

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

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

DOE COVER PAGE (Part of Project Narrative)

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

- The project title:
- Applicant/Institution:
- Street Address/City/State/Zip:
- PI name:
- Position title for the PI
- PI telephone number, email
- DOE National Laboratory Announcement Number: LAB 20-2173
- DOE/SC Program Office: (ASCR, BER, BES, FES, HEP, or NP)
- Topic Area\*:
- Topic Area Program Manager:
- Year Doctorate Awarded:
- Eligibility Extension Included in Approved Pre-proposal: (Yes or No)
- Number of Times Previously Applied†:
- PAMS Preproposal (Preproposal) Number§:
- PECASE Eligible\*\*: (Yes or No)?
- Proposal Contains Biosketch in Appendix 1 (Yes or No)?
- Proposal Contains Data Management Plan in Appendix 6§: (Yes or No)?
- Signature of Laboratory Director\*\*\*:
- Printed name of Laboratory Director:

<sup>\*</sup> The topic area can be found in Section I, Supplementary Information, of this Program Announcement. For example, the topic area might be *Synthesis and Processing Science* or

Magnetic Fusion Energy Science Theory and Simulation. Please select from the list in Section I.

† Indicate how many times the PI has previously submitted a full proposal in the SC Early Career Research Program. The program has been offered in ten previous years, FY 2010 - FY 2019. Participation in the competition is defined as submission of a full, formal proposal that was not withdrawn from consideration prior to official declination of the proposal. A PI who has participated in three past SC Early Career Research Program competitions is not eligible.

\*\* The White House Office of Science and Technology Policy may ask federal agencies each year to nominate candidates for the Presidential Early Career Awards for Scientists and Engineers (PECASE). Investigators from the top proposals in the SC Early Career Research Award competition may be nominated for PECASE if they are eligible. A PI is PECASE-eligible if he or she is, as of the closing date of this National Laboratory Announcement, a U.S. citizen, U.S. national or permanent resident and if she or he has not received a PECASE previously through any agency. PECASE eligibility is not required for an award under the current National Laboratory Announcement.

§ SC will decline without review any proposal without an encouraged pre-proposal or without a data management plan.

\*\*\* The signature of the Laboratory Director confirms that the proposed research idea fits within the scope of Office-of-Science-funded programs at the national laboratory.

PROJECT NARRATIVE (NO MORE THAN 15 PAGES LONG)

The project narrative **must not exceed 15 pages** of technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right). The font must not be smaller than 11 point. Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph. This page limit does not apply to the Cover Page, Budget Page(s), Budget Justification, Table of Contents, biographical material, publications and references, and appendices, each of which may have its own page limit.

The Project Narrative comprises the research plan for the project. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The narrative should provide a clear, concise statement of the specific objectives/aims of the proposed project. 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.

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. Part D for instructions on how to mark proprietary proposal information. To attach a Project Narrative, click "Add Attachment."

#### APPENDIX 1: BIOGRAPHICAL SKETCH

- Provide the biographical sketch information as an appendix to your project narrative.
- Do not attach a separate file.
- The biographical sketch appendix will not count in the project narrative page limitation.
- The biographical information (curriculum vitae) must not exceed three pages when printed on 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include:

A biographical sketch for the PI must be included as an appendix to the technical narrative. Failure to include this information will result in the proposal being declined without review. As part of the sketch, provide information that can be used by reviewers to evaluate the PI's potential for leadership within the scientific community. The biographical information (curriculum vitae) must include:

- **Education and Training**: Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.
- **Research and Professional Experience**: Beginning with the current position list, in chronological order, professional/academic positions with a brief description.
- **Publications**: Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications. An abbreviated style such as the Physical Review Letters (PRL) convention for citations (list only the first author) may be used for publications with more than 10 authors.
- Synergistic Activities: List professional and scholarly activities related to the effort proposed. Some examples might be invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society membership and/or activities, special international or industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences.

In addition, the biographical sketch must include information to permit DOE to identify individuals who are conflicted with or potentially biased (favorably or unfavorably) against the investigator. Include a section entitled "Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers" that will not count in a page limit. Provide the following information in this section:

• Collaborators and Co-editors: List in alphabetical order all persons, including their current organizational affiliation, who are, or who have been, collaborators or co-authors with you on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of this proposal. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the PI interacted on a regular basis while the research was being done. Also, list any individuals who are currently, or have been, co-editors with you on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of

- this proposal. If there are no collaborators or co-editors to report, state "None."
- **Graduate and Postdoctoral Advisors and Advisees**: List the names and current organizational affiliations of your graduate advisor(s) and principal postdoctoral sponsor(s). Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates.

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

#### APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support (both Federal and non-Federal) for the PI for ongoing projects and pending proposals. List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid. Do not list start-up funds provided to the PI by the employing academic institution. If the PI has submitted a similar research proposal to an early career program at another agency or foundation, this proposal must be included as a pending proposal, with the required explanation of the similarities and/or differences with the current Early Career Research Program proposal.

For every activity, list the following items:

- The sponsor of the activity or the source of funding
- The award or other identifying number
- The title of the award or activity
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The award period (start date end date).
- The person-months of effort per year being dedicated to the award or activity
- Briefly describe the research being performed (or planned for pending proposals) and explicitly identify any similarities, differences, overlaps, or synergies with the proposed research.

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

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

#### APPENDIX 3: BIBLIOGRAPHY & REFERENCES CITED

Provide a bibliography of any references cited in the Project Narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. For research areas where there are routinely more than ten coauthors of archival publications, you may use an abbreviated style such as the Physical Review Letters (PRL) convention for citations (listing only the first author). 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 available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. For proposed investigations requiring access to experimental user facilities maintained by institutions other than the applicant, please provide a document from the facility manager confirming that the researchers will have access to the facility. Please provide the Facility and Other Resource information as an appendix to your project narrative.

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

# APPENDIX 5: EQUIPMENT

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

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

### APPENDIX 6: DATA MANAGEMENT PLAN

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

- 1. DMPs should describe whether and how data generated in the course of the proposed research will be shared and preserved. If the plan is not to share and/or preserve certain data, then the plan must explain the basis of the decision (for example, cost/benefit considerations, other parameters of feasibility, scientific appropriateness, or limitations discussed in #4). At a minimum, DMPs must describe how data sharing and preservation will enable validation of results, or how results could be validated if data are not shared or preserved.
  - 2. DMPs should provide a plan for making all research data displayed in publications resulting from the proposed research digitally accessible to the public at the time of publication. This includes data that are displayed in charts, figures, images, etc. In addition, the underlying digital research data used to generate the displayed data should be made as accessible as possible to the public in accordance with the principles stated in the Office of Science Statement on Digital Data Management (<a href="https://science.osti.gov/Funding-Opportunities/Digital-Data-Management">https://science.osti.gov/Funding-Opportunities/Digital-Data-Management</a>). This requirement could be met by including the data as supplementary information to the

published article, or through other means. The published article should indicate how these data can be accessed.

- 3. DMPs should consult and reference available information about data management resources to be used in the course of the proposed research. In particular, DMPs that explicitly or implicitly commit data management resources at a facility beyond what is conventionally made available to approved users should be accompanied by written approval from that facility. In determining the resources available for data management at SC User Facilities, researchers should consult the published description of data management resources and practices at that facility and reference it in the DMP. Information about other SC facilities can be found in the additional guidance from the sponsoring program.
- 4. DMPs must protect confidentiality, personal privacy, Personally Identifiable Information, and U.S. national, homeland, and economic security; recognize proprietary interests, business confidential information, and intellectual property rights; avoid significant negative impact on innovation, and U.S. competitiveness; and otherwise be consistent with all applicable laws, regulations, and DOE orders and policies. There is no requirement to share proprietary data.
- 5. Proposals must meet the published additional requirements of the program office to which the proposal is submitted, as identified on the DOE Cover Page of the proposal. Program office requirements will be considered during merit review and award selection. Advanced Scientific Computing Research (ASCR) and Biological and Environmental Research (BER) have published additional requirements, available through <a href="https://science.osti.gov/Funding-Opportunities/Digital-Data-Management">https://science.osti.gov/Funding-Opportunities/Digital-Data-Management</a>. Proposals will not be transferred between program offices.

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: <a href="https://science.osti.gov/Funding-Opportunities/Digital-Data-Management">https://science.osti.gov/Funding-Opportunities/Digital-Data-Management</a>.

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

#### **APPENDIX 7: OTHER ATTACHMENT**

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, and reviewers may not have time to read extensive appendix materials with the same care they would use with the proposal proper. Do not include scientific publications.

Although the preference of this program is to support PI-led efforts without paid
collaborators, if a funded or unfunded collaboration is proposed, an optional letter of
collaboration may be included in this appendix. Letters of collaboration should state the
intent to participate and nothing else. They should not be written as recommendation or
endorsement letters, which are not allowed. Each optional letter of collaboration may
contain two and only two sentences and must use the format shown in Section IV D.

Content and Proposal Forms, under the Letters subheading. Do not attach a separate file.

• This appendix will not count in the project narrative page limitation.

# Follow the above instructions to include the information as appendices to the project narrative file.

- These appendices will not count toward the project narrative's page limitation.
- Do not attach any files to fields 9, 10, 11, or 12.

# 3. Detailed Instructions for the Budget

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

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

# Section A. Senior/Key Person (Required)

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

# **Section B. Other Personnel**

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

# **Section C. Equipment Description**

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

#### Section D. Travel

In the budget justification, list each trip's destination, dates, estimated costs including

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

# **Section E. Participant/Trainee Support Costs:**

If applicable, submit training support costs. Educational projects that intend to support trainees (precollege, college, graduate and post graduate) must list each trainee cost that includes stipend levels and amounts, cost of tuition for each trainee, cost of any travel (provide the same information as needed under the regular travel category), and costs for any related training expenses. Participant costs are those costs associated with conferences, workshops, symposia or institutes and breakout items should indicate the number of participants, cost for each participant, purpose of the conference, dates and places of meetings and any related administrative expenses. In the budget justification, indicate whether trainee cost estimates are based upon past experience of support of similar number of trainees on similar projects; past experience of support of similar number of participants attending similar conferences/workshops/symposia; or something else (describe).

## **Section F. Other Direct Costs:**

Enter Other Direct Costs information for each item listed.

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

- institution; or something else (describe).
- Subawards/Consortium/Contractual Costs: Enter total costs for all subawards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details.
- Equipment or Facility Rental/User Fees: Enter total funds requested for Equipment or Facility Rental/User Fees. In the budget justification, identify each rental/user fee and justify. In the budget justification, indicate whether cost estimates are based upon past experience with similar or like items; vendor quotes of similar items; or something else (describe).
- Alterations and Renovations: Enter total funds requested for Alterations and Renovations.
- In the budget justification, itemize by category and justify the costs of alterations and renovations, including repairs, painting, removal or installation of partitions, shielding, or air conditioning. Where applicable, provide the square footage and costs.
- Other: Add text to describe any other Direct Costs not requested above. Enter costs associated with "Other" item(s). Use the budget justification to further itemize and justify.

#### **Section G. Direct Costs**

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

## **Section H. Other Indirect Costs**

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

#### **Section I. Total Direct and Indirect Costs**

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

## D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS

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

## E. SUBMISSION DATES AND TIMES

# 1. Letter of Intent Due Date

A letter of intent is not required.

# 2. Pre-proposal Due Date

January 7, 2020 at 5:00 PM Eastern Time

A Pre-Proposal is required.

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

# 3. Proposal Due Date

March 30, 2020 at 5:00 PM Eastern Time

You are encouraged to transmit your proposal well before the deadline. Modifications to the proposal are not allowed after the proposal due date.

#### 4. Late Submissions

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

- Failure to begin submission process early enough.
- Failure to provide sufficient time to complete the process.
- Failure to understand the submission process.
- Failure to understand the deadlines for submissions.
- Failure to satisfy prerequisite registrations.
- Unavailability of administrative personnel.

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

Scheduled medical events that are known at the time this FOA is published do not justify late submissions: Applicants should draft their submissions in sufficient time to meet the deadlines.

Applicants must email <u>SC.Early@science.doe.gov</u> to discuss the option of a late submission in the case of unavoidable circumstances. DOE notes that not all requests for late submission will be approved.

## F. FUNDING RESTRICTIONS

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

Support for paid collaborators of the PI will be considered only in rare cases where a collaborator (either early career or senior) brings something unique to the project. However, preference will be given to PI-led efforts without paid collaborators for which the budget covers research support staff (e.g., students and postdoctoral fellows), travel, supplies, equipment, and other expenses necessary for the Principal-Investigator-led project.

Preference will be given to proposals without subawards with the exception of those that propose

small subawards for essential supporting work such as sample analysis. Subawards that pay salary for scientific collaborators outside the proposing institution are discouraged.

# G. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS

#### 1. Where to Submit

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

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

# 2. Registration Process

ONE-TIME REGISTRATION PROCESS

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

For help with PAMS, click the "External User Guide" link on the PAMS website, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submission and inquiries about this DOE National Laboratory Program Announcement should reference LAB 20-2173.

# 3. Proposal Receipt Notices

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

## 4. Viewing Submitted Proposals

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

## Section V - PROPOSAL REVIEW INFORMATION

#### A. CRITERIA

#### 1. Initial Review Criteria

Prior to a comprehensive merit evaluation, DOE will perform an initial review to determine that (1) the applicant is eligible for the award; (2) the information required by this National Laboratory Announcement has been submitted; (3) all mandatory requirements are satisfied including having an approved pre-proposal and attachment of a biographical sketch, current and pending support, and data management plan; (4) the proposed project is responsive to the objectives of this National Laboratory 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.

A proposal declined without merit review by the DOE SC will not count as one of the three allowed submissions to the Early Career Research Program. Likewise, a proposal withdrawn prior to being officially declined by the DOE SC will not count as one of the three allowed submissions.

## 2. Merit Review Criteria

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

- 1. Scientific and/or Technical Merit of the Project;
- 2. Appropriateness of the Proposed Method or Approach;
- 3. Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
- 4. Reasonableness and Appropriateness of the Proposed Budget.

The following FOA-specific evaluation criteria will also be used during the scientific merit review (peer review):

- 5. Relevance to the mission of the specific program (e.g., ASCR, BER, BES, FES, HEP, or NP) to which the proposal is submitted.
- 6. Potential for leadership within the 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 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:

- 1. SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROPOSED RESEARCH What is the scientific innovation of proposed research? How does the proposed research compare with other research in its field, both in terms of scientific and/or technical merit and originality? How might the results of the proposed research impact the direction, progress, and thinking in relevant scientific fields of research? What is the likelihood of achieving influential results? Is the Data Management Plan suitable for the proposed research and to what extent does it support the validation of research results?
- 2. APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH Does the proposed research employ innovative concepts or methods? How logical and feasible are the research approaches? Are the conceptual framework, methods, and analyses well justified, adequately developed, and likely to lead to scientifically valid conclusions? Does the applicant recognize significant potential problems and consider alternative strategies?
- 3. Competency of Applicant's Personnel and Adequacy of Proposed Resources What are the past performance and potential of the Principal Investigator (PI)? How well qualified is the research team to carry out the proposed research? Are the research environment and facilities adequate for performing the research? Does the proposed work take advantage of unique facilities and capabilities?
- 4. REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET
  Are the proposed budget and staffing levels adequate to carry out the proposed research? Is the budget reasonable and appropriate for the scope?
- 5. RELEVANCE TO THE MISSION OF THE SPECIFIC PROGRAM (E.G., ASCR, BER, BES, FES, HEP, OR NP) TO WHICH THE PROPOSAL IS SUBMITTED

  How does the proposed research contribute to the mission of the program in which the proposal is being evaluated? Is the proposed research aligned with the program office's priorities as described in advisory committee reports?
- 6. POTENTIAL FOR LEADERSHIP WITHIN THE SCIENTIFIC COMMUNITY Scientific leadership can be defined very broadly and can include direct research contributions. How has the PI demonstrated the potential for scientific leadership and creative vision? How has the PI been recognized as a leader?

For criterion 5, the missions of the program areas are:

**Advanced Scientific Computing Research (ASCR)**: To advance applied mathematics and computer science; deliver the most advanced computational scientific proposals in partnership with disciplinary science; advance computing and networking capabilities; and develop future

generations of computing hardware and software tools for science, in partnership with the research community, including U.S. industry.

**Biological and Environmental Research (BER):** To support transformative science and scientific user facilities to achieve a predictive understanding of complex biological, earth, and environmental systems for energy and infrastructure security and resilience.

**Basic Energy Sciences (BES):** To support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security.

**Fusion Energy Sciences (FES):** To expand the fundamental understanding of matter at very high temperatures and densities and to build the scientific foundation needed to develop a fusion energy source. This is accomplished through the study of plasma, the fourth state of matter, and how it interacts with its surroundings.

**High Energy Physics (HEP):** To understand how the universe works at its most fundamental level by discovering the elementary constituents of matter and energy, probing the interactions between them, and exploring the basic nature of space and time.

**Nuclear Physics (NP):** To discover, explore, and understand all forms of nuclear matter. Although the fundamental particles that compose nuclear matter—quarks and gluons—are themselves relatively well understood, exactly how they interact and combine to form the different types of matter observed in the universe today and during its evolution remains largely unknown.

In addition to providing narrative comments associated with each of the six merit review criteria, each reviewer will be asked to provide an overall integer numerical rating between 1 and 6 for each proposal, where the scale follows:

Strongly Encourage Funding (5 or 6);

Encourage Funding (3 or 4); or

Discourage Funding (1 or 2).

#### **B. REVIEW AND SELECTION PROCESS**

#### 1. Merit Review

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

# 2. Program Policy Factors

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

- Relevance of the proposed activity to SC priorities
- Ensuring an appropriate balance of activities within SC programs
- Fostering the development of a diverse cadre of supported Principal Investigators
- The availability of funds
- Institutional history of training and mentoring early-career researchers
- Providing career pathways for the next generation of researchers
- Ensuring opportunities to investigators not currently supported by DOE
- Commitment to sharing the results of research

#### 3. Selection

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

## 4. Discussions and Award

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

## C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES

It is anticipated that the award selection will be completed by September 30, 2020. It is expected that awards will be made in Fiscal Year 2020.

## Section VI - AWARD ADMINISTRATION INFORMATION

Office of Science Early Career Research Program investigators intending to transfer to a new institution must submit a request for transfer along with a new proposal. If the scope of work has not changed, the award may be transferred. If the scope of work has changed, the new proposal will be subject to merit review as described below. Transfer awards will be for the remaining award period only, and the requested budget cannot exceed the remaining budget for the original award. If a laboratory employee transfers to a university, the requested budget should be as close to \$150,000 per year as possible for each remaining year. While a transfer proposal can be submitted any time of the year, it should be submitted at least six months before the transfer to allow time for execution of merit review.

To transfer an award to an academic institution, the investigator must move into a tenure-track or tenured position at the academic institution.

To transfer an award to a DOE National Laboratory, the investigator must move into a full-time, permanent, non-postdoctoral national laboratory position. The transfer proposal must be accompanied by a letter from the national laboratory director to the technical point of contact confirming that the proposed research idea fits within the scope of Office-of-Science-funded programs at the national laboratory. Transferring research that falls within this category ensures that investigators have the opportunity to belong to or join, at the laboratory's discretion, funded research groups. Making sure that DOE National Laboratory investigators have potential connections with Office-of-Science funded programs encourages the laboratory to actively plan to address funding transition issues that may arise when an award ends.

To retain an award at a DOE National Laboratory, the investigator must remain in a full-time, permanent, non-postdoctoral national laboratory position.

Execution of the annual funding is at the discretion of the principal investigator in accordance with the DOE-approved budget and the requirements of the national laboratory.

The award period is five years, conditional on adequate annual progress and appropriation of funds. At the end of this period, the DOE national laboratory employing the principal investigator has the primary responsibility to address funding transition issues that arise when the award ends.

A minimum of 50% and up to 100% of the Principal Investigator's salary must be charged to the award annually.

#### A. AWARD NOTICES

#### 1. Notice of Selection

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

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

# 2. Notice of Award

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

# **B. REPORTING**

Annual progress reports and a final technical report from the award investigator will be required. Annual progress reports will be due 90 days before the end of each budget year. A final technical report will be required 90 days after the award ends.

## **Section VII - OUESTIONS/AGENCY CONTACTS**

# **A. QUESTIONS**

For help with PAMS, click the "External User Guide" link on the PAMS website, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submission and inquiries about this DOE National Laboratory Program Announcement should reference LAB 20-2173.

Please contact the PAMS help desk for technological issues with the PAMS system.

Questions regarding the specific program areas and technical requirements may be directed to the technical contacts listed for each program within the DOE National Laboratory Program Announcement or below.

Please contact the program staff with all questions not directly related to the PAMS system.

#### **B. AGENCY CONTACTS**

PAMS	855-818-1846 (toll-free)
Customer Support	301-903-9610
	sc.pams-helpdesk@science.doe.gov
Administrative Contact	Questions about program rules should be sent to
	SC.Early@science.doe.gov
Program Manager	Questions regarding the specific program areas/technical
Scientific Contact	requirements can be directed to the program managers /
	technical contacts listed for each program within the FOA.

# 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 <a href="mailto:ighotline@hq.doe.gov">ighotline@hq.doe.gov</a>. Allegations may be reported by DOE employees, DOE contractors, or the general public. OIG contact information is available at <a href="http://energy.gov/ig/services">http://energy.gov/ig/services</a>.

## **Section VIII - OTHER INFORMATION**

## A. MODIFICATIONS

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

## B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE

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

## C. COMMITMENT OF PUBLIC FUNDS

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

## D. PROPRIETARY PROPOSAL INFORMATION

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

"The data contained in pages\_\_\_\_\_\_of this proposal have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes."

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

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

#### E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL

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

## F. AVAILABILITY OF FUNDS

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