DEPARTMENT OF ENERGY OFFICE OF SCIENCE



EARLY CAREER RESEARCH PROGRAM

FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER: DE-FOA-0002563

FOA TYPE: INITIAL CFDA NUMBER: 81.049

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Submission Deadline for Pre-Applications:	October 21, 2021 at 5:00 PM Eastern Time
	A Pre-Application is required
Pre-Application Response Date:	December 1, 2021 at 11:59 PM Eastern
	Time
Submission Deadline for Applications:	January 20, 2022 at 11:59 PM Eastern
	Time

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<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 (LOIs), preapplications, and applications well before the deadline.

CURRENT AND PENDING SUPPORT AND BIOSKETCHES

The instructions for the content of current and pending support and biosketches have changed. Please read the instructions carefully and follow them.

REPORTING AND ADMINISTRATIVE REQUIREMENTS

DOE is implementing enhanced reporting requirements for applications and awards. Reporting and administrative requirements, including but not limited to those pertaining to other sources of support and potential conflicts of interest or commitment, are subject to change before the Federal award date. The terms and conditions of award will specify changed requirements: Applicants have the right to reject any proposed awards. Terms and conditions may be modified at the time of an award modification. Recipients have the right to reject such modifications and allow an award to expire.

Unique Entity Identifier (UEI)

The Federal Government is transitioning from the Data Universal Numbering System (DUNS), assigned by Dun and Bradstreet at https://fedgov.dnb.com/ to the UEI, assigned by the System for Award Management (SAM) at <a href="https://www.gsa.gov/about-us/organization/federal-acquisition-service/office-of-systems-management/integrated-award-environment-iae/iae-information-kit/unique-entity-identifier-update. Information systems including SAM.gov, Grants.gov and PAMS (https://pamspublic.science.energy.gov) are being updated: Please follow the on-screen instructions or contact each system's Help Desk for additional information. Detailed information about the transition is available at <a href="https://www.gsa.gov/about-us/organization/federal-acquisition-service/office-of-systems-management/integrated-award-environment-iae/iae-information-kit/unique-entity-identifier-update.

ACKNOWLEDGMENT OF FEDERAL SUPPORT

SC guidance about how its support should be acknowledged is published at https://science.osti.gov/funding-opportunities/acknowledgements/.

PUBLIC ACCESS

Awards made under this FOA are subject to DOE's Public Access Plan (https://www.energy.gov/downloads/doe-public-access-plan). Full-text version of scientific publications must be made publicly accessible at no charge to readers.

SC STATEMENT OF COMMITMENT

The DOE SC is fully and unconditionally committed to fostering safe, diverse, equitable, and inclusive work, research, and funding environments that value mutual respect and personal integrity. Discrimination and harassment undermine SC's ability to achieve its mission by reducing productivity, discouraging, or inhibiting talent retention and career advancement, and weakening the integrity of the SC enterprise overall. SC does not tolerate discrimination or harassment of any kind, including sexual or non-sexual harassment, bullying, intimidation, violence, threats of violence, retaliation, or other disruptive behavior in the federal workplace, including DOE field site offices, or at national laboratories, scientific user facilities, academic institutions, other institutions receiving SC funding, or other locations where activities funded by SC are carried out. All applicants and collaborators should familiarize themselves with the SC Statement of Commitment available at https://science.osti.gov/sc-2/Research-and-Conduct-Policies/Diversity-Equity-and-Inclusion/SC-Statement-of-Commitment.

UPDATING YOUR PAMS PROFILE

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

PDF GENERATION

The research narrative in an application must be one single machine-readable PDF file that contains the DOE Title Page, project narrative, biographical sketch, current and pending support, bibliography and references cited, facilities and other resources, equipment, data management plan, and other attachments. This single PDF file may not be scanned from a printed document and must be attached in Field 8 on the Grants.gov form. You are strongly encouraged to submit the combined research narrative file through a "Print to PDF" or equivalent process to ensure that all content is visible in one PDF file.

Checklist for Avoiding Common Errors:

Item	Issue
Page Limits	Strictly followed throughout application,
	including particular attention to:
	- Research Narrative
	- Appendix 2 Narrative, if any
	- Biosketches
	- Data Management Plan(s) (DMPs)
	- Letter(s) of Recommendation, if any
Personally Identifiable Information	None present in the application
Research Narrative	Composed of one PDF file including all
	appendices
Project Summary / Abstract	Name(s) of applicant, PI(s), PI's institutional
	affiliation(s), Co-Investigator(s), Co-
	Investigator's institutional affiliation(s)
DOE Title Page	Follow instructions closely
Budget	Use current negotiated indirect cost and fringe
8	benefit rates
Budget Justification (attached to budget)	Justify all requested costs
Biographical Sketches	Follow page limits strictly
Current and Pending Support	Ensure complete listing of all activities,
	regardless of source of funding
Data Management Plans (DMP)	- If referring to an experiment's DMP,
()	describe the relationship to the proposed
	research
	- Include a DMP even if no experimental
	data is expected
Institutions capable of being funded through	If National Laboratories and/or DOE sites are
the DOE Field Work System	permitted to submit under this FOA:
, and the second	- Do not create new institutions in the
	PAMS website
	- Submit applications in Grants.gov using
	the name of the laboratory or site in Field
	5 of the SF-424(R&R) application form,
	not the contractor operating the laboratory
	or site
	Submissions under this FOA will be
	evaluated for technical merit, but any
	resulting funding, work, or awards will be
	made under the laboratory or site's contract
	with DOE. No separate financial assistance
	awards will be made. No administrative
	provisions of this FOA will apply to the
	laboratory or any laboratory subcontractor.

Section I – FUNDING OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS FOA SHOULD BE DIRECTED TO:

Technical/Scientific Program Contact:

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

Administrative Contact (questions about program rules):

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

STATUTORY AUTHORITY

Section 646 of Public Law 95-91, U.S. Department of Energy Organization Act Section 901, et seq., of Public Law 109-58, Energy Policy Act of 2005

APPLICABLE REGULATIONS

Uniform Administrative Requirements, Cost Principles, and Audit Requirements for Federal Awards, codified at 2 CFR 200

U.S. Department of Energy Financial Assistance Rules, codified at 2 CFR 910 U.S. Department of Energy, Office of Science Financial Assistance Program Rule, codified at 10 CFR 605

SUMMARY

DOE SC hereby invites applications for support under the Early Career Research Program in the following program areas: Advanced Scientific Computing Research (ASCR); Basic Energy Sciences (BES); Biological and Environmental Research (BER); Fusion Energy Sciences (FES); High Energy Physics (HEP); Nuclear Physics (NP); Isotope R&D and Production (DOE IP); or Accelerator R&D and Production (ARDAP). 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.

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 28 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.

RESEARCH OPPORTUNITIES

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.

- A. Advanced Scientific Computing Research (ASCR);
- B. Basic Energy Sciences (BES);
- C. Biological and Environmental Research (BER);
- D. Fusion Energy Sciences (FES);
- E. High Energy Physics (HEP);
- F. Nuclear Physics (NP);
- G. Isotope R&D and Production (DOE IP); and
- H. Accelerator R&D and Production (ARDAP)

The research topics for this FOA are indicated by numbers (1, 2, 3, etc.) under each Program Office name (A, B, C, etc.). For example, under ASCR, the first topic (1) is "Extreme-Scale Algorithms for Scientific Computing."

A. Advanced Scientific Computing Research (ASCR)

Program Website: https://www.energy.gov/science/ascr/advanced-scientific-computing-research or https://science.osti.gov/ascr

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, 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, 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.

Proposed research under ASCR for the Early Career Research Program 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:

(1) Extreme-Scale Algorithms for Scientific Computing Technical Contact: Steven Lee, <u>Steven.Lee@science.doe.gov</u>

The scientific computing research community faces a broad array of challenges in the development of high-performance algorithms and solvers for emerging computing architectures. Because algorithms, solvers, and decision support methods (e.g., Priority Research Direction (PRD) #6 in [3]) can dominate the overall execution time of computational and data science applications, research in developing efficient, robust, resilient, and portable techniques is essential for scientific advances over the next decade [5, 6]. Research areas of interest include novel approaches identified in the recent ASCR workshop on Randomized Algorithms for Scientific Computing [2] and that address:

- High computational and communication complexity and the development of efficient algorithms;
- Better algorithm scalability for low-power, high-performance computing;
- Reduced ill-conditioning and sensitivity for inverse problems; and
- Improved algorithm reliability and robustness to noise on emerging computer architectures [4].

Topics and research areas that are out of scope include:

- Pre-applications and applications that do not address research for creating a body of knowledge and understanding that will inform future advances in extreme-scale science, and
- Research in cryptography and quantum computing algorithms.

(2) Scalable Scientific Data Analysis and Reduction Technical Contact: William Spotz, William.Spotz@science.doe.gov

Rigorous mathematical and computationally efficient approaches are needed for analyzing and extracting information and insight from large-scale data relevant to the DOE missions. Data-Intensive Scientific Machine Learning is Priority Research Direction (PRD) #4 from the 2019 workshop report [3]. The 2021 workshop report on Data Reduction in Science identifies the research and development challenges in that area [1]. This overall topic area is specifically focused on the research and development of scientific machine learning and data reduction in two different scenarios: Models and analysis 1) for large-scale distributed data sets that occurs without moving the data (static), and 2) in real-time, streaming environments (dynamic).

Rigorous mathematical and computationally efficient approaches are needed for analyzing and extracting information and insight from large-scale data relevant to the DOE missions. The principal focus of this topic area is algorithms and techniques that can improve data analysis or reliably reduce the volume of scientific data by finding signals, patterns, or structure under such challenges as high-dimensionality, noise, or uncertainty. Research areas of interest include novel approaches that address PRDs from two recent ASCR workshop reports.

PRDs #1-4 from the Data Reduction for Science workshop [1]:

- Effective algorithms and tools that can be trusted by scientists for accuracy and efficiency;
- Progressive reduction algorithms that enable data to be prioritized for efficient streaming;
- Algorithms which can preserve information in features and quantities of interest with quantified uncertainty; and
- Reduction techniques that map to new architectures and use cases.

PRD #4 from the Scientific Machine Learning workshop [3]:

• Data-intensive scientific machine learning for automated scientific inference and data analysis.

(3) Multiscale Mathematics for the Modeling and Simulation of Complex Systems

Technical Contact: William Spotz, William.Spotz@science.doe.gov

Innovative mathematics research is needed 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. This topic area is focused on the challenges of accurately coupling different multi-physics systems, the rigorous development of hybrid or hierarchical mathematical models that incorporate machine learning or reduced order models, and other approaches that bring together multiple facets of more realistic, predictive modeling and simulation [7, 8] and [3, see PRD #5]. Topics and research areas that are out of scope include:

- Pre-applications and applications that do not address innovation in coupling or multifaceted mathematical models;
- Approaches for specific scientific or engineering problems that are not applicable to a broader class of problems;
- Approaches with a primary emphasis on tailoring, or the implementation of, existing numerical methods for specific scientific problems;
- Computational implementation or frameworks for scientific or engineering problems that are primarily based on specific programming models or architecture; and
- Research that results in incremental improvements to the existing state of practice.

<u>Important note for encourage and discourage decisions</u>: Pre-applications 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.

See <u>Section IV.B</u> for details regarding the pre-application submission and review process.

References:

- [1] Workshop report on Data Reduction for Science, https://doi.org/10.2172/1770192
- [2] Workshop report on Randomized Algorithms for Scientific Computing, https://arxiv.org/pdf/2104.11079.pdf
- [3] Workshop Report on 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
- [4] 2018 Basic Research Needs Workshop on Extreme Heterogeneity, https://doi.org/10.2172/1473756
- [5] Report on Applied Mathematics Research for Exascale Computing, https://doi.org/10.2172/1149042
- [6] Report on the Extreme-Scale Solvers Workshop https://science.osti.gov/-/media/ascr/pdf/program-documents/docs/reportExtremeScaleSolvers2012.pdf
- [7] Report on A Multifaceted Mathematical Approach for Complex Systems https://science.osti.gov/-/media/ascr/pdf/program-documents/docs/Multifaceted Mathematical Approach for Complex Systems.pdf

[8] DOE Workshop Report on Multiphysics Simulations

https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/MultiPhysics-Simulations- Report.pdf

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:

(4) Systems

Technical Contact: Hal Finkel, Hal.Finkel@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, high-bandwidth memory [HBM], scratchpads, and heterogeneity of processing (e.g., Graphics Processing Units [GPUs], Field-Programmable Gate Arrays [FPGAs], Coarse-Grained Reconfigurable Architectures [CGRAs], 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. All phases of the software-development cycle are relevant, including but not limited to, design, implementation, verification, optimization, and integration. Particularly welcome are methods 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 highly-parallel software and workflow-management systems, and that facilitates effective and efficient use of heterogeneous computing technologies, including diverse execution models, processors, accelerators, memory, and storage systems. Target workloads include modeling and simulation, data analysis, and the processing of large-scale, streaming data from experiments.
- c. **Performance Portability and Co-design**: Methods that support performance portability, which provides the ability to efficiently use diverse kinds of hardware platforms with minimal changes to the application source code, and/or hardware/software co-design, which is a method for designing and/or adapting both hardware and software design as part of a holistic process. These methods include automated and semi-automated refinements from high-level specification of an application and/or hardware design to low-level code, optimized when compiled and/or, for software, at runtime, to different HPC platforms. The focus is on enabling performance portability of, and/or the design of future hardware for, applications developed for extreme-scale computing and beyond.

Applications 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.

(5) Data Management, Visualization, and Analytics Technical Contact: Margaret Lentz, <u>Margaret.Lentz@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.

Topics that are out of scope include:

- Pre-applications and applications that do not address the specific Computer Science topics described above;
- Pre-applications and applications 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-applications and applications 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 research or capabilities without also proposing a generalization of this research 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; and
- Research focused on quantum computing.

References:

[1] DOE Workshop report: Productive Computational Science in the Era of Extreme Heterogeneity, https://www.osti.gov/biblio/1473756

[2] DOE Workshop report: Management, Analysis and Visualization of Experimental and

Observational Data: The Convergence of Data and Computing, https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/2015-report_160524.pdf
[3] DOE Workshop report: Crosscut Report: Exascale Requirements Reviews, March 2017. https://science.osti.gov/~/media/ascr/pdf/programdocuments/docs/2018/DOE-ExascaleReport-CrossCut.pdf

[4] DOE Workshop report: Report of the HPC Correctness Summit, https://www.osti.gov/biblio/1470989

[5] DOE Workshop report: In Situ Data Management: Enabling Scientific Discovery from Diverse Data Sources, https://www.osti.gov/biblio/1493245-workshop-report-situ-data-management

[6] DOE Workshop report: Storage Systems and Input/Output: Organizing, Storing, and Accessing Data for Scientific Discovery. https://www.osti.gov/biblio/1491994/
[7] DOE Workshop report: Data and Models: A Framework for Advancing AI in Science, https://www.osti.gov/biblio/1579323

Advanced Computing Technologies

This activity supports Quantum efforts and Research and Evaluation Prototypes (REP). 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.

(1) Quantum Computing

Technical Contact: Claire Cramer, Claire.Cramer@science.doe.gov

Research to evaluate the suitability of specific quantum computing hardware architectures for science applications, including resource estimates for quantum computing applications of interest to SC. Theoretical methods and software tools to assess the performance of real-world quantum processors, facilitate device-specific optimization of individual operations ranging from state preparation and measurement through gate implementation and compilation, suppress noise, mitigate crosstalk, control errors, and maintain optimally high-fidelity operations in the absence of formal error correction.

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-applications and applications 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;
- Development of integrated circuits for quantum computing;
- 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

[1] ASCR Report on Quantum Computing for Science, February 2015.

https://science.osti.gov/-

/media/ascr/pdf/programdocuments/docs/ASCRQuantumReport-final.pdf

[2] ASCR Report on a Quantum Computing Testbed for Science, February 2017.

https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/2017/QTSWReport.pdf

(2) Emerging Computing Technologies

Technical Contact: Robinson Pino, Robinson.Pino@science.doe.gov

- a. **Advanced Wireless for Science**: The focus of this subtopic is on communications that cover higher frequencies, THz, of 5G+ or WiFi6+ and software defined capabilities. The expanding national rollout of advanced wireless networks is creating opportunities for scientific applications.
- b. **Microelectronics for Scientific Computing**: For continued advances in computing technologies, a fundamental rethinking is needed of the science behind computing processor synthesis, placement, architectures, and algorithms. No longer can the approach be modular and linear, as it has been in the past. Rather, these advances must be developed collectively, in a spirit of co-design, where each scientific discipline informs and engages the other to achieve orders of magnitude improvements in system-level performance.

Topics that are out of scope include:

- Pre-applications and applications that do not address the specific topics described above;
- Pre-applications and applications that do not explain/describe their relevance to current and future high performance computing platforms and/or research-centric science as well as their relevance to the mission of SC and ASCR;
- Pre-applications and applications with primary emphasis on materials science, biology, devices, circuits; sensors; crossbar arrays; quantum computing;
- Research primarily focused on advancing discipline-specific research or capabilities without also proposing a generalization of this research 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; social networks; reservoir

- computing; statistical-based approaches; blockchain; Internet of Things (IoT);
- Research that is only applicable to hand-held, tablets, laptops, mobile phones, desktop, or cloud computing; and
- Pre-applications and applications with a primary focus on development or deployment activities; or that suggest incremental upgrades to existing computer or network architectures, protocols, tools, or services.

Notice: This year, the emerging computing technologies will focus on microelectronics and advanced wireless. Applications focusing on neuromorphic computing or HPC cybersecurity will NOT be considered responsive, but these topics are anticipated to be the focus in next year's call.

References:

[1] DOE Workshop report: 5G Enabled Energy Innovation Workshop, March 2020. https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/2020/5G_Workshop_Report_2020.pdf
[2] DOE Workshop report: Basic Research Needs Workshop for Microelectronics, October 2018. https://science.osti.gov/-/media/bes/pdf/reports/2019/BRN_Microelectronics_rpt.pdf

B. Basic Energy Sciences (BES)

Program Website: https://www.energy.gov/science/bes/basic-energy-sciences or https://science.osti.gov/bes/

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 Investigator (PI) 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 PI Meetings: http://science.osti.gov/bes/mse/principal-investigators-meetings/

Chemical Sciences, Geosciences, & Biosciences Division PI

Meetings: http://science.osti.gov/bes/csgb/principal-investigators-

meetings/

Scientific User Facilities Division web page:

http://science.osti.gov/bes/suf/

Proposed research must be responsive to a supported topic in one of the core research areas listed below. Many of the core research areas limit early career Applications to a subset of topics within their regular research activities. In those cases, the intention is to rotate topics on an annual basis. Overarching research priorities for BES that are relevant to multiple core research areas are described in the bulleted list below. The individual program descriptions further define research directions relevant to these priorities.

- Clean Energy: Research to provide understanding and scientific foundations for clean energy, including direct air capture of carbon dioxide; hydrogen production, storage, and use; solar energy conversion to electricity and fuels; and electrical and thermal energy storage.
- Critical Materials/Minerals: Research to understand the fundamental properties of rare earth and platinum group elements to improve separation and extraction processes and to enable discovery and design of alternates to critical materials that will reduce or eliminate their need.
- Fundamental Science to Transform Manufacturing: Research to understand fundamental chemical and materials processes for circular, clean, and scalable synthesis and processing; to advance transformational operando characterization and multiscale models and tools; and to co-design materials, processes, and products for functionality and use.
- **Revolutionizing Polymer Upcycling**: Research to provide the foundational knowledge for the selective deconstruction of the polymers that constitute plastics, followed by reassembly into high-value chemicals, fuels, or materials in a repeating cycle.
- Artificial Intelligence and Machine Learning (AI/ML): Research to advance the approaches and use of data science and AI/ML to accelerate fundamental research for the discovery of new chemical mechanisms and material systems with exceptional properties and function, and to apply these techniques for effective user facility operations and interpretation of massive data sets.
- Quantum Information Science (QIS): Research to advance understanding of quantum phenomena in systems that could be used for quantum information science, and the use of quantum computing in chemical and materials sciences research.

(1) Materials Chemistry

Technical Contacts: Michael Sennett, <u>Michael Sennett@science.doe.gov</u> (select Michael Sennett in PAMS) and Craig Henderson, <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 and a view to elucidating fundamental chemical 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 understanding the *chemistry* and *chemical* control of composition, structure, and function across the range of length scales from atomic to mesoscopic, and consequent materials properties. The desired outcome is fundamental knowledge of the chemistry of materials, which may be widely applied to the development of next-generation clean energy technologies in one or more of the BES priority areas.

For the early career program, the topic for applications in response to this year's FOA is strictly limited to scientific understanding of chemical phenomena observed to play a role in the synthesis, function, or degradation of energy-relevant materials. To be considered, applications to the FY 2022 BES Materials Chemistry Early Career Research Program must propose research involving chemical aspects of materials that meet ALL of the following criteria:

- a) identifies one or more specific scientific hypotheses, defined here for the purposes of this topic as a plausible explanation for an observed phenomenon, which may be a newly discovered effect or a well-known effect that remains unexplained;
- b) describes a program of research that will definitively test the proposed hypotheses and targets understanding of chemical phenomena that could lead to new models, theories, or scientific principles for materials chemistry;
- c) can be expected to have a positive impact on one or more of the following topical areas, which are described elsewhere in this FOA and in documents included by reference: Clean Energy, Critical Materials and Minerals, Transformative Manufacturing, Polymer Upcycling or Quantum Information Science.

Relevant chemical phenomena may have been observed experimentally, computationally, or both at any length or time scale, but must be applicable to materials with chemical structures beyond small molecules. Applications that focus on identifying, quantifying, and/or tuning structure-property relationships for materials to optimize performance without impacting the understanding of why such relationships exist 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.

(2) Biomolecular Materials

Technical Contact: Michael Markowitz, mike.markowitz@science.doe.gov

This activity supports basic research in the discovery, design and synthesis of functional materials and complex structures based on principles and concepts of biology. Biology provides a blueprint for translating atomic and nanoscale phenomena into mesoscale materials that display complex yet well-coordinated collective behavior. The major programmatic direction is on the science-driven creation of resilient materials and multiscale systems that exhibit well-coordinated functionality and information content approaching that of biological materials but capable of functioning under harsher, non-biological environments.

Biomolecular Materials research activity seeks fundamental knowledge needed for co-design and scalable synthesis of materials for clean energy and quantum information science that coherently

manage and self-regulate multiple complex and simultaneous functions and tolerate abuse. An area of emphasis will be activities to understand and control assembly mechanisms to seamlessly integrate capabilities developed over one length scale across multiple length scales as the material is constructed. Included is development of predictive models and AI/ML for data-driven science that accelerate materials discovery and support fundamental science to direct clean, energy efficient scalable synthesis with real-time adaptive control.

For the Early Career Research Program, two separate topics (A and B shown below) are planned for alternate fiscal years in pursuit of these goals. Science-driven coupling of theory and experiment to achieve Topic objectives are encouraged. For this announcement, only applications focused on Topic B will be considered.

- Topic A (Alternate years): The specific focus will be on fundamental science underpinning design and scalable creation of next-generation materials and systems that incorporate low-energy mechanisms for electrical energy, thermal energy, ion and fluid transport with programmable selectivity based on biological gating and pumping functions.
- Topic B (This year): The focus will be control of fundamental mechanisms for precise synthesis and assembly, including self-replication approaches, of multiscale and multicomponent materials and systems that self-regulate structure repair and rebuild functions and/or energy transfer, transport, and communication pathways.

For both of these topics, bio-centric research **will be de-emphasized**, including activities focused on understanding of underlying biological synthetic or assembly processes, or creation of bio-hybrid materials. The program **will not** support projects that lack a clear focus on fundamental materials science or are aimed at optimization of materials properties for any applications, device fabrication, sensor development, tissue engineering, biological research, 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.

(3) Synthesis and Processing Science Technical Contact: Tim Fitzsimmons, <u>tim.fitzsimmons@science.doe.gov</u>

This program supports basic scientific research on materials to understand the physical principles that underpin materials synthesis and processing including diffusion, nucleation, and phase transitions, often using *in situ* diagnostics and new techniques. An important element of this activity is the use 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 reports on *Synthesis Science* and *Transformative Manufacturing*, have identified the needs and challenges in

synthesis and processing science that are most relevant to clean energy technologies.

This year's Early Career Research Program FOA invites applicants to submit hypothesis driven applications that present novel understanding and creative approaches that underpin the science advances for scalability and co-design in manufacturing processes as defined in the Basic Research Needs Report for Transformative Manufacturing. Applications that integrate a creative experimental methodology with a theoretical-based approach to accelerate progress in understanding unifying principles for synthesis and/or processing of clean energy technologies 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 applications that involve biological materials or that are aimed at *optimization* of material properties for specific applications. In addition, the program **will not** support applications with a primary goal of engineering development, device fabrication, nanoparticle synthesis, tribology, or fluid dynamics. For this year's FOA, applications must both specifically target manufacturing or processing science AND refer to a clean energy technology for the material.

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.

(4) Experimental Condensed Matter Physics Technical Contact: Michael Pechan, 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 FOA in ECMP will focus on nanostructured and low dimensional quantum materials wherein electronic, structural, charge and magnetic states are controlled to produce novel functionality. Of particular interest are topics related to 1) critical materials in magnetism; and 2) quantum phononics and magnonics for quantum information science and dissipation-less energy transfer. Applications focusing on synthesis and characterization of <u>bulk</u> quantum materials will <u>NOT</u> be considered responsive to this year's FOA but are anticipated to be the focus in next year's FOA.

The ECMP Program does not support applications 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 applications on topics in the following areas: conventional semiconductors, heavy fermion (non-topological) 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.

(5) Theoretical Condensed Matter Physics Technical Contact: Matthias Graf, <u>matthias.graf@science.doe.gov</u>

This program supports research in theoretical condensed matter physics developing quantum methods and techniques for quantum materials, quantum computing, quantum systems out of equilibrium (including quantum transport and dynamics), materials discovery, and fundamental research in materials related to clean energy technologies. Examples of current research include correlated electron systems, topological states and quantum phases of matter, magnetism, superconductivity, computational and data driven materials design, optical response, and excited states phenomena including photon and neutron scattering. Novel, physics-based AI/ML computational techniques are supported for quantum many-body problems and quantum information science.

For this year's FOA, applications are sought only in targeted areas of quantum computing/simulation for many-body correlated electron systems on current and near-term available quantum computing/simulation platforms, and AI/ML approaches for the dynamics of quantum systems far from equilibrium. For next year's FOA, the plan is to invite applications in the areas of physics-based AI/ML approaches to computational and data-driven functional materials discovery and materials theory solely related to fundamental research for clean energy related to solar, electrical and thermal energy storage.

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.

(6) Physical Behavior of Materials

Technical Contacts: Refik Kortan, <u>refik.kortan@science.doe.gov</u> (select Refik Kortan in PAMS) and Athena Sefat, <u>athena.sefat@science.doe.gov</u>

This program broadly supports fundamental research on the physical behavior of materials. This year, the program invites applications for transformational basic research that may enable tomorrow's Clean Energy technologies, specifically those focusing on light-matter interactions. Additionally, the program calls for applications relevant to topics of Quantum Photonics and Quantum Information Science, which may include research on creation, transport, and control of novel quantum coherent phenomena to enhance transduction of quantum coherent states to demonstrate high fidelity. All applications should heavily emphasize transformative and hypothesis-driven basic science. This program supports research that involves theory, modeling, and simulation, specifically projects that combine theoretical and experimental research. The program **does not** support projects aimed at optimization of materials properties for any applications, device fabrication, or conventional 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.

(7) Mechanical Behavior and Radiation Effects Technical Contact: John Vetrano, iohn.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 understanding mechanisms dictating strength, formability, and fracture in energy relevant materials. The goals are to develop the scientific underpinning for predictive design of materials having superior mechanical properties. These fundamental science efforts will impact Clean Energy topics in general, and may also impact Fundamental Science to Transform Manufacturing, Polymer Upcycling, or Artificial Intelligence/Machine Learning.

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 interest in 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. Applications taking advantage of advanced synthesis methods to create tailored structures 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 supported in this program at this time. Applications 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.

(8) X-ray Scattering Technical Contact: Lane Wilson, lane.wilson@science.doe.gov

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 and extend the capabilities at the DOE facilities by providing support for novel instrumentation, techniques, and research. For example, research is sought that will take advantage of unprecedented levels of coherent brightness and of controlled timing structures at upgraded light source facilities. New investments in ultrafast science will also 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. Additionally, new approaches to improve the collection, processing and analysis of large data sets obtained with high repetition-rate pulsed sources or with fast multi-mega-pixel detector arrays are encouraged under the cross-cutting emerging domain of Data Sciences. Novel X-ray techniques are sought that enable detailed investigations of the fundamental dynamic mechanisms of clean energy conversion systems and their active material components.

The program will not support research considered "mature use" of existing X-ray or ultrafast techniques. Typically, the emphasis on new techniques enables new access to inhomogeneous and dynamic systems and therefore the program will de-emphasize steady-state research of bulk and equilibrium systems.

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.

(9) Neutron Scattering Technical Contact: P. Thiyagarajan (Thiyaga), 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 data science 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 research on materials that exhibit novel emergent phenomena or unique properties that could impact clean energy technologies. Characterizing and controlling such emergent behavior are keys to optimizing and exploiting a wide range of materials' performance and functionality. *In situ* and *operando* characterization can measure structure and dynamics of materials in the appropriate environment and at realistic conditions, yielding direct data for comparison to predictions. The program will develop novel measurement techniques that will exploit the unique aspects of neutron scattering for materials research. AI/ML and data science approaches could enable development of data analysis tools for better utilization of the large amount of scattering data from the BES facilities.

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.

(10) Electron and Scanning Probe Microscopies Technical Contact: Jane Zhu, 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 clean energy applications. The goal is to develop a fundamental understanding of materials through advanced microscopy and spectroscopy.

This year's Early Career Research Program FOA invites applicants to submit hypothesis driven applications that present fundamental understanding of quantum materials and phenomena in systems that could be used for quantum information science using innovative electron and scanning probe microscopy approaches. New methods and approaches could provide an array of opportunities for groundbreaking science that will accelerate discovery and technological deployment of quantum materials. These include understanding and controlling quantum systems, nano- or meso-scale inhomogeneity, and the interplay between charge, orbital, spin and lattice degrees of freedom. Research opportunities also include characterization and manipulation of individual atoms in matter at the atomic scale or controlled introduction and manipulation of complex defect systems, combined with atomic and nanometer scale measurements of quantum behavior or machine learning/artificial intelligence/data science methods in microscopy.

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.

(11) Atomic, Molecular, and Optical Sciences (AMOS) Technical Contact: Tom Settersten, thomas.settersten@science.doe.gov

The DOE AMOS program is focused on fundamental, hypothesis-driven research in ultrafast chemical sciences. The program supports basic experimental and theoretical research aimed at understanding the structural and dynamical properties of atomic and molecular systems. The research targets fundamental interactions of photons and electrons with atomic and molecular systems to characterize and control their behavior. The program aims to develop accurate quantum-mechanical descriptions of ultrafast dynamical processes, such as charge migration and transfer, chemical bond breaking and forming, and interactions in strong fields, where electron-electron and electron-nuclei correlations are important. Topics of interest include the development and use of novel, ultrafast probes of matter; the interactions of atoms and molecules with intense electromagnetic fields; and control of quantum coherence/decoherence and entanglement in molecular systems.

The AMOS activity will continue to support science that advances DOE and BES mission priorities, including research that contributes to the BES priority on Clean Energy by developing a fundamental understanding of excitation dynamics and charge transfer relevant to the initial steps in clean solar energy conversion. The AMOS program 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. Closely related experimental and theoretical efforts are encouraged. The AMOS program will consider ECRP applications that contribute to the BES priority on Quantum Information Science by focusing on fundamental research aimed to advance understanding and control of quantum coherence/decoherence and entanglement in molecular systems. Projects involving technical development of sources or instrumentation must include a well-integrated scientific research focus.

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. The program encourages research exploiting next-generation capabilities of X-ray free electron lasers and modern data science approaches to provide new insights to electronic and molecular dynamics occurring on the attosecond-to-femtosecond time scale and to reveal key intermediate states in chemical reactions. 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 applications in the areas of plasma physics, nanoscience, bioscience, and science of ultracold systems.

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.

(12) Gas Phase Chemical Physics (GPCP) Technical Contact: Wade Sisk, wade.sisk@science.doe.gov

This program supports research on fundamental gas-phase chemical processes that provide understanding and scientific foundations for clean energy. Research in this program explores chemical reactivity, kinetics and dynamics in the gas phase at the level of electrons, atoms, molecules and nanoparticles. A continuing goal of this program is to understand energy flow and reaction mechanisms in complex, nonequilibrium, gas-phase environments. A new goal for this program is to understand how these gas-phase processes can influence and be influenced by surface phenomena.

The major focus of research in this area is in five thrust areas: Light-Matter Interactions, Chemical Reactivity, Gas-Particle Interconversion, Gas-Surface Chemical Physics, and Ultrafast

Imaging/Spectroscopy.

- 1. Light-Matter Interactions includes research in the development and application of novel tools, such as molecular spectroscopy, for probing the nuclear and electronic structure of gasphase molecules to enable chemical and physical analysis of heterogeneous and dynamic gasphase environments and to understand the dynamic behavior of isolated molecules, such as energy flow (e.g., relaxation of excited states), nuclear rearrangements, and loss of coherence and entanglement. Applications are encouraged that develop automated methods based on artificial intelligence and machine learning (AI/ML) methods to facilitate the analysis of complex molecular spectra, or seek to improve the understanding of quantum phenomena in systems that could be used for quantum information science. (OPEN)
- 2. Chemical Reactivity comprises research in chemical kinetics and mechanisms, chemical dynamics, collisional energy transfer, and construction of, and calculations on, molecular potential energy surfaces to develop fundamental insight into energy flow and chemical reactions important in clean energy processes. Applications are encouraged that develop AI/ML methods for the construction of potential energy surfaces and optimization of chemical kinetic mechanisms. (OPEN)
- 3. Gas-Particle Interconversions comprises research on the chemistry of small gas-phase particles, including their interactions with gas-phase molecules and dynamic evolution to understand the molecular mechanisms of formation, growth and transformation (such as evaporation, phase transition, and reactive processing) of small particles. (CLOSED)
- 4. Gas-Surface Chemical Physics retains a strong emphasis on molecular-scale investigations of gas-phase chemical processes with the goal of gaining a better understanding of the cooperative effects of coupling gas phase chemistry with surface chemistry. (CLOSED)
- 5. Ultrafast Imaging/Spectroscopy includes studies of the short timescale phenomena underlying photochemical and photophysical processes, such as photodissociation, isomerization, and nonadiabatic dynamics. Applications are encouraged that develop AI/ML methods for analyzing ultrafast images/spectra or to provide insight into chemical systems associated with clean energy. (OPEN)

Research Applications will be accepted from only a subset of the selected five research thrusts in response to each year's FOA, with the remaining thrusts offered in alternate years. For this FOA, only Applications focused on thrusts 1, 2 and 5 will be considered. Research Applications 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.

(13) Computational and Theoretical Chemistry Technical Contact: Aaron Holder, <u>aaron.holder@science.doe.gov</u>

Computational and Theoretical Chemistry (CTC) 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 dynamical processes that are so complex that efficient computational implementation must be accomplished in concert with development of new theories and algorithms. Efforts must be tightly integrated with the research and goals of BES and provide theories and computational approaches to advance the fundamental science of at least one of the six overarching research priorities for BES in FY 2022 listed in the introductory section above. Applications 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, coherent 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 time-independent and timedependent simulation approaches. FY 2022 topics of interest include:

- Novel non-classical or non-perturbative theories and approaches for the predictive simulation and control of vibrationally-mediated chemical dynamics in non-equilibrium and/or fielddriven complex open systems.
- Practical and hierarchical theories and methods for the high fidelity simulation of nonlocal
 chemical interactions and emergent phenomena occurring in complex molecular ensembles
 and environments, including; stochastic and correlated quantum chemical approaches for the
 accurate simulation and prescriptive design of emergent functionality, non-biological
 autocatalytic cooperative reaction networks, such as those leading to directed molecular
 assembly and/or replication processes, or correlated multi-electron and/or multi-photon
 governed chemical transformation and energy transduction processes.

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.

(14) Condensed Phase and Interfacial Molecular Science (CPIMS) Technical Contact: Gregory Fiechtner, 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 and physical processes in liquids and at interfaces. With its foundation in chemical physics, the impact of this crosscutting program is far reaching, providing understanding and scientific foundations underpinning a variety of areas of importance to the DOE, including clean energy, catalytic and separation processes, energy storage, chemical synthesis and manufacturing, and microelectronics. The CPIMS program also supports efforts related to BES research priorities such as Artificial Intelligence and Machine Learning and Quantum Information Science.

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 condensedphase 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. Investigations at model interfaces seek to understand processes underlying atomically precise synthesis, which could have an impact ranging from heterogeneous catalysis to future electronic devices.

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, including entanglement preservation at interfaces; (2) examine rare electrochemical events (such as nucleation and self-assembly) using machine learning and advanced sampling techniques of large data sets; (3) investigate the effect of the chemical environment on oxidation and spin states as well as the influence of native solvation environments on spin dynamics of solvated complexes; (4) study hydrogen bonding and solvation of ions in liquid electrolytes (including in conventional dipolar solvents, ionic liquids and deep eutectic solvents); (5) study manipulation of electrochemical reactivity on layered 2D materials by tuning the electronic structure via band structure manipulation and tunable electrostatic effects; (6) demonstrate photoredox chemistry of excited polaritonic states along with studies of long-range energy and electron transport made possible by cavity polaritons; (7) seek an understanding of chemical bond dynamics in solution

using mixed quantum/classical molecular dynamics simulations; and (8) study the enhanced reactivity at the air-liquid interface of microdroplets and aerosols. Descriptions of earlier awards are found in Chemical Sciences, Geosciences, & Biosciences Division PI Meetings under "Condensed-Phase and Interfacial Molecular Science". A more extensive description of program evolution can be found at the link: https://science.osti.gov/bes/csgb/Research-Areas/Condensed-Phase-and-Interfacial-Molecular-Sciences.

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 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.

(15) Catalysis Science

Technical Contacts: Viviane Schwartz, <u>viviane.schwartz@science.doe.gov</u> and Chris Bradley, <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 FOA strongly **encourages** applicants to submit hypothesis-driven Applications in fundamental catalysis science that underpins the following areas:

• Sustainable chemical manufacturing, circular processing (such as polymer upcycling), clean energy (including electro-driven transformations that use clean H₂), catalysis by Earth-abundant metals, and utilization of data science and Machine Learning approaches to mechanism identification and catalyst discovery.

Topics specifically **excluded** this year:

• Chemical transformations primarily based on electrocatalytic or photo-electrocatalytic approaches that do not include the use of clean H₂.

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 on the 'Chemical Sciences, Geosciences, & Biosciences Division PI Meetings' webpage (search for "catalysis" in the title), and in the BES Research Summaries (https://science.osti.gov/bes/csgb/Research-Areas/Catalysis-Science). 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 as well as a 2019 BES roundtable report on Chemical Upcycling of Polymers, discussing the challenges of polymer deconstruction and redesign.

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.

(16) Separation Science (SEP)

Technical Contact: Daniel Matuszak, <u>Daniel.Matuszak@science.doe.gov</u>

This program supports hypothesis-driven experimental and computational research to discover, understand, predict, and control de-mixing transitions, with the goal of enabling chemical separation paradigms that may become the basis for solutions to the nation's energy challenges – these include the utilization of clean energy (renewable energy or fossil energy that is offset by carbon removal approaches) as well as enabling the availability of critical elements while mitigating environmental impacts. Basic research activity in these areas relies on understanding molecular interactions and energy exchanges that determine the efficiency of chemical separations. Advancing the understanding of basic chemical and physical principles at the atomic-, electronic-, molecular-, nano-, and meso-scales is essential.

Energy-relevant separation science topics that are of interest to the Separation Science Program are outlined in six recent National Academies of Science, Engineering, and Medicine (NASEM) and DOE BES reports:

- NASEM 2019 A Research Agenda for Transforming Separation Science (https://www.nap.edu/catalog/25421/a-research-agenda-for-transforming-separation-science)
- NASEM 2019 Negative Emissions Technologies and Reliable Sequestration: A Research Agenda (https://www.nap.edu/catalog/25259/negative-emissions-technologies-and-reliable-sequestration-a-research-agenda)
- NASEM 2019 Gaseous Carbon Waste Streams Utilization
 https://www.nap.edu/catalog/25232/gaseous-carbon-waste-streams-utilization-status-and-research-needs)
- BES 2015 Basic Research Needs for Environmental Management
- BES 2017 The Water-Energy Nexus
- BES 2010 Carbon Capture Beyond 2020.

The Program also supports emerging fundamental scientific areas within separation science that are in a nascent stage. Selected topics of interest include:

- elucidating factors that cause a separation system to approach mass transfer limitation in the source phase
- enabling and enhancing strategies for critical materials recovery from natural and unconventional feedstocks; for water and environmental management of heavy elements and nuclear waste; and for carbon removal from low-concentration sources
- understanding non-thermal mechanisms that have the potential to drive efficient and selective energy-relevant separations, such as electromagnetic, electrochemical, magneto-reactive, and other means to affect transport and bonding selectively
- discovering and advancing strategies for removal of dilute constituents from a mixture, including but not limited to reactive separation approaches
- generating specific and long-range interactions among trace constituents with the aim of promoting nucleation of a new phase that is enriched in the target species
- discovering novel approaches for dehydration of heterogeneous systems without the application of heat
- designing separation systems that have high selectivity, capacity, and throughput
- understanding temporal changes that occur in separation systems

The above topics are agnostic to the separation system and may include, for example, membranes, framework materials (e.g., metal-organic framework materials), zeolites, ionic liquids, and molecular complexes. Issues of selectivity, capacity, throughput, durability, and energy input are important for most separations, and should be of concern in separation science research, although they may not be the singular focus.

Based on programmatic priorities, this activity *does not* support the following areas: engineering design or scale-up, development of narrowly defined processes or devices, desalination, microfluidics, or sensors.

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.

(17) Heavy Element Chemistry (HEC) Technical Contact: Philip Wilk, philip.wilk@science.doe.gov

This activity supports actinide and transactinide fundamental chemical research that underpins the DOE missions in energy, environment, and national security. The unique molecular bonding of these elements is explored using experiment and theory to elucidate electronic and molecular structure, reaction thermodynamics, as well as quantum phenomena, such as coherence and entanglement. 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. Theoretical Applications are considered that

integrate closely with experimental research or otherwise demonstrate impact outside the theory community. The HEC program does not fund code development.

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. Catalytic reactivity involving actinides is of current interest to this program, if the project yields insight into f-electron behavior, and is not better aligned with the BES Catalysis Science program described in section (15). Exotic catalytic and redox behavior exhibited by actinides in extreme environments, such as the legacy nuclear waste tanks or molten salts, is also of particular interest to this program. Also of particular interest is the exploitation of the unique electronic properties of the f-elements for quantum information science purposes (e.g. actinide qubits or the synthesis and investigation of strongly correlated multidimensional lattices).

The inclusion of machine learning, artificial intelligence, and quantum computing methods are particularly desirable and aligned with current BES priorities. Applications that will further our understanding and provide scientific foundations for clean energy are also desirable and aligned with BES priorities. 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, data science efforts without chemical experimentation, or biological systems; which are all more appropriately supported through other DOE programs. The HEC program will consider Applications to understand how the unique electronic structure of rare earth elements, including the role of f-electrons, determines the physical and chemical properties of molecules and materials, with the goal of accelerating their design to reduce or eliminate the use of critical elements. 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 (SEP) program, which is described in section (16). More information about the Heavy Element Chemistry program can be found at https://science.osti.gov/bes/csgb/Research- Areas/Heavy-Element-Chemistry.

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.

(18) Geosciences (GEO)

Technical Contact: Jim Rustad, <u>iames.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 requires applicants to address fundamental questions directed to one of the following areas:

- (1) Critical elements that underlie key energy technologies. We seek applications aimed at understanding the molecular-level origins of critical element behavior that governs their distribution and separation in minerals and fluids in the Earth via natural processes. Particular critical elements are not specified here but must be a non-fuel mineral or earth materials essential to clean energy technologies for which the supply chain is vulnerable to disruption. Examples would include, but are not limited to, platinum group elements, rare earth elements, lithium, and cobalt. Both the pre-application and the application need to make strong arguments for the clean energy relevance of the system chosen (for example by referring to needs specified in DOE reports and workshops). Applications that do not focus on understanding molecular-level speciation and distribution will not be considered. Purely theoretical/computational investigations will not be considered unless they make well-defined connections to parallel experimental research.
- (2) Issues related to hydrogen storage in subsurface geological reservoirs. Focus must be at the molecular level and specifically examine mechanisms of interaction of H₂ with earth materials governing transformation and migration of hydrogen in subsurface formations.
- (3) Data Science approaches to understanding time-dependent shallow crustal rheology. Applications must demonstrate the ability to generate/have access to large datasets that show substantial promise for understanding mechanistic processes in the shallow crust. Purely computational studies (where, for example, datasets are generated by forward models) will not be considered.

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

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.

(19) Solar Photochemistry

Technical Contact: Chris Fecko, christopher.fecko@science.doe.gov

This activity supports fundamental, molecular-level research on solar energy capture and conversion in the condensed phase and at interfaces. Photochemical approaches may ultimately offer new routes for generating electricity or fuels from sunlight using closed, renewable, clean energy cycles. Advances in these areas will require a thorough understanding of elementary processes such as light absorption, charge separation, and charge transport within a number of chemical systems, including those with significant nanostructured composition.

Supported research areas include organic and inorganic photochemistry, light-driven electron and energy transfer in condensed phase and interfacial molecular systems, electrocatalysis and photocatalysis of solar fuels reactions, semiconductor photoelectrochemistry, light-driven generation or manipulation of quantum coherence in artificial molecular systems, and artificial assemblies that mimic natural photosynthetic systems. An enhanced theory and modeling effort is needed to improve current understanding of many photochemical phenomena.

To advance the science of light-driven fuels production, knowledge gained in photoinduced charge transfer needs to be applied in a meaningful way to activation of small molecules including oxidation or reduction of H_2O , as well as the reduction of CO_2 or N_2 to fuels.

Considerable challenges remain in understanding degradation mechanisms to enhance photochemical durability, designing catalytic microenvironments that promote selective production of energy-rich solar fuels, exploiting direct coupling of light-driven phenomena and chemical processes to enhance performance, and tailoring interactions of complex phenomena to achieve integrated multicomponent assemblies for solar fuels production.

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.

(20) Photosynthetic Systems Technical Contact: Stephen Herbert, 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 the photosynthetic systems of plants, algae, and photosynthetic microbes. Topics of study 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 and self-repair of photosynthetic proteins, complexes, and membranes. The goal of the program is to foster greater knowledge of the useful chemistry exhibited by the diverse photosynthetic systems found in nature. Examples include capture of CO₂ by carboxylase enzymes and bicarbonate transport systems, light-driven production of H₂ by hydrogenase enzymes, prolonged coherence at room temperature exhibited by energy transfers in photosystems, oxidation of water to provide electrons for solar fuels and other reduced carbon compounds, and the protein-protein interactions that drive self-assembly and

self-repair of the complex molecular components of photosynthesis.

All submitted applications must clearly state the relevance of the proposed basic research for clean energy 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.

(21) Physical Biosciences

Technical Contact: Gail McLean, gail.mclean@science.doe.gov

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 CO₂/CH₄, N₂/NH₃, and H⁺/H₂), 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.

The fundamental research supported by this program can provide foundational knowledge for clean energy, for instance, through a mechanistic understanding of processes and identification of unique principles in biological systems that could guide design of highly selective and efficient bioinspired catalysts and chemical pathways for direct air capture of carbon dioxide, hydrogen production and use, and solar energy conversion into fuels.

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 applications 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.

(22) Nanoscale Science Research Centers Technical Contact: George Maracas, george.maracas@science.doe.gov

The program is open to national laboratory applications only. University PIs interested in research on nanoscale science should consider topics (1) through (21) listed above for BES.

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. Applications will not be accepted to establish new, unrelated types of facilities or to develop techniques that do not relate to the missions of the Nanoscale Science Research Centers. (https://science.osti.gov/bes/suf/userfacilities/nanoscale-science-research-centers/). Research is supported across the spectrum of NSRC-relevant 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 sensors, and integration from nano to meso to micro 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.

New approaches to probe, understand, synthesize, and build at the nanoscale are needed. In-situ, operando approaches that could eventually be adapted for real-time monitoring and control of experiments are preferred. 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, chemical processes and structures for clean energy and security applications. Leveraging complementary modalities at co-located X-ray, neutron, high-performance computing and microfabrication facilities are of interest. Closely coupling theory and modeling with experiment to accelerate understanding nanoscale phenomena and their resulting innovations is encouraged. Relevant BES Reports are *Challenges at the Frontier of Matter and Energy report: Transformative Opportunities for Discovery Science, Future of Electron Scattering and Diffraction, Synthesis Science for Energy Technologies, Innovation and Discovery of Transformative Experimental Tools, Catalysis Science to Transform Energy*

Technologies, Chemical Upcycling of Polymers, Producing and Managing Large Scientific Data with Artificial Intelligence and Machine Learning, Quantum Materials for Energy Relevant Technology, and From Quanta to the Continuum: Opportunities for Mesoscale Science, Opportunities for Quantum Computing in Chemical and Materials Sciences, Microelectronics, and Workshop for Transformative Manufacturing.

Allowed topics for novel instrumentation and technique development efforts must be scientifically justified and are limited to scanning, transmission, and scanning transmission electron microscopes, atom probes, related field ion instruments, surface characterization apparatus, scanning probe microscopes, and material and chemical synthesis.

The proposed research must fit within the BES Scientific User Facilities (SUF) Division funded programs at the laboratory of the applicant.

(23) Accelerator and Detector Research Technical Contact: Eliane Lessner, <u>eliane.lessner@science.doe.gov</u>

This program supports work that advances the instruments, techniques, and capabilities of the existing and/or future BES SUFs. We do not intend to support applications 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. Of interest are techniques leading to Terawatt power radiation and source-generated THz beams. The second component is detectors, which 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 (AI/ML). Using the rapidly growing data stream produced at the SUFs to its full potential will require new innovations to solve a variety of technical challenges in data acquisition, control, modeling, and analysis. AI/ML-based methods are needed to efficiently search large, complex parameter spaces in real time and to predict the health and failure of instruments at high-power sources and the experiments that are run on those instruments. Such capabilities will dramatically reduce facility tuning time and downtime, improve facility performance, and maximize the productivity of BES SUFs.

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 *BES Workshop on Future Electron Sources* report, the *BES Workshop on Neutron and X-ray Detectors* report, and the *Basic Energy Sciences Roundtable on Producing and Managing Large Scientific Data with Artificial Intelligence and Machine Learning* report.

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.

(24) X-ray Instrumentation and Technique Development Technical Contacts: P. Thiyagarajan (Thiyaga), <u>p.thiyagarajan@science.doe.gov</u> (select Pappannan Thiyagarajan in PAMS) and Eliane Lessner, <u>eliane.lessner@science.doe.gov</u>

The program is open to national laboratory applications only. University PIs interested in X-ray instrumentation technique development should consider the topics discussed above under (8) X-ray Scattering.

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 Applications 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).

In order to fully exploit the wide range of advanced capabilities at the BES X-ray facilities, this program emphasizes the development of novel concepts for new types of X-ray instruments and innovative uses of existing instruments. The main priorities will be the development of novel measurement techniques for innovative clean energy research advanced X-ray optics, and powerful tools for data visualization and analysis. *In situ* and *operando*, and high-throughput techniques are powerful tools in revealing mechanisms, and synthesis-structure and structure-property relationships. Artificial intelligence and machine learning (AI/ML) can enable

automated experimental approaches to guide scientific discovery and accelerate the realization of the full potential of current and next-generation light sources.

The proposed research must fit within the BES SUF Division funded programs at the laboratory of the applicant.

(25) Neutron Scattering Instrumentation and Technique Development Technical Contact: P. Thiyagarajan, p.thiyagarajan@science.doe.gov

The program is open to national laboratory applications only. University PIs interested in neutron scattering instrumentation and technique development should consider the topics discussed above under (9) Neutron Scattering.

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

Neutron scattering is a unique and effective tool for probing many aspects of the atomic structure and dynamics of materials over wide length and time scales. 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 develop novel measurement techniques that will exploit the unique aspects of neutron scattering and polarized neutrons for impactful research for future clean energy technologies. It 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. AI/ML and data science approaches will enable development of data analysis tools for better utilization of the large amount of scattering data from the BES facilities.

The proposed research must fit within the BES SUF Division funded programs at the laboratory of the applicant.

C. Biological and Environmental Research (BER)

Program Website: https://www.energy.gov/science/ber/biological-and-environmental-research or https://science.osti.gov/ber

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 and 'omics research to understand, predict, manipulate, and design biological processes that underpin innovations for bioenergy and bioproduct research. Building on a foundation of multi-omic data and combining systems and synthetic biology, experimental physiology, genome-scale editing and engineering, and computational approaches, it becomes possible to harness the power of microorganisms and microbial communities as cellular factories. An important goal of the Division is to meet the challenges associated with microbial production of advanced biofuels, bioproducts, and biomaterials from plant biomass, synthetic polymers, or as a byproduct of photosynthesis through highly interdisciplinary and integrated research projects.

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

(1) Systems biology and biosystems design of bioenergy-relevant microbes to enable production of next-generation biofuels, bioproducts, and biomaterials Technical Contact: Pablo Rabinowicz, pablo.rabinowicz@science.doe.gov

Applications are requested for systems biology research to advance the development of emerging eukaryote or prokaryote model microorganisms and/or microbial communities relevant for the production of biofuels, bioproducts, and/or biomaterials by converting lignocellulosic biomass, upcycling synthetic (petroleum-derived) polymers, or as a byproduct of photosynthesis. Applications that propose multi-omics approaches coupled with genome-wide design and editing technology development, in vivo or cell-free engineering, advanced predictive modeling, and high-throughput screening to understand and re-design biological systems with novel functional capabilities and biosynthetic potential are encouraged. Proposed studies could include, but are not limited to: i) elucidation and/or engineering of relevant regulatory and metabolic networks, metabolic pathways, and/or signal processing related to bioproduct synthesis by microbes or multispecies consortia; ii) development of synthetic biology tools to facilitate the study and manipulation of emerging microbial model systems; iii) understanding and modification of phenotypes involved in the deconstruction and conversion of plant cell walls or synthetic, petroleum-derived polymers, the tolerance to stresses induced by altered biosynthetic pathways or culture conditions, and/or the synthesis of biofuels, bioproduct, and material precursors; and iv) engineering microorganisms for the production of biominerals, inorganic-organic composites, and composites of inorganic materials and living cells (living materials), with wholly new properties not found in nature.

A focus on emerging model systems to expand the breadth of platform microorganisms for genome engineering is encouraged. Genome engineering approaches that may contribute to carbon capture and sequestration to reduce atmospheric CO₂ are also encouraged. Research on traditional model systems should be kept to a minimum. Applications should address biocontainment of the engineered organisms and consider potential unintended outcomes and biological escapes.

The following topics are NOT within the scope of the BSSD research area: Starch-, waste-, natural gas-, petroleum-, or coal-derived biofuels, bioproducts or biomaterials; microbial fuel

cells; electrosynthesis; wastewater; municipal solid waste; bioremediation; bioprospecting; biomimetics/biohybrids; production of ethanol, biogas, hydrogen, pharmaceuticals, nutraceuticals, cosmetics, or food products. Projects focused on titer/yield improvement or scale-up production in established microbial systems are not within the scope of BSSD. Research that would result in only incremental knowledge or technological advances, or applications focused solely on technology development will not be considered.

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; http://www.kbase.us), the National Microbiome Data Collaborative (NMDC; https://microbiomedata.org/), the DOE Environmental Molecular Sciences Laboratory (EMSL; https://www.emsl.pnnl.gov/emslweb/), the National Energy Research Scientific Computing Center (NERSC; http://www.nersc.gov), the DOE Structural Biology and Imaging Resources (https://berstructuralbioportal.org), and the DOE Joint Genome Institute (JGI; https://jgi.doe.gov). Awarded projects will receive prioritized consideration for use of JGI capabilities through the Biological and Environmental Research Support Science (BERSS) user program (https://jgi.doe.gov/user-programs/other-programs/). To determine the feasibility of the planned work to be done by JGI, applicants should contact JGI before submitting their application.

Annual Principal Investigator (PI) meeting: if an award is made, at least one project participant will be expected 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

Environmental System Science (ESS) research within BER's Earth and Environmental Systems Sciences Division (EESSD) seeks to develop an integrated framework using a systems approach to elucidate the complex processes and controls on the structure, function, feedbacks, and dynamics of terrestrial ecosystems that span from the bedrock through the rhizosphere and vegetation to the atmospheric interface. The program scope advances foundational process knowledge from molecular to global scales and the interplay of key system components to enable an improved understanding of understudied ecosystems and environmental interfaces such as coastal zones. This effort requires the linking of system components and their interfaces with ecological, watershed, and biogeochemical sciences to address key knowledge gaps across a range of spatial and temporal scales. Incorporation of process understanding into a range of models improves predictive understanding and future projections of the terrestrial system, which in turn enables the identification of new research questions and directions (https://ess.science.energy.gov/program/).

BER is seeking ESS research in the following area:

(2) Environmental Process Research in Urban-Influenced Coastal Systems Technical Contact: Jennifer Arrigo, <u>Jennifer.arrigo@science.doe.gov</u> and Daniel Stover, <u>Daniel.stover@science.doe.gov</u>

Applications are sought within the scope of the ESS program that will improve fundamental understanding of ecological and hydro-biogeochemical processes in urban influenced coastal systems. Structurally, coastal systems include a wide variety of landforms, including beaches, sand dunes, cliffs, estuaries, marshes, wetlands, tidal zones, deltas, intracoastal waterways, and barrier islands. In addition, they include a wide variety of vegetation types, soil types, subsurface formations and groundwater resources, and interfacial areas of the land margin to either salt/tidal waters or dynamically varying freshwater systems. Research solicited under this topic is limited to coastal systems consisting of urban to suburban environments and urban transition zones that include a U.S. shoreline on the continental coastal margins and/or on the Great Lakes. Where appropriate, these environments could include constructed wetlands and partially channeled waters and armored shorelines.

While coastal systems function naturally due to a variety of physical, chemical, and biological processes, urban coastal systems are also exposed to numerous anthropogenic influences that affect not only the ecology and hydro-biogeochemistry of the coastal zone but also how these processes interact with other system components in the complex coastal environment and broader domains. Intermittent or periodic natural perturbations and disturbances (such as extreme and compounding storm events, precipitation shifts and/or extremes, drought, increasing temperature, flooding/inundation, saltwater intrusion, sea level rise, wildfires, and wind extremes) coupled with increasing anthropogenic influences and impacts (e.g., the presence and development of the built environment, land use change, pollution, water and resource extraction, and energy sector and food production) can result in both sudden or gradual shifts and long-term changes in the resilience of urban coastal systems. Current understanding of the functioning of urban-influenced coastal systems is inadequate to predict future coastal system behavior, responses, and evolution under changing conditions and increasing urbanization and disturbance. Increased predictive understanding might also be helpful for addressing built environment challenges and environmental justice issues often found in these urban coastal locations.

Applications must focus on changes in the functioning and vulnerability of ecological and hydro-biogeochemical processes in urban-influenced coastal systems due to critically important disturbances (i.e., extreme and compounding storm events, drought, temperature extremes, flooding/inundation, saltwater intrusion, wildfires, and wind extremes). ESS has particular interest in studies that address how contemporaneous chronic shifts (i.e., chronic sea level rise, precipitation shifts, and/or increasing temperatures) compound these episodic events to affect the resilience of natural systems within the context of urban environments.

Submissions to this topic must plan a significant field and/or lab effort to collect and make use of new measurements from field and/or laboratory experiments in a clearly delineated integrative, hypothesis-driven approach. All applications are required to describe the existing needs/gaps in state-of-the-art models that motivate the proposed research, and combine the data/information obtained from the field and/or laboratory work with modeling/simulation efforts in a coupled modeling-experimental (ModEx) approach (https://ess.science.energy.gov/program/). Applications should provide details on how the results will enable advances in predictive, scale-aware understanding of ecological and hydro-biogeochemical processes in ecosystem, watershed, and regional models of urban-influenced coastal systems.

Pre-applications and applications for this topic must:

- be focused on ecological and/or hydro-biogeochemical processes;
- be focused on coastal urban/suburban/transitional environments located on a U.S. continental margin saltwater coast and/or a U.S. shoreline of the Great Lakes;
- delineate an integrative, hypothesis-driven approach and describe the existing needs/gaps in state-of-the-art models that motivate the proposed research;
- make use of new measurements from field and/or laboratory experiments, and combine the data/information with modeling/simulation efforts; and
- include enough information to enable evaluation of responsiveness to the terms of this announcement.

Applicants could make use of existing infrastructure/data, including those supported by other agencies/entities, but this would require a letter of support from the collaborating entity. Applicants may want to propose linkages to on-going studies supported by EESSD such as the COMPASS (https://compass.pnnl.gov/fme) and ICoM (https://climatemodeling.science.energy.gov/projects/integrated-coastal-modeling-icom) projects, the AmeriFlux network (https://ameriflux.lbl.gov/), and/or others.

Note: Research that would result in only incremental knowledge or technology advances or applications solely focused on technology development are not encouraged.

The following topics are NOT within the scope of the EESSD research area: studies focused primarily on multi-sector dynamics, integrated assessments, the built environment, socioeconomics, land-use (including agricultural enhancements), human populations, noise pollution, or economic disparity/environmental injustice; urban design, planning or architecture; ecosystem or watershed engineering; sedimentation/erosion studies; land-locked/non-continental margin coastal areas other than the Great Lakes; water-column-only studies focused on harmful algal blooms, contaminant/pollutant/pesticide runoff or impacts, or aquatic organism impacts; riverine- or lacustrine-only studies; characterization of invasive macro-organisms or their mitigation; terrestrial-aquatic interfaces of completely channeled waters or armored shorelines; and studies that propose to primarily use or develop models without equally obtaining new data/parameters.

<u>DOE Office of Science User Facilities and Other Community Resources</u>: Applicants are encouraged to consider the use of resources provided by SC User Facilities and Community Resources. These include the BER User Facilities (https://science.osti.gov/ber/Facilities) and a variety of Community Resources (https://science.osti.gov/ber/Community-Resources/BER-Community-Research-Infrastructure and https://ess.science.energy.gov/research-approach/).

<u>Data Management Plan</u>: A Data Management Plan (DMP) is a required element of the application and is considered in the review process. ESS has established the Environmental System Science – Data Infrastructure for a Virtual Ecosystems (ESS-DIVE) data archive (https://essdive.lbl.gov/) for ESS-funded projects that allows data contributors to archive and

share data, and to obtain digital object identifiers (DOIs) that can be used to cite and track usage of the data. Successful applicants are required to share their data, data products, and metadata from their funded project with ESS-DIVE. If successful applicants store some or all of their data in an established, public, long-term archive other than ESS-DIVE (e.g., AmeriFlux Archive, NASA DAAC, NCBI, DOE user facilities), they are also required to, at a minimum, archive metadata describing the data with ESS-DIVE including links/DOI's to the archived data. These archiving requirements are not intended to interfere with data management activities at the home institution of the project PI.

<u>Software – Productivity and Sustainability Improvement Plan</u>: To increase the pace of scientific discovery and promote more efficient and effective use of government funding and resources, software/code development and enhancement efforts are expected to be open source and made available to the scientific community. Applications that propose to undertake development of new software/code or modification/enhancement of existing software/code and to then use that new or modified/enhanced software/code for modeling/simulation as part of the proposed effort are required to include a Software-Productivity and Sustainability Improvement Plan (S-PSIP) as an appendix to the research narrative. Applicants are encouraged to follow best practices outlined in the materials posted on the Better Scientific Software site (https://bssw.io/).

<u>Annual PI Meeting</u>: Reasonable travel expenses to attend the annual ESS Principal Investigator meeting should be included as part of each year of the project budget.

More detailed information about BER Earth and Environmental Systems Sciences sponsored research can be found at: https://science.osti.gov/ber/Research/eessd.

D. Fusion Energy Sciences (FES)

Program Website: https://science.osti.gov/fes or https://science.osti.gov/fes

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, future blanket concepts and tritium fuel cycle, and invention of new measurement techniques.

In addition to its fusion energy mission, FES also supports discovery plasma science, which is focused on research at the frontiers of basic and low temperature plasma science (with

applications to microelectronics) and high-energy-density laboratory plasmas. Finally, FES invests in transformational technologies such as artificial intelligence and machine learning (AI/ML), fundamental science to transform advanced manufacturing, and quantum information science (QIS), that have the potential to accelerate progress in several mission areas.

References

FES research is guided by the 2021 Long-Range Plan "Powering the Future: Fusion and Plasmas" developed by the Fusion Energy Sciences Advisory Committee (FESAC): https://science.osti.gov/-

/media/fes/fesac/pdf/2020/202012/FESAC Report 2020 Powering the Future.pdf

Additional resources include:

- a series of community engagement workshops (https://science.osti.gov/fes/Community-Resources/Workshop-Reports),
- National Academies reports such as:
 - o the 2018 report on a Strategic Plan for U.S. Burning Plasma Research
 - o the 2018 report on Opportunities in Intense Ultrafast Lasers
 - o the 2020 Decadal Assessment of Plasma Science report; and
 - o the 2021 report on "Bringing Fusion to the U.S. Grid, https://www.nap.edu/catalog/25991/bringing-fusion-to-the-us-grid

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:

(1) Advanced Tokamak Experimental Research Technical Contact: Matthew Lanctot, <u>matthew.lanctot@science.doe.gov</u>

The Advanced Tokamak Experimental Research program seeks to utilize domestic tokamak research facilities with conventional aspect ratios to develop the knowledge needed to advance the FES energy mission. The effort involves the operation of experimental tokamak facilities ranging from small-scale university experiments to large national user facilities. The plasma diagnostic and technology systems operating on these facilities provide the experimental data required to study fusion and plasma science and technology. 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 and technology issues relevant to sustaining a burning plasma, engineering for extreme fusion conditions, developing technology for a fusion pilot plant, and preparing for plasma operations on the ITER facility.

Applications to this area must have a primary focus on experimental research and address critical issues for the advanced tokamak approach to a fusion energy source or investigate topics common to all fusion power plant concepts. Applications aimed at *closing* critical gaps in the

advanced tokamak physics basis to enable the development of a low-capital-cost fusion pilot plant are strongly encouraged. Applicants are urged to pursue innovative and transformational approaches to surmount high-priority challenges.

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.

(2) Spherical Tokamak Research Technical Contact: Josh King, 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 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 (i.e., NSTX-U, MAST-U, LTX-β, ST40, Pegasus-III, and QUEST). The largest domestic facility (i.e., NSTX-U) is currently down for an extended outage, but experimental operations is anticipated to resume within the term of new awards. The experimental focus of both large and smaller-scale domestic facilities will be focused on research relevant to the Fusion Energy Sciences Long-Range Plan.

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.

Applications to this area must focus on experimental research and/or model validation pertaining to spherical tokamak plasmas.

(3) Stellarator Research in Magnetic Fusion Energy Sciences Technical Contact: Samuel Barish, sam.barish@science.doe.gov

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.

(4) Magnetic Fusion Energy Science Theory and Simulation Technical Contact: John Mandrekas, john.mandrekas@science.doe.gov

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. Applications focused on transformative approaches, such as fusion-relevant computing aspects of quantum information science (QIS), are also encouraged.

(5) Measurement Innovation

Technical Contact: Curt Bolton, curt.bolton@science.doe.gov

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.

(6) High-Energy-Density Plasma Science Technical Contact: Kramer Akli, 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. Applications focusing on developing high energy density materials relevant to QIS are strongly encouraged. Applications focusing on inertial fusion energy sciences are also encouraged.

(7) General Plasma Science Experiment and Theory Technical Contact: Nirmol Podder, nirmol.podder@science.doe.gov

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.

(8) Fusion Nuclear Science, Materials Research, and Enabling R&D Programs for Fusion Technical Contact for Fusion Nuclear Science and Enabling R&D: Guinevere Shaw, guinevere.shaw@science.doe.gov

Technical Contact for Materials Research: Daniel Clark, <u>Daniel.clark@science.doe.gov</u>

Fusion science and technology has reached a level of maturity that calls for research to broaden from the plasma core of a fusion reactor toward a comprehensive fusion energy system. A Fusion Pilot Plant is one such system, and is expected to produce heat, particle, and neutron fluxes that significantly exceed those in present confinement facilities, requiring new approaches and materials to be developed and engineered for the anticipated extreme reactor conditions. Interlinked with this requirement are the key systems required to harness fusion power, breed

fuel, and ensure the safe operation of a reactor. In addition, magnets and heating/current drive system are integral features of magnetic fusion confinement systems and require advancement for a successful Fusion Pilot Plant. This research topic focuses on foundational fusion materials and technology research opportunities to enable improved performance and/or lower the costs of a Fusion Pilot Plant. This includes a focus on both experimental and theory/modeling efforts (including machine learning and artificial intelligence) that support advancing technology readiness levels in the specifical topical areas below:

- Development of plasma-facing materials and components
- Development of advanced structural and functional materials (including diagnostic materials)
- Development of breeder blanket concepts
- Development of tritium fuel cycle technologies
- Development of superconducting magnet technologies
- Development of plasma heating and current drive technologies
- Development of balance of plant technologies, including remote handling
 For more information, please refer to the 2021 FESAC Long-Range Plan and the following
 community reports: the 2012 Fusion Energy Sciences Advisory Committee (FESAC) report
 titled Opportunities for Fusion Materials Science and Technology Research Now and During the
 ITER Era (https://science.osti.gov/-/media/fes/pdf/workshop-reports/20120309/FESAC-Materials-Science-final-report.pdf), the 2015 workshop Report on Science Challenges and
 Research Opportunities in Plasma Materials Interactions https://science.osti.gov/-/media/fes/pdf/workshop-reports/2016/PMI_fullreport_21Aug2015.pdf), 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).

(9) Artificial Intelligence and Machine Learning for Fusion Energy Sciences Technical Contact: Matthew Lanctot, <u>matthew.lanctot@science.doe.gov</u>

The objective of the FES Artificial Intelligence and Machine Learning (AI/ML) activity is to support research on the development and application of AI/ML techniques that can have a transformative impact on FES mission areas. Among the areas supported are prediction of key plasma phenomena and plant states; plasma optimization and active plasma control augmented by AI/ML; plasma diagnostics enhanced by AI/ML methods; extraction of models from experimental and simulation data; and extreme data algorithms able to handle the amount and rate of data generated by fusion simulations and experiments at both existing and planned fusion user facilities.

Supported activities encompass multiple FES areas, including magnetic fusion, materials science, and discovery plasma science. Therefore, applications submitted to this topic should seek to advance not only a specific FES area through the application of existing AI/ML techniques, but should also further develop AI/ML techniques so they are adequate for fusion energy applications.

E. High Energy Physics (HEP)

Program Website: https://science.osti.gov/hep/
or https://science.osti.gov/hep/

The mission of the HEP program is to understand how the universe works at its most fundamental level, which is done 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: https://science.osti.gov/~/media/hep/hepap/pdf/May-2014/FINAL P5 Report Interactive 060214.pdf.

The HEP program focuses on three (3) experimental scientific frontiers:

<u>The Energy Frontier</u> - where powerful accelerators are used to create new particles, reveal their interactions, and investigate fundamental forces using highly sensitive experimental detectors;

<u>The Intensity Frontier</u> - where intense particle beams and highly sensitive detectors are used to pursue alternate pathways to investigate fundamental forces and particle interactions by studying events that occur rarely in nature, and to provide precision measurements of these phenomena; and

<u>The Cosmic Frontier</u> - where non-accelerator-based experiments use measurements of naturally occurring cosmic particles and observations of the universe to probe fundamental physics questions and offer new insight about the nature of dark matter, cosmic acceleration in the forms of dark energy and inflation in the early universe, neutrino properties, and other phenomena.

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 crosscutting research areas that enable new scientific opportunities by developing the necessary tools and methods for discoveries:

<u>Theoretical High Energy Physics</u>, 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

<u>Detector Research and Development</u>, 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 crosscutting research areas are collectively the six core research

subprograms supported by HEP. All applications should address specific research goals in one or more of the six research subprograms (as in the examples given below), explain how the proposed research or technology development supports the broad scientific objectives and mission of the HEP program, and aligns with its priorities. Applications where the investigator is proposing to conduct research across multiple HEP research subprograms during the project period will be considered, but PIs should note that in initial merit review of the applications, all applications are assigned to groups in one (and only one) subprogram area. In addition, applications that use modern data science approaches (e.g., artificial intelligence, machine learning, graph theory, uncertainty quantification, etc.) to accelerate scientific discovery of any of the HEP subprograms would be considered to be within the scope of that subprogram.

Additional information about the HEP research subprogram areas described above, and in areas (1) through (6) given below, may be found at https://science.osti.gov/hep/research/. Each of the research frontiers is described with a list of currently-supported experiments and facilities. PIs are encouraged to discuss their particular research interests, and how they relate to HEP's subprograms, with one of the technical contacts listed below.

Applications submitted to this FOA for support of *generic* (i.e., broadly applicable) HEP detector R&D efforts should be directed to the Detector Research and Development subprogram research area described below. However, applicants proposing physics studies and/or R&D efforts directed towards a *specific experiment* within an experimental frontier should submit their application to the relevant HEP scientific frontier subprogram research area.

HEP Research Subprogram Areas:

(1) Experimental Research at the Energy Frontier in High Energy Physics Technical Contact: Abid Patwa, 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, applications 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. Applications addressing physics studies and pre-conceptual R&D directed towards specific future Energy Frontier collider experiments are also accepted. Support for Heavy Ion Physics research is not provided under this research area.

(2) Experimental Research at the Intensity Frontier in High Energy Physics Technical Contact: Brian Beckford, brian.beckford@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. Applications addressing physics studies and pre-conceptual R&D directed towards specific future Intensity Frontier experiments are also accepted. Support for the Large Hadron Collider beauty experiment (LHCb) research or studies of neutrinoless double beta decay is <u>not</u> provided under this research area.

(3) Experimental Research at the Cosmic Frontier in High Energy Physics Technical Contact: Kathy Turner, 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 the study of cosmic acceleration by studying the nature of dark energy, planning the next-generation ground-based cosmic microwave background experiment to explore the inflationary epoch, and using direct-detection experiments to search for dark matter particles. Many of the experiments in the program also place constraints on neutrino masses. Measurements using high-energy cosmic rays, gamma rays and other phenomena are included, but at a lower priority. Applications 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 applications not specifically carried out as part of a particular Cosmic Frontier experimental collaboration should be directed to the *Theoretical Research in High Energy Physics* 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 not included in this research area.

(4) Theoretical Research in High Energy Physics Technical Contact: William Kilgore, <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 not included in this research area.

(5) Accelerator Science and Technology Research & Development in High Energy Physics Technical Contact: L.K. Len, lk.len@science.doe.gov

The Accelerator Science and 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, early-stage 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-power targets; 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 applications which are focused on accelerator uses outside of high-energy physics are now coordinated through the Accelerator Stewardship program under the DOE SC Engineering and Technology Office and are outside the scope of this program.

(6) Detector Research and Development in High Energy Physics Technical Contact: Helmut Marsiske, helmut.marsiske@science.doe.gov

The Detector R&D subprogram develops the next generation of instrumentation for HEP and fosters the next generation of detector experts. It supports research leading to fundamental advances in the science of particle and radiation detection, and the development of new, HEP-relevant technologies and 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. Applications should broadly align with the priority research directions identified in the report of the FY 2020 HEP Detector R&D Basic Research Needs study. Moreover, applications for "Blue-Sky" scientific research on innovative technologies not already in contention for implementation in

future HEP projects are strongly encouraged.

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.

F. Nuclear Physics (NP)

Program Website: https://science.osti.gov/np or https://science.osti.gov/np

The mission of the Nuclear Physics (NP) program is to discover, explore, and understand all forms of nuclear matter.

One of the enduring mysteries of the universe is the nature of matter—what are its basic constituents and how do they interact to form the properties we observe? The largest contribution by far to the mass of the matter we are familiar with comes from protons and heavier nuclei. 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.

The priority areas for NP include the following:

- Understanding how nucleons—protons and neutrons—combine to form atomic nuclei and what are the limits of nuclear existence in nature,
- Understanding how heavy nuclei have emerged since the origin of the Universe and continue to be created via nucleo-synthesis in cataclysmic cosmic events,
- Using particle accelerators to carry out tomography of the nucleon—the core building block of matter to understand how the quark and gluon fields inside the nucleon dynamically generate its properties including its mass and spin,
- Searching for undiscovered forms of nuclear matter,
- Searching for new physics via high precision, very high sensitivity measurements illuminating fundamental properties of the neutron and the neutrino as well as possible violations of well-established symmetries of nature, and
- Conceiving, constructing, and operating national scientific user facilities and developing novel detector and accelerator instrumentation.

Within each of these priority areas, unique nuclear physics opportunities to advance or benefit from Artificial Intelligence or Machine Learning, and new developments in Microelectronics are also of NP programmatic interest. Applicants are encouraged to contact the relevant subprogram manager.

To carry out its mission and address these priorities, the NP program addresses three broad, yet tightly interrelated, scientific thrusts: Quantum Chromodynamics; Nuclei and Nuclear Astrophysics; and Fundamental Symmetries and Neutrinos. NP supports basic research in seven subprograms or areas: Medium Energy, Heavy Ion, Nuclear Structure and Astrophysics, Fundamental Symmetries, Nuclear Theory and Nuclear Theory Computing, and Nuclear Data (1 through 6). The program is also the steward of Accelerator Research and Development for Current and Future Nuclear Physics Facilities (7). A comparatively new initiative in Quantum Information Science (QIS) (8) has been established to support this priority initiative of SC and leverage opportunities for Nuclear Physics to benefit from advances in this topical area.

The NP subprograms and their objectives follow:

(1) Medium Energy Nuclear Physics

Technical Contact: Gulshan Rai, gulshan.rai@science.doe.gov

Website: https://science.osti.gov/np/research/

The Medium Energy Nuclear Physics subprogram focuses primarily on understanding the structure of hadrons, how quarks move within a hadron and tests of the theory of the strong interaction, known as Quantum Chromodynamics (QCD). According to QCD, all observed nuclear particles, collectively known as hadrons, arise from the strong interaction of quarks, antiquarks, and gluons. The protons and neutrons inside nuclei are the best-known examples of hadrons. QCD, although difficult to solve computationally, predicts what hadrons exist in nature, and how they interact and decay. Specific questions addressed include: What is the internal landscape of the protons and neutrons (collectively known as nucleons)? What does QCD predict for the properties of strongly interacting matter? What governs the transition of quarks and gluons into pions (hadronic subatomic particle) and nucleons? What is the role of gluons and gluon self-interactions in nucleons and nuclei? The objectives of this subprogram are to develop a comprehensive picture of the spatial, momentum and angular momentum structure of the nucleon, elucidate quark confinement and hadron excitations, and understand the strong interaction in nuclei. Various experimental approaches are used to determine the distribution of "up", "down", and "strange" quarks, their antiquarks, and gluons within protons and neutrons, as well as clarifying the role of gluons in confining the quarks and antiquarks within hadrons. Polarized electron and proton beams are typically used to study the effects of the quark and gluon spins within nucleons, and the effect of the nuclear environment on the quarks and gluons. The subprogram also supports experimental searches for higher-mass "excited state" and exotic hadrons predicted by QCD, as well as studies of their various production mechanisms and decay properties. In pursuing these topics, the Medium Energy subprogram supports experimental research at the subprogram's primary research facility, the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF), and at other facilities, including the Relativistic Heavy Ion Collider (RHIC)

at Brookhaven National Laboratory (BNL) and the High Intensity Gamma Source (HIGS) at the Triangle Universities Nuclear Laboratory (TUNL). Also of interest are R&D of concepts and emerging technologies in Machine Learning and Artificial Intelligence that go beyond the simple use case for available software packages.

(2) Heavy Ion Nuclear Physics

Technical Contact: Kenneth Hicks, Kenneth. Hicks@science.doe.gov

Website: https://science.osti.gov/np/research/

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. Only two facilities in the world are capable of exploring the properties nuclear matter in these conditions, the U.S. Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory and the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN). 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 its temperature, the energy loss mechanism for quarks and gluons traversing the plasma, determining the speed of sound in the plasma, measuring the effect of the chiral magnetic force, understanding how quarks fragment and recombine to form hadronic matter (hadronization), and locating a possible critical point for the transition between the plasma and normal matter. Experimental research is carried out primarily using the RHIC facility and the Large Hadron Collider (LHC) at the European Organization for Nuclear Research (CERN).

Low Energy Nuclear Physics

The Low Energy subprogram has been separated into two distinct portfolios: that of Nuclear Structure and Astrophysics and Fundamental Symmetries.

(3) Nuclear Structure and Astrophysics

Technical Contact: Sharon Stephenson, sharon.stephenson@science.doe.gov

Website: https://science.osti.gov/np/research/

Nuclear Structure and Astrophysics addresses frontiers identified in the 2015 Long Range Plan for Nuclear Science: Nuclear Structure and Reactions, and Nuclear Astrophysics.

The atomic nucleus is at the core of all visible matter and comprises 99.9% of its mass. Its relevance spans dimensions from the proton radius to objects as large as stars, and covers the evolutionary history of the universe from fractions of a second after the Big Bang to today, 13.8 billion years later. The subfield of nuclear structure and reactions strives to measure, explain, and use nuclei to meet society's scientific interests and needs. The research addresses the underlying nature of atomic nuclei and the limits of their existence. It also aims to describe dynamical processes such as nuclear reactions and fission. The ultimate goal is to develop a predictive understanding of nuclei and their interactions grounded in fundamental QCD and electroweak

theory; furthermore, this understanding must be based on experimental data from a wide variety of nuclei.

Nuclear astrophysics addresses the role of nuclear physics in our universe. As a field at the interface of astrophysics and nuclear physics, it is concerned with the impact of nuclear processes on the evolution of the universe, the role of nuclear structure in influencing the evolution of the cosmos, and the cosmogenic origin of elements that are the building blocks of life. It is a broad discipline that can identify new observational signatures probing our universe. Nuclear astrophysics can identify the conditions at the very core of stars and provide a record of the violent history of the universe.

Major goals of this subprogram are to develop a comprehensive description of nuclei across the entire nuclear chart, to utilize rare isotope beams to reveal new nuclear phenomena and structures unlike those that are derived from studies using stable ion beams, and to measure the cross sections of nuclear reactions that power stars and spectacular stellar explosions and are responsible for the synthesis of the elements. Experimental research is currently carried out primarily using the Argonne Tandem Linac Accelerator System (ATLAS), a premier stable beam facility, as well as the Triangle Universities Nuclear Laboratory (TUNL), and the Texas A&M University Cyclotron Institute.

(4) Fundamental Symmetries

Technical Contact: Paul Sorensen, paul.sorensen@science.doe.gov

Website: https://science.osti.gov/np/research/

This subprogram investigates aspects of the third thrust, Fundamental Symmetries and Neutrinos. Questions addressed in Fundamental Symmetries 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? Specifically, the subprogram seeks to support: research to measure the neutrino mass and to determine if the neutrino is its own antiparticle; experiments with cold and ultra-cold neutrons to investigate the dominance of matter over antimatter in the universe, and to determine the lifetime of the neutron; experiments to illuminate the fundamental symmetries of nature through precise measurements of beta decay and searches for anomalous parity violation; research on other aspects of Fundamental Symmetries and Interactions involving nuclei. A major focus of this sub program is furthering progress towards a major priority of the 2015 Long Range Plan for Nuclear Physics, Reaching for the Horizon: the implementation of a ton-scale neutrino-less double beta decay experiment to determine whether the neutrino is its own anti-particle.

(5) Nuclear Theory and Nuclear Theory Computing

Technical Contact: Xiaofeng Guo, xiaofeng.guo@science.doe.gov; Paul Sorensen,

Paul.Sorensen@science.doe.gov;

Website: https://science.osti.gov/np/esearch/

The Nuclear Theory subprogram provides the theoretical support needed to interpret the wide

range of data obtained from the experimental nuclear science subprograms and to advance new ideas and hypotheses that identify potential areas for future experimental investigations. 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 OCD (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, internal structure of nucleons and nuclei at sub-femtometer distance in terms of quarks and gluons and their dynamics, 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 highprecision studies of cold neutrons.

Nuclear Theory Computing supports research in nuclear physics with "extreme" computational requirements, which has been enabled by the advent of high performance computing (HPC). Funding for HPC-driven NP research is provided primarily through the programs Scientific Discovery through Advanced Computation (SciDAC) and the new Exascale Computing Project (ECP), through joint projects with the ASCR. The NP SciDAC projects are five-year multisite collaborations on specific projects in computational nuclear physics, funded jointly by NP and ASCR, and closely aligned with the needs of the NP experimental program. These projects investigate 1) the properties of nuclei, using state-of-the- art models and numerical techniques; 2) the properties of strongly interacting particles (hadrons) composed of quarks and gluons, as predicted by the fundamental theory QCD; 3) the internal structure of nucleons and nuclei at subfemtometer distance in terms of quarks and gluons; 4) computational nuclear astrophysics, including the synthesis of the heavier elements in supernovae and neutron star mergers, and their observables effects. The two current NP ECP projects are addressing changes needed in computational NP practice in the Exascale Era, in the areas of 1) lattice QCD, and 2) nuclear astrophysics. Some computational resources needed for HPC research on NP

(6) Nuclear Data

Technical Contact: Keith Jankowski, Keith.Jankowski@science.doe.gov

Website: https://science.osti.gov/np/research/

The mission of the United States Nuclear Data Program (USNDP) is to provide current, accurate, authoritative data for workers in pure and applied areas of nuclear science and engineering. This is accomplished primarily through the compilation, evaluation, dissemination, and archiving of extensive nuclear datasets. The USNDP also addresses gaps in the data, through targeted experimental studies and the use of theoretical models. A continuing interagency program of

experiments led by NP continues to address critical gaps in nuclear data and modernization of nuclear data curation by incorporating new tools such as AI/ML. The USNDP involves the efforts of ~ 50 nuclear physicists at ~ 15 national labs, research centers, institutes and universities, and is an important resource for workers in a wide range of pure and applied topics in nuclear physics. Research opportunities in Nuclear Data include both experimental and theoretical work in areas including, but not limited to basic nuclear science, nuclear energy, and nuclear non-proliferation applications, as well as improvements to the nuclear data pipeline (data collection, curation, evaluation, and dissemination).

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

Technical Contact: Manouchehr Farkhondeh, <u>manouchehr.farkhondeh@science.doe.gov</u> Website: <u>https://science.osti.gov/np/research/</u>

The 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 R&D of technologies for the Brookhaven National Laboratory's Relativistic Heavy Ion Collider (RHIC), with heavy ion and polarized proton beams; linear accelerators such as the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF); development of devices and/or methods that would be useful in the generation of intense rare isotope beams for 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), and R&D in accelerator science and technology in support of next generation Nuclear Physics accelerator facilities such as an electron-ion collider (EIC). Also of interests are 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. Research aimed at transformative advances in ion sources, superconducting radiofrequency, and beam cooling is also encouraged.

(8) NP - Quantum Information Science (QIS)

Technical Contact: Gulshan Rai, gulshan.rai@science.doe.gov

Website: https://science.osti.gov/np/Research/Quantum-Information-Science

Quantum Horizons: QIS Research and Innovation for Nuclear Science is a new initiative to identify, prioritize, and coordinate emerging opportunities in both fundamental research and applied challenges at the interface of Nuclear Physics and Quantum Information Science and Technology (QIST). QIS is a rapidly developing interdisciplinary field and has been identified as an important cross-cutting topic and where continued leadership is critically important to our nation's national security and economic competitiveness. Emerging priority areas in QIS provide new opportunities to address challenges of enormous interest and complexity in NP.

NP's Quantum Horizons emphasizes the science-first approach and supports research that could, in the long-term, have a transformative impact on the NP mission area and/or advance QIS development 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. Topics may include quantum computation, quantum simulations and simulators, quantum sensing, quantum-enhanced nuclear physics detectors, nuclear many-body problems, 'squeezed' quantum states, nuclear qubits, quantum entanglement, and implementation of NP theories on quantum hardware, as well as other novel areas of basic research and technologies. Topics and subject areas which are outside the scope of NP's Quantum Horizons initiative are listed in the Financial Assistance Opportunity (FOA) 0002514. This document may be accessed at: https://science.osti.gov/-/media/grants/pdf/foas/2021/SC FOA 0002514.pdf

This subprogram specifically encourages the exploitation of the interdisciplinary nature of Quantum Computing and QIST to expand the frontiers of the NP program and the national QIS enterprise through partnerships with Universities, National Laboratories and Industry. Prospective investigators are encouraged to contact the subprogram manager.

G. Isotope R&D and Production (DOE IP)

Program Website: https://science.osti.gov/Isotope-Research-Development-and-Production

The mission of the DOE Isotope Program (DOE IP) is to produce and distribute critical radioactive and enriched stable isotopes that are in short supply or not produced in the U.S. The DOE IP ensures national preparedness for isotope production and distribution by maintaining mission readiness of relevant national infrastructure and core competencies to ensure functionality even during times of national crisis; conducts advanced R&D to develop innovative technology and advanced radiochemical separations and purifications and mitigates U.S. dependence on foreign supplies of isotopes to ensure robust domestic supply chains. The DOE IP lies at the intersection of many scientific areas including nuclear and radiochemistry, nuclear physics, accelerator and nuclear reactor science, materials science and engineering, separations science, and nuclear data to name a few.

Isotopes are high-priority commodities of strategic importance for the Nation and are essential in medical diagnosis and treatment, discovery science, national security and preparedness, industrial processes and advanced manufacturing, space exploration and communications, biology, archaeology, quantum science, clean energy, environmental science, and other fields. Isotopes can directly enable emerging technology and contribute to the economic, technical and scientific strength of the United States. Facilities utilized include particle accelerators, nuclear research reactors, enrichment technologies, and radiochemical processing capabilities throughout the national laboratory complex and at universities. Unique facilities stewarded by the DOE IP are located at Brookhaven National Laboratory, Los Alamos National Laboratory, Argonne National Laboratory, and Oak Ridge National Laboratory.

DOE IP supports world-leading R&D associated with creating innovative and more efficient isotope production and processing techniques, including advanced targetry, artificial intelligence (AI) and machine learning (ML), robotics, automation and advanced manufacturing concepts. Research, development, and fabrication of equipment directed toward research in any DOE IP relevant topic may be proposed, but applications including extensive projects requiring detailed

review of scope, budget, and schedule beyond the procedures for this announcement will not be considered. Applications 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, DOE IP does not support investigations into the development of particle accelerators or nuclear reactors for purposes outside the scope of the DOE IP topics listed below. It is also important to note that applications related to the production of Mo-99 are specifically excluded from this solicitation, as this isotope is under the purview of the National Nuclear Security Administration Office of Materials Management and Minimization.

A primary document released by the Nuclear Science Advisory Committee - Subcommittee on Isotopes (NSAC-I) which is currently guiding DOE IP priorities is entitled "Meeting Isotope Needs and Capturing Opportunities for the Future: The 2015 Long Range Plan for the DOE-NP Isotope Program." The document may be accessed at: https://science.osti.gov/~/media/np/nsac/pdf/docs/2015/2015_NSACI_Report_to_NSAC_Final.pdf.

While not an exhaustive list, below are five broad topics of interest to the DOE IP research and development portfolio. These topics seek development of advanced, cost-effective, and efficient technologies for producing, processing (including isotopic separations, and the development of biological tracers), extracting. recycling, and distributing isotopes in short supply.

(1) Isotope Production Research Technical Contact: Ethan Balkin, ethan.balkin@science.doe.gov

Applications to this topic should be focused on novel or improved capabilities for inducing transmutation of atoms in targets to create radioisotopes. This includes aspects of targetry and target fabrication, as well as the development of innovative approaches, including integration of Artificial Intelligence and Machine Learning techniques to model and predict the behavior of targets undergoing irradiation to optimize yield and minimize target failures during routine isotope production. It is understood that accelerator- and reactor-based isotope production have different considerations. Applications to this topic can address either production modality. Robotics and advanced manufacturing techniques, as they apply to isotope production and processing, may also be proposed.

(2) Isotope Processing and Purification Technical Contact: Ethan Balkin, ethan.balkin@science.doe.gov

This topic includes, but is not limited to, the improvement and/or development of novel chemical and physical processes to recover and purify radioisotopes from activated targets. Development of automated production and processing techniques to enhance the efficiency and safety of radioisotope production (including uses of Artificial Intelligence or Machine Learning) are also encouraged.

(3) Nuclear Chemistry and Radiochemical Separations Technical Contact: Ethan Balkin, ethan.balkin@science.doe.gov

Work in this topic might be directed toward isotopes not necessarily resulting from direct transmutation of target material (e.g., the recovery and purification of radioisotopes from legacy materials, facility components, used nuclear fuel, or waste streams of other processing efforts). Automation of production and processing techniques or facilities to enhance the efficiency and safety (including uses of Artificial Intelligence or Machine Learning) would also be applicable here.

(4) Biological Tracers and Imaging

Technical Contact: Ethan Balkin, ethan.balkin@science.doe.gov

Work in this topic should be focused on the development of isotopes and or chemical constructs which have physical or chemical properties that make them particularly useful as biological tracers and/or imaging agents. Included in this topic are the synthesis and development of novel chelating agents or other ligands. Please note that the DOE IP funds only basic science R&D. Studies investigating the applications of isotopes will not be considered for funding.

(5) Isotopic Enrichment Technology Technical Contacts: April Gillens, <u>april.gillens@science.doe.gov</u>

DOE IP is presently making significant investments in the establishment of a broad-scope stable isotope enrichment capability using gas centrifuge and electromagnetic ion separation (EMIS) technologies, as well as a modest radioisotope EMIS investment. Therefore, new applications aimed at stable and radioisotope enrichment should utilize technologies other than gas centrifuge and electromagnetic ion separation. Applications involving energy and feedstock efficient enrichment technologies are also acceptable.

H. Accelerator R&D and Production (ARDAP)

(1) Accelerator R&D and Production

Technical Contact: Eric Colby, Eric.Colby@science.doe.gov

The mission of the Office of Accelerator R&D and Production (ARDAP) program is to ensure a robust pipeline of next-generation Accelerator Science & Technology to support physical sciences research while providing technology advances and industrial strength that position the U.S. to lead the world for decades to come. A key aspect of this mission is to develop a workforce with expertise in effective technology transfer R&D and accelerator component engineering, including manufacturing risk and cost reduction and high efficiency accelerator technologies.

ARDAP is particularly interested in early career scientists and engineers who can bridge the gap between basic research and industrial adoption and production of accelerator technology. In addition to strong accelerator science and engineering skills, closely-coupled expertise in design

for manufacture, manufacturing risk reduction, supply chain analysis and risk reduction, application of advanced manufacturing techniques, and application of data science techniques to improve accelerator component production are each of interest.

The successful applicant will be expected to work on cross-cutting R&D in accelerator science and technology that benefits multiple Office of Science programs and to devote a significant portion of the Early Career Award effort to working closely with one or more domestic technology companies on collaborative R&D, technology transfer, and the eventual industrialization of accelerator technology.

Applicants who seek to focus on accelerator science or engineering for a specific Office of Science facility should apply under that program's research topic.

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.

All entities submitting applications to this FOA must recognize the moral and legal obligations to comply with export controls and policies that limit the transfer of technologies with potential dual use. Applicants are reminded that international activities must comply with nonproliferation, sanction, and other protocols described at https://www.export.gov.

International activities related to special nuclear materials (SNM) are subject to additional requirements. Please see 10 CFR 810 for further information.

This FOA is to support scientific endeavors that could be described in scholarly publications. Do not submit applications containing restricted data or unclassified nuclear information as defined in the Atomic Energy Act of 1954, as amended, 42 USC 2011 et seq., 10 CFR 1017, 10 CFR 1045.

Section II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT

DOE anticipates awarding grants and National Laboratory authorizations under this FOA.

B. ESTIMATED FUNDING

DOE anticipates that, subject to the availability of future year appropriates, a total of \$100,000,000 in current and future fiscal year funds will be used to support awards under this FOA.

DOE is under no obligation to pay for any costs associated with preparation or submission of applications. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this FOA.

C. MAXIMUM AND MINIMUM AWARD SIZE

The award size will depend on the number of meritorious applications and the availability of appropriated funds. The ceiling and floor described in this FOA represent the expected range of award sizes.

Ceiling

Historically, the average award for an Institution of Higher Education has been \$750,000 for five years and the average award for a DOE National Laboratory has been \$2,500,000 for five years. Requests for budget amounts larger than the average require sufficient justification.

Floor

The minimum request for awards to an Institute of Higher Education is approximately \$750,000 over five years and the minimum request for awards to a DOE National Laboratory is approximately \$2,500,000 over five years. DOE National Laboratories awards must cover at least 50% of the PI salary.

Additional Notes

Requested funding may vary year-by-year to accommodate the real and expected needs of the proposed research. The average Early Career Research award supports the PI (i.e., up to three months summer salary for university-based PIs, and at least 50% of time and effort for other PIs), research staff under the PI's direction (including postdocs and graduate students), equipment (including fabrication), and other necessary costs (materials, supplies, and travel).

D. EXPECTED NUMBER OF AWARDS

DOE anticipates up to 65 awards under this FOA. Historically, there have been an average of approximately 20 national laboratory awards and 45 university awards each year. The exact

number of awards will depend on the number of meritorious applications and the availability of appropriated funds.

E. ANTICIPATED AWARD SIZE

DOE expects the typical award size will be in a narrow range around \$750,000 over five years for an Institute of Higher Education and around \$2,500,000 over five years for a DOE National Laboratory.

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 application; (3) submission of required reports; and (4) compliance with the terms and conditions of the award.

G. TYPE OF APPLICATION

DOE will accept new applications under this FOA.

Section III – ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS

In accordance with 2 CFR 910.126, Competition, eligibility for award is restricted to U.S. Institutes of Higher Education and DOE National Laboratories.

Applicants must adhere to the eligibility standards below.

The act of submitting an application implies that the submitting institution has checked, confirmed, and certifies that the PI is eligible, as outlined in Section III C and D.

1. DOE/NNSA National Laboratories

DOE/NNSA National Laboratories are eligible to submit applications under this FOA. If recommended for funding as a lead applicant, funding will be provided through the DOE Field-Work Proposal System. If recommended for funding as a proposed subawardee, the value of the proposed subaward will be removed from the prime applicant's award and will be provided to the laboratory through the DOE Field-Work Proposal System. Additional instructions for securing authorization from the cognizant Contracting Officer are found in Section VIII of this FOA.

The cover page for each pre-application and the title page of each application must be signed by the national laboratory director confirming that the proposed research idea fits within the scope of SC-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. In the case that a different senior lab official must sign, documentation must be included that indicates authorization from the director to the signing official.

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 SC funded programs encourages the laboratory to actively plan to address funding transition issues that may arise when an award ends.

Applications 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.

2. Institutes of Higher Education

U.S. academic institutions are eligible to submit applications under this FOA. 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 above must also be met.

B. COST SHARING

Cost sharing for basic and fundamental research is not required pursuant to an exclusion from the requirements of Section 988 of the Energy Policy Act of 2005.

C. ELIGIBLE INDIVIDUALS

Eligible individuals with the skills, knowledge, and resources necessary to carry out the proposed research as a PI are invited to work with their organizations to develop an application for assistance. Individuals from underrepresented groups as well as individuals with disabilities are always encouraged to apply for assistance.

There can be no co-PIs.

PIs who have received awards previously under the SC Early Career Research Program are not eligible. PIs 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.

No more than 10 years can have passed between the year the PI's Ph.D. was awarded and 2021. For the present competition, those who received doctorates no earlier than 2011 are eligible. If a PI 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 (three 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 and Medical Leave Act. Requests for extended eligibility must be made by including in the pre-application a letter signed by the dean, research vice president, laboratory division director, or equivalent official stating that the proposed PI will have, as of the application deadline, no more than 10 years of full-time professional work experience in positions requiring a Ph.D. in the field in which the application will be submitted. The request for an eligibility extension will be evaluated as part of the pre-application assessment.

PIs from DOE National Laboratories and Institutes of Higher Education must adhere to the respective eligibility standards below.

The eligibility requirements improve the quality of applications submitted and encourages those who are strong candidates to submit applications to the program.

1. PIs from DOE National Laboratories

The PI must be a full-time, permanent, non-postdoctoral national laboratory employee as of the deadline for the application. If a PI has multiple doctorates, the discipline of the one they have earned within the 10-year eligibility window should be relevant to the proposed research.

2. PIs from Institutes of Higher Education

The PI must be an **untenured** Assistant Professor on the tenure track or an **untenured** Associate Professor on the tenure track at a U.S. academic institution as of the deadline for the application. The PI must be employed in the eligible position as of the closing date for this FOA. If a PI has multiple doctorates, the discipline of the one they have earned within the 10-year eligibility window should be relevant to the proposed research.

D. LIMITATIONS ON SUBMISSIONS

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

Only one application on behalf of a PI may be submitted in any given SC Early Career Research Program competition. A PI may not participate in more than three SC Early Career Research Program competitions.

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

Letters of recommendation and department chair letters are not allowed. Applications that include recommendation or department chair letters will be subject to elimination from consideration during DOE's initial review.

Section IV – APPLICATION AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST APPLICATION PACKAGE

Application forms and instructions are available at Grants.gov. To access these materials, go to https://www.Grants.gov, select "Search Grants", and then enter the Catalog of Federal Domestic Assistance (CFDA) number (81.049) and/or the FOA number shown on the cover of this FOA. Select the "Apply" button to access the application package.

Applications submitted through <u>www.FedConnect.net</u> will not be accepted. Applications may not be submitted through PAMS at https://pamspublic.science.energy.gov.

B. LETTER OF INTENT (LOI) AND PRE-APPLICATION

1. Letter of Intent (LOI)

Not applicable.

2. Pre-application

PRE-APPLICATION DUE DATE

The pre-application due date is printed on the cover of the FOA.

ENCOURAGE/DISCOURAGE DATE

The pre-application response date is printed on the cover of the FOA.

A pre-application is required and must be submitted by the date indicated on the cover of the FOA.

Pre-applications will be reviewed for responsiveness of the proposed work to the research topics identified in this FOA. DOE will send a response by email to each applicant encouraging or discouraging the submission of an application by the date indicated on the cover of the FOA. Applicants who have not received a response regarding the status of their pre-application by this date are responsible for contacting the program to confirm this status.

Applications that have not been encouraged by DOE may be declined without merit review.

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

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

Year Doctorate Awarded: XXXX Number of Times Previously Applied†: Topic Area*:

Eligibility Extension Requested: (Yes/No – see below**)
FOA Number: Include the FOA Number indicated on the cover of this FOA

- † Indicate how many times the PI has previously submitted a full application in the SC Early Career Research Program. The program has been offered in twelve previous years, FY 2010 FY 2021. Participation in the competition is defined as submission of a full, formal application that was not withdrawn prior to official declination of the application. A PI who has participated in three past SC Early Career Research Program competitions is not eligible.
- ** Extensions to eligibility will be considered for individuals who have had a major life event requiring an extended absence (three months or longer) from the workplace, including active military service or an absence due to personal disability or covered by the Family Medical Leave Act, or other similar reasons. Requests for extended eligibility must be made by including in the pre-application a letter signed by the dean, research vice president, laboratory division director, or equivalent official stating that the proposed PI will have, as of the application deadline, no more than 10 years of full-time professional work experience in positions requiring a Ph.D. in the field in which the application will be submitted. The request for an eligibility extension will be evaluated as part of the pre-application assessment.
- * The topic area descriptions can be found in <u>Section I, Funding Opportunity Description</u> 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 Section I.

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

In addition, the pre-application must include a listing of individuals who should or should not serve as merit reviewers of a subsequent application. Detailed instructions for how to craft such a listing are provided in <u>Section VIII</u> of this FOA. This listing will not count toward the pre-application's page limit. The list of individuals must be converted to a PDF file and appended to your pre-application for submission through the PAMS website at https://pamspublic.science.energy.gov.

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

PRE-APPLICATION REVIEW

Program Managers may evaluate all or some portion of pre-applications to determine their competitiveness within a scientific topic.

Any review will be based on the following criteria:

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

Any such review will be conducted by no less than three federal program managers chosen for their topical knowledge and diversity of perspective.

Reviews within a topical field will be a comparative review with priority given to scientifically innovative and forward-looking basic research with the highest likelihood of success as an application. The results of the review will be documented.

Applicants with the highest rated pre-applications will be encouraged to submit applications; others will be discouraged from submitting applications. Written feedback about pre-applications will be provided after the deadline for the receipt of applications.

Topics with comparatively few pre-applications may not make use of such pre-application reviews. The ratio of encourage/discourage results will differ between topical subjects.

SC is committed to ensuring that a sufficient number of applicants will be encouraged to submit applications to foster a competitive merit review of the applications. SC's intent in discouraging submission of certain applications is to save the time and effort of applicants in preparing and submitting applications with a negligible likelihood of success.

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

PRE-APPLICATION SUBMISSION

The pre-application must be submitted electronically through the DOE SC Portfolio Analysis and Management System (PAMS) website https://pamspublic.science.energy.gov/.

Applicants are strongly encouraged to inform their DOE Program Manager if teaming arrangements, proposed personnel, topics, or the anticipated title change between submitting the

pre-application and when an application is submitted, to ensure that their application is properly linked to their pre-application and that reviewers are properly assigned to the application.

Detailed instructions about how to submit a pre-application are in <u>Section VIII</u> of this FOA.

C. GRANTS.GOV APPLICATION SUBMISSION AND RECEIPT PROCEDURES

Applications in response to this FOA must be submitted through Grants.gov. Detailed instructions for registering in and using Grants.gov are in <u>Section VIII</u> of this FOA.

D. CONTENT AND APPLICATION FORMS

LETTERS

Letters of recommendation are not allowed. A department chair letter is not required and should not be included. Applications 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. SF-424 (R&R)

Complete this form first to populate data in other forms. Complete all the required fields in accordance with the pop-up instructions on the form. The list of certifications and assurances referenced in Field 17 is available on the DOE Financial Assistance Forms Page at https://energy.gov/management/office-management/operational-management/financial-assistance-forms under Certifications and Assurances. Applicants are bound by their representations and certifications in SAM.gov.

DUNS/UEI AND EIN NUMBERS (FIELDS 5 AND 6)

The DUNS/UEI and Employer Identification Number (EIN) fields on the SF-424 (R&R) form are used in PAMS to confirm the identity of the individual or organization submitting an application.

- Enter each number as a nine-digit number.
- Do not use hyphens or dashes.
- SC does not use the 12-digit EIN format required by some other agencies.
- SC does not use the DUNS+4 format.

Type of Application (Field 8)

A **new** application is one in which DOE support for the proposed research is being requested for the first time.

Only new applications will be accepted under this FOA.

SC does not make use of the Resubmission or Continuation options.

Please answer "yes" to the question "Is this application being submitted to other agencies?" if substantially similar, identical, or closely related research objectives are being submitted to another Federal agency. Indicate the agency or agencies to which the similar objectives have been submitted.

2. Research and Related Other Project Information

Complete questions in fields 1 through 6 of the SF-424 Research and Related Other Project Information form.

Note regarding question 4.a. and 4.b.:

If any environmental impact, positive or negative, is anticipated, indicate "yes" in response to question 4.a., "potential impact – positive or negative - on the environment." Disclosure of the impact should be provided in response to question 4.b. First indicate whether the impact is positive or negative and then identify the area of concern (e.g., air, water, exposure to radiation, etc.). Should the applicant have any uncertainty, they should check "yes."

DOE understands the phrase in field 4.a., "potential impact ... negative" to apply if the work described in the application could potentially have any of the impacts listed in (1) through (5) of 10 CFR 1021, Appendix B, Conditions that Are Integral Elements of the Classes of Action in Appendix B. (https://www.ecfr.gov)

Additionally, for actions which could have any other adverse impacts to the environment or have any possibility for adverse impacts to human health (e.g., use of human subjects, Biosafety Level 3-4 laboratory construction/operation, manufacture or use of certain nanoscale materials which are known to impact human health, or any activities involving transuranic or high level radioactive waste, or use of or exposure to any radioactive materials beyond de minimis levels), applicants should indicate a "negative" impact on the environment.

Lastly, 1) if there would be extraordinary circumstances (i.e., scientific or public controversy) related to the significance of environmental effects (10 CFR 1021.410 (b)(2)), 2) if the work is connected to other actions with potentially significant impacts (10 CFR 1021.410 (b)(3), or 3) if the work is related to other nearby actions with the potential for cumulatively significant impacts (10 CFR 1021.410 (b)(3)), applicants should indicate a "negative" impact on the environment.

The bulk of your application will consist of files attached to the Research and Related Other Project Information form. The files must comply with the following instructions:

PROJECT SUMMARY/ABSTRACT (FIELD 7 ON THE FORM)

The project summary/abstract is a summary of the proposed activity suitable for distribution to the public and sufficient to permit potential reviewers to identify conflicts of interest. It must be a self-contained document. Provide the name of the applicant, the project title, the PI and the PI's institutional affiliation, any coinvestigators and their institutional affiliations, the objectives of the project, a description of the project, including methods to be employed, and the potential impact of the project (i.e., benefits, outcomes). A sample is provided below:

Project Title

A. Smith, Lead Institution (Principal Investigator)
A. Brown, Institution 2 (Co-Investigator)
A. Jones, Institution 3 (Co-Investigator)

Text of abstract

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

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

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

DOE TITLE PAGE

(PART OF PROJECT NARRATIVE ATTACHED TO FIELD 8 ON THE FORM)

The application narrative must begin with a title page that will not count toward the project narrative page limitation. The title page must include the following items:

- The project title:
- Applicant/Institution:
- Street Address/City/State/Zip:
- Postal Address:
- Principal Investigator (PI) name:
- Position title for PI:
- PI telephone number, email:
- Administrative Point of Contact name, telephone number, email:
- FOA Number:
- DOE/SC Program Office (ASCR, BER, BES, FES, HEP, NP, DOE IP, or ARDAP):
- Topic Area*:
- DOE/SC Program Office Technical Contact:
- Year Doctorate Awarded:
- Eligibility Extension Included in Approved Pre-application: (yes or no)
- If at a University, is the PI in a tenure-track appointment?: (yes or no)
- Does the PI have tenure: (Yes or No)?
- Number of Times Previously Applied†:
- PAMS Preproposal (Pre-application) 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)?
- * The topic area can be found in Section I 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.
- † Indicate how many times the PI has previously submitted a full application in the SC Early Career Research Program. The program has been offered in twelve previous years, FY 2010 FY 2021. Participation in the competition is defined as submission of a full, formal application that was not withdrawn from consideration prior to official declination of the application. 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 applications 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 FOA, 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 FOA.
- ↓ SC will decline without review any application without an encouraged pre-application and may decline without review any application without a data management plan.

Important Instructions to the Sponsored Research Office of Submitting Institutions: SC requires that you create one single machine-readable PDF file that contains the DOE Title Page, project narrative, biographical sketch, current and pending support, bibliography and references cited, facilities and other resources, equipment, data management plan, and other attachments. This single PDF file may not be scanned from a printed document and must be attached in Field 8 on the Grants.gov form. You are strongly encouraged to submit the combined research narrative file through a "Print to PDF" or equivalent process to ensure that all content is visible in the one PDF file. Do not attach any of the items listed in this paragraph separately in any other field in Grants.gov. If you do, these additional attachments will not become part of the application in PAMS.

PROJECT NARRATIVE (FIELD 8 ON THE FORM)

The project narrative **must not exceed a page limit of 15 pages** of technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard letter-size (8.5 inch x 11 inch) paper with 1-inch margins (top, bottom, left, and right). The 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 Title Page, Budget Page(s), Budget Justification, biographical material, publications and references, and appendices, each of which may have its own page limit defined later in this FOA.

Do not include any websites (URLs) that provide supplementary or additional information that constitutes a part of the application. Merit reviewers are not required to access websites; however, Internet publications in a list of references will be treated identically to print publications. See Section VIII for instructions on how to mark proprietary application information. To attach a Project Narrative, click "Add Attachment."

The Project Narrative comprises the research plan for the project. It should contain enough background material in the Introduction, including a brief review of the relevant literature and any prior research in this area, to demonstrate sufficient knowledge of the state of the science. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also include a timeline for the major activities of the proposed project, and should indicate which project personnel will

be responsible for which activities. There should be no ambiguity about which personnel will perform particular parts of the project, and the time at which these activities will take place.

The following organization of the Project Narrative is suggested:

- **Background/Introduction**: Explanation of the importance and relevance of the proposed work as well as a review of the relevant literature.
- **Project Objectives:** This section should provide a clear, concise statement of the specific objectives/aims of the proposed project.
- **Proposed Research and Methods**: Identify the hypotheses to be tested (if any) and details of the methods to be used including the integration of experiments with theoretical and computational research efforts.
- **Timetable of Activities**: Timeline for all major activities including anticipated milestones and deliverables.

The Project Narrative is considered the intellectual work of the proposed researchers. Concurrent submission of the same or substantially similar narratives attributed to different researchers may constitute academic dishonesty or research misconduct.

Do not attach any of the requested appendices described below as files for fields 9, 10, 11, and 12 in Grants.gov. Follow the below instructions to include the information as appendices in the single, bundled project narrative file.

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the PI and each senior/key person listed in Section A on the R&R Budget form.

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

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

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

The PI and each senior/key person at the prime applicant and any proposed subaward must provide a list of all sponsored activities, awards, and appointments, whether paid or unpaid; provided as a gift with terms or conditions or provided as a gift without terms or conditions; full-time, part-time, or

voluntary; faculty, visiting, adjunct, or honorary; cash or in-kind; foreign or domestic; governmental or private-sector; directly supporting the individual's research or indirectly supporting the individual by supporting students, research staff, space, equipment, or other research expenses. All foreign government-sponsored talent recruitment programs must be identified in current and pending support.

APPENDIX 2: CURRENT AND PENDING SUPPORT

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

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

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

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 10 coauthors of archival publications, you may use an abbreviated style such as the *Physical Review Letters* (PRL) convention for citations (listing only the first author). For example, your paper may be listed as, "A Really Important New Result," A. Aardvark et. al. (MONGO Collaboration), PRL 999. Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the application. Provide the Bibliography and References Cited information as an appendix to your project narrative.

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

APPENDIX 4: FACILITIES & OTHER RESOURCES

This information is used to assess the capability of the organizational resources, including subrecipient 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. Such documents, provided that they do not become letters of support or recommendation, may be printed on any letterhead. Please provide the Facility and Other Resource information as an appendix to your project narrative.

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

APPENDIX 5: EQUIPMENT

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

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

APPENDIX 6: DATA MANAGEMENT PLAN

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

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

The standard requirements for a DMP may be found in Section VIII of this FOA.

APPENDIX 7: OTHER ATTACHMENT

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

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

REMINDERS REGARDING ALL APPENDICES

- 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. Research and Related Budget

Complete the Research and Related Budget form in accordance with the instructions on the form (Activate Help Mode to see instructions) and the following instructions. You must complete a separate budget for each year of support requested. The form will generate a cumulative budget for the total project period. You must complete all the mandatory information on the form before the NEXT PERIOD button is activated. You may request funds under any of the categories listed as long as the item and amount are necessary to perform the proposed work, meet all the criteria for allowability under the applicable Federal cost principles, and are not prohibited by the funding restrictions in this FOA.

Additional information is found in Section VIII of this FOA.

BUDGET JUSTIFICATION (FIELD L ON THE FORM)

Provide a justification that explains all costs proposed in the budget. The following items of advice are offered to assist you in developing a justification.

- Organize the justification by listing items in the same order as presented on the budget.
- Ensure that the narrative matches the budget in dollar amounts and language.
- Explain the line items. If costs are estimated, provide a basis for the estimate. Explain if costs are based on prior experience of similar activities. If a cost is based on the product of two numbers (such as a number of items at a per-item price), ensure that your math is correct.
- If including an inflationary factor for future budget periods, explain the basis for the inflationary factor.

Provide any other information you wish to submit to justify your budget request. Including items in the budget justification is not considered a form of cost-sharing: Provide the details of all personnel (key or other) who will be working on the award, regardless of their source(s) of compensation. Explain their source(s) of compensation if it is not from this award. Include the indirect cost rate agreement as a part of the budget justification.

Attach a single budget justification file for the entire project period in field L. The file automatically carries over to each budget year.

Additional information is found in Section VIII of this FOA.

4. R&R Subaward Budget Attachment(s) Form

Budgets for Subawards: You must provide a separate R&R budget and budget justification for each subrecipient. Download the R&R Budget Attachment from the R&R SUBAWARD BUDGET ATTACHMENT(S) FORM and either email it to each subrecipient that is required to submit a separate budget or use the collaborative features of Workspace. After the subrecipient has either emailed its completed budget back to you or completed it within Workspace, attach it to one of the blocks provided on the form. Use up to 10 letters of the subrecipient's name

(plus.pdf) as the file name (e.g., ucla.pdf or energyres.pdf). Filenames must not exceed 50 characters.

If the project involves more subrecipients than there are places in the SUBAWARD BUDGET ATTACHMENT(S) FORM, the additional subaward budgets may be saved as PDF files and appended to the Budget Justification attached to Field L.

Applicants should consult their local information technology ("IT") support resources for any necessary assistance in converting the forms downloaded from Grants.gov into plain PDF files that can be combined into one non-Portfolio PDF file (the Budget Justification).

Ensure that any files received from subrecipients are the PDF files extracted from the SUBAWARD BUDGET ATTACHMENT(S) FORM. Errors will be created if a subrecipient sends a prime applicant a budget form that was not extracted from the application package.

Note: If an application proposes subawards to a DOE/NNSA National Laboratory, a Federal agency, or another Federal agency's FFRDC, the value of such proposed subawards may be deducted from any resulting award: Those classes of organizations may be paid directly by SC. However, the details of such proposed budgets are an essential for understanding and analyzing the proposed research.

5. Project/Performance Site Location(s)

Indicate the primary site where the work will be performed. If a portion of the project will be performed at any other site(s), identify the site location(s) in the blocks provided.

Note that the Project/Performance Site Congressional District is entered in the format of the two-digit state code followed by a dash and a three-digit Congressional district code, for example VA-001. Hover over this field for additional instructions.

Use the Next Site button to expand the form to add additional Project/Performance Site Locations.

6. Disclosure of Lobbying Activities (SF-LLL)

If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the grant/cooperative agreement, you must complete and submit Standard Form - LLL, "Disclosure Form to Report Lobbying."

7. Identification of Merit Reviewer Conflicts

Provide a list of individuals who should or should not serve as merit reviewers of this application, following the instructions in <u>Section VIII</u> of this FOA. Attach this information to Field 12 of the Research and Related Other Project Information Form.

8. Summary of Required Forms/Files

Your application must include the following items:

Name of Document	Format	Attach to
SF 424 (R&R)	Form	N/A
RESEARCH AND RELATED Other Project Information	Form	N/A
Project Summary/Abstract	PDF	Field 7
Project Narrative, including required appendices	PDF	Field 8
Identification of Merit Review Conflicts	Excel template	Field 12
RESEARCH & RELATED BUDGET	Form	N/A
Budget Justification	PDF	Field L
R&R SUBAWARD BUDGET ATTACHMENT(S) FORM (if applicable)	Form	N/A
Subaward Budget Justification (if applicable)	PDF	Field L of the subaward budget
PROJECT/PERFORMANCE SITE LOCATION(S)	Form	N/A
SF-LLL Disclosure of Lobbying Activities, if applicable	Form	N/A

E. SUBMISSIONS FROM SUCCESSFUL APPLICANTS

If selected for award, DOE reserves the right to request additional or clarifying information for any reason deemed necessary, including, but not limited to:

- Indirect cost information
- Other budget information
- Name and phone number of the Designated Responsible Employee for complying with national policies prohibiting discrimination (See 10 CFR 1040.5)
- Representation of Limited Rights Data and Restricted Software, if applicable
- Commitment Letter from Third Parties Contributing to Cost Sharing, if applicable
- Environmental Information

Applicants that are not institutions of higher education, that request indirect costs, and that do not already have an Indirect Cost Rate Agreement with their Cognizant Federal Agency or documentation of rates accepted for estimating purposes by DOE or another Federal agency, are advised to begin preparing an Indirect Cost Rate Proposal for submission, upon request, to the DOE contract specialist/grants management specialist who will evaluate your application if you are selected for award.

F. SUBMISSION DATES AND TIMES

1. Letter of Intent Due Date

Not applicable.

2. Pre-application Due Date

The pre-application due date is printed on the cover of this FOA.

You are encouraged to submit your pre-application well before the deadline. Pre-applications may be submitted at any time between the publication of this FOA and the stated deadline.

3. Application Due Date

The application due date is printed on the cover of this FOA.

You are encouraged to transmit your application well before the deadline. Applications may be submitted at any time between the publication of this FOA and the stated deadline.

4. Late Submissions

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

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

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

Applicants must email SC.Early@science.doe.gov 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.

You may be able to submit your application in response to the currently available SC Annual

Solicitation. Please contact the Program Office/Manager listed in this FOA to discuss this option.

Section V - APPLICATION REVIEW INFORMATION

A. CRITERIA

1. Initial Review Criteria

Prior to a comprehensive merit evaluation, DOE will perform an initial review in accordance with 10 CFR 605.10(b) to determine that (1) the applicant is eligible for the award; (2) the information required by the FOA, including LOIs or pre-applications, has been submitted; (3) all mandatory requirements are satisfied; (4) the proposed project is responsive to the objectives of the FOA, and (5) the proposed project is not duplicative of programmatic work. Applications that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

2. Merit Review Criteria

Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria as found in 10 CFR 605.10 (d), the Office of Science Financial Assistance Program Rule.

- Scientific and/or Technical Merit of the Project;
- Appropriateness of the Proposed Method or Approach;
- Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
- Reasonableness and Appropriateness of the Proposed Budget.
- Merit reviewers will be asked to evaluate two additional criterion of equal significance to the criteria established by regulation: Relevance to the mission of the specific program (e.g., ASCR, BER, BES, FES, HEP, NP, DOE IP, or ARDAP) to which the application is submitted.
- 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 an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

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

SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROJECT

- What is the scientific innovation of the proposed research?
- What is the likelihood of achieving valuable results?
- How might the results of the proposed work impact the direction, progress, and thinking in relevant scientific fields of research?
- How does the proposed work compare with other efforts in its field, both in terms of

- scientific and/or technical merit and originality?
- Is the Data Management Plan suitable for the proposed research? To what extent does it support the validation of research results? To what extent will research products, including data, be made available and reusable to advance the field of research?

APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

- How logical and feasible are the research approaches?
- Does the proposed research employ innovative concepts or methods?
- 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?

COMPETENCY OF APPLICANT'S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES

- What is the past performance and potential of the research team?
- 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?

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?

RELEVANCE TO THE MISSION OF THE SPECIFIC PROGRAM (E.G., ASCR, BER, BES, FES, HEP, NP, DOE IP, OR ARDAP) TO WHICH THE APPLICATION IS SUBMITTED

- How does the proposed research contribute to the mission of the program in which the application is being evaluated?
- Is the proposed research aligned with the program office's priorities as described in advisory committee reports?

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?

B. REVIEW AND SELECTION PROCESS

1. Merit Review

Applications that pass the initial review will be subjected to a formal merit review and will be evaluated based on the criteria codified at 10 CFR 605.10(d) in accordance with the guidance provided in the "Office of Science Merit Review System for Financial Assistance," which is available at: https://science.osti.gov/grants/policy-and-guidance/merit-review-system/.

2. Program Policy Factors

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

- Availability of funds
- Relevance of the proposed activity to SC priorities
- Ensuring an appropriate balance of activities within SC programs
- Institutional history of training and mentoring early-career researchers
- Providing placement for postdoctoral researchers
- Training graduate students in conduct of basic research
- Training the next generation of researchers
- Maximizing the use of DOE user facilities
- Ensuring opportunities to investigators not currently supported by DOE
- Commitment to sharing the results of research
- Promoting the diversity of supported investigators
- Promoting the diversity of institutions receiving awards
- Institutional history of hiring, promoting, and placing scientists from underrepresented communities in the scientific workforce

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. Review of Risk

Pursuant to 2 CFR 200.206, DOE will conduct an additional review of the risk posed by applications submitted under this FOA. Such review of risk will include:

- Quality of the application,
- Reports and findings from audits performed under 2 CFR 200 or OMB Circular A-133, and
- Systems maintained under 2 CFR 180.

DOE may make use of other publicly available information and the history of an applicant's performance under DOE or other Federal agency awards.

Applicants with no prior performance of DOE awards may be asked to provide information about their financial stability and or their ability to comply with the management standards of 2 CFR 200.

5. Discussions and Award

The Government may enter into discussions with a selected applicant for any reason deemed necessary, including but not limited to the following: (1) the budget is not appropriate or reasonable for the requirement; (2) only a portion of the application is selected for award; (3) the Government needs additional information to determine that the recipient is capable of complying with the requirements in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation); and/or (4) special terms and conditions are required. 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 July 2022. It is expected that awards will be made in Fiscal Year 2022.

DOE is interested in seeing projects supported under this FOA begin work by August 2022.

Section VI – AWARD ADMINISTRATION INFORMATION

A. AWARD NOTICES

1. Notice of Selection

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

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

2. Notice of Award

An Assistance Agreement issued by the DOE Contracting Officer is the authorizing award document. It normally includes, either as an attachment or by reference, the following items: (1) Special Terms and Conditions, (2) Intellectual Property Provisions, (3) Federal Assistance Reporting Checklist and Instructions, (4) Budget Pages, (5) The Research Terms and Conditions, available at https://www.nsf.gov/pubs/policydocs/rtc/rtcoverlay_march17.pdf, and DOE Agency Specific Requirements, available at https://www.nsf.gov/awards/managing/rtc.jsp, (6) Applicable program regulations, 10 CFR 605 at https://www.ecfr.gov/, (7) DOE Assistance Regulations, 2 CFR part 200 as amended by 2 CFR part 910 at https://www.ecfr.gov/, (8) Application/proposal as approved by DOE, (9) National Policy Assurances to Be Incorporated as Award Terms in effect on date of award at https://www.nsf.gov/awards/managing/rtc.jsp.

TERMS AND CONDITIONS

Sample DOE Special Terms and Conditions for Use in Most Grants and Cooperative Agreements are located at https://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms under Award Terms.

The standard DOE financial assistance intellectual property provisions applicable to various types of recipients are located at:

https://energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards

NATIONAL POLICY ASSURANCES

The National Policy Assurances To Be Incorporated As Award Terms are located at https://energy.gov/management/office-management/office-management/operational-management/financial-assistance-forms under Award Terms.

B. ADMINISTRATIVE AND NATIONAL POLICY REQUIREMENTS

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

- 1. Evaluation and Administration by Non-Federal Personnel
- 2. Government Right to Reject or Negotiate
- 3. Intergovernmental Review
- 4. Modifications

Awards made under this FOA are subject to the following Administrative and National Policy Requirements. The full text of each provision is in <u>Section VIII</u> of this FOA and may be accessed by navigating to the hyperlinks below:

- 1. Administrative Requirements
- 2. Availability of Funds
- 3. Conference Spending (February 2015)
- 4. Commitment of Public Funds
- 5. Corporate Felony Conviction and Federal Tax Liability Representations (March 2014)
- 6. Environmental, Safety and Health (ES&H) Performance of Work at DOE Facilities
- 7. Federal, State, and Local Requirements
- 8. Funding Restrictions
- 9. National Environmental Policy Act (NEPA) Compliance
- 10. Nondisclosure and Confidentiality Agreements Representations (June 2015)
- 11. Notice Regarding Eligible/Ineligible Activities
- 12. Prohibition on Discrimination and Harassment
- 13. Prohibition on Lobbying Activity
- 14. Proprietary Application Information
- 15. Publications
- 16. Registration Requirements
- 17. Research Misconduct
- 18. Rights in Technical Data
- 19. Subaward and Executive Reporting
- 20. Title to Subject Inventions

C. REPORTING

Reporting requirements are identified on the Federal Assistance Reporting Checklist, DOE F 4600.2, attached to the award agreement. The standard checklist is available at http://energy.gov/management/office-management/operational-management/financial-assistance-forms under Award Forms: Individual awards may impose additional requirements.

D. REPORTING OF MATTERS RELATED TO RECIPIENT INTEGRITY AND PERFORMANCE (DECEMBER 2015)

DOE, prior to making a Federal award with a total amount of Federal share greater than the simplified acquisition threshold, is required to review and consider any information about the applicant that is in the designated integrity and performance system accessible through SAM (currently FAPIIS) (see 41 USC 2313).

The applicant, at its option, may review information in the designated integrity and performance systems accessible through SAM and comment on any information about itself that a Federal awarding agency previously entered and is currently in the designated integrity and performance system accessible through SAM.

DOE will consider any written comments by the applicant, in addition to the other information in the designated integrity and performance system, in making a judgment about the applicant's integrity, business ethics, and record of performance under Federal awards when completing the review of risk posed by applicants as described in 2 CFR 200.206 Federal awarding agency review of risk posed by applicants.

Section VII - QUESTIONS/AGENCY CONTACTS

A. QUESTIONS

Questions relating to the Grants.gov registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@Grants.gov. DOE cannot answer these questions. Please only contact the Grants.gov help desk for questions related to Grants.gov.

For help with PAMS, click the "External User Guide" link on the PAMS website, https://pamspublic.science.energy.gov/. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this FOA should reference the FOA number on the cover of this Announcement. 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 FOA or below. Please contact the program staff with all questions not directly related to the Grants.gov or PAMS systems.

B. AGENCY CONTACTS

Grants.gov	800-518-4726 (toll-free)
Customer Support	support@Grants.gov
PAMS	855-818-1846 (toll-free)
Customer Support	301-903-9610
	sc.pams-helpdesk@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.

Section VIII – SUPPLEMENTARY MATERIAL

A. HOW-TO GUIDES

1. How to Distinguish Between a New and Renewal Application

New Application: An application must be submitted as "new" in the following circumstances:

- When applying for funding to create a new research award that has not previously received DOE funding, including any funding for the current year.
- When applying for funding to support continued research from the same applicant institution as the current grant but with a significant change in fundamental nature of the research.
- When applying for funding to support continued research supported by an existing DOE award but at a new applicant institution.

Renewal Application: A renewal application is appropriate when funds are requested for an award that has no changes in the following items:

- The recipient/applicant institution.
- The award's senior leadership.
- The fundamental nature of the award.

A change in an award's PI does not necessarily require submission as a new application: The change in personnel must be considered in light of other changes.

Renewal applications compete for funds with all other peer-reviewed applications and must be developed as fully as though the applicant were applying for the first time. Renewal applications must be submitted by the same sponsoring institution as that holding the current award for which renewal funding is requested, and the proposed research topic must be logical scientific extensions of the research that has been performed in the current award.

2. How Federally Affiliated Organizations May Participate and Be Funded

VALUE/FUNDING FOR DOE/NNSA NATIONAL LABORATORIES AND NON-DOE/NNSA FFRDCS

For grant awards, the value of, and funding for, a DOE/NNSA National Laboratory contractor, a non-DOE/NNSA Federally Funded Research and Development Center (FFRDC) contractor, or another Federal agency's portion of the work will not be included in the award to the successful applicant. DOE will fund a DOE/NNSA National Laboratory contractor through the DOE field work authorization system or other appropriate process and may fund non-DOE/NNSA FFRDC contractors and other Federal agencies through an interagency agreement in accordance with the Economy Act, 31 USC 1535, or other statutory authority.

DISPUTES AND CLAIMS

The successful prime applicant/awardee (lead organization) will be the responsible authority

regarding the settlement and satisfaction of all contractual and administrative issues, including but not limited to, Disputes and Claims arising out of any agreement between the applicant and any team member, and/or subrecipient.

If an award is made to a DOE/NNSA National Laboratory, all Disputes and Claims will be resolved in accordance with the terms and conditions of the DOE/NNSA National Laboratory's management and operating (M&O) contract, as applicable, in consultation between DOE and the prime awardee.

If an award is made to another Federal agency or its FFRDC contractor, all Disputes and Claims will be resolved in accordance with the terms and conditions of the interagency agreement in consultation between DOE and the prime awardee.

3. How Federally Affiliated Organizations May Apply

DOE/NNSA NATIONAL LABORATORIES

DOE/NNSA National Laboratories, if eligible either as a prime applicant or a proposed team member on another entity's application, should ensure that their cognizant DOE/NNSA Contracting Officer provides written authorization. This authorization should be submitted with the application as part of the Budget Justification for DOE/NNSA National Laboratory Contractor File. [This is not required for the National Energy Technology Laboratory because it is a Government Owned/Government Operated (GOGO).] **Please note that failure to provide this authorization may result in rejection of an application prior to merit review.** If a DOE/NNSA National Laboratory Contractor is selected for award, or proposed as a team member, the proposed work will be authorized under the DOE field work authorization system or other appropriate process and performed under the laboratory Contractor's M&O contract, as applicable. The following wording is acceptable for the authorization:

"Authorization is granted for the	Laboratory to participate in the
proposed project. The work proposed for the labo	ratory is consistent with or
complementary to the missions of the laboratory	and will not adversely impact execution
of the DOE/NNSA assigned programs at the labo	ratory."

(end of acceptable authorization)

If required by the language in <u>Section III</u>, in addition to the cognizant DOE Contracting Officer, SC Laboratories¹ are required to provide written authorization from the Director of Laboratory Policy (SC-42) with the application in order to be eligible to apply for funding under this FOA.

¹ SC Laboratories are Ames Laboratory, Argonne National Laboratory, Brookhaven National Laboratory, Fermi National Accelerator Laboratory, Lawrence Berkeley National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Princeton Plasma Physics Laboratory, SCAC National Accelerator Laboratory, and Thomas Jefferson National Accelerator Facility.

The following wording is acceptable for the authorization:
"Authorization is granted for theLaboratory to participate in the proposed project. The work proposed for the laboratory is consistent with or complementary to the missions of the laboratory and will not adversely impact execution of the DOE assigned programs at the laboratory."
(end of acceptable authorization)
If a DOE/NNSA FFRDC is selected for award negotiation, the proposed work will be authorized under the DOE work authorization process and performed under the laboratory's Management and Operating (M&O) contract.
Non-DOE/NNSA FFRDCs
Non-DOE/NNSA FFRDCs, if eligible either as a prime applicant or a proposed team member on another entity's application, should follow the following guidelines:
The prime applicant must obtain written authorization for non-DOE/NNSA FFRDC participation. The cognizant Contracting Officer for the Federal agency sponsoring the FFRDC contractor must authorize in writing the participation of the FFRDC contractor on the proposed project and this authorization should be submitted with the application. The written authorization must also contain a determination that the use of a FFRDC contractor is consistent with the contractor's authority under its award and does not place the FFRDC contractor in direct competition with the private sector, in accordance with FAR Part 17.5. Please note that failure to provide this authorization may result in rejection of an application prior to merit review. The following wording is acceptable for the authorization:
"Authorization is granted for the Laboratory to participate in the proposed project. The work proposed for the laboratory is consistent with or complementary to the missions of the laboratory and will not adversely impact execution of the (insert agency) assigned programs at the laboratory. This laboratory is authorized to perform the work proposed in the application submitted under DOE Funding Opportunity Announcement < <include cover="" foa="" number="" on="" page="" the="">> by the following statutory authority (insert statute name, citation, and section)."</include>

OTHER FEDERAL AGENCIES

Other Federal Agencies, if eligible either as a prime applicant or a proposed team member on another entity's application, must include in their budget justifications any specific statutory authorization (other than the Economy Act) that permits their receipt of an Inter-Agency Agreement or that authorizes the payment of certain costs.

4. How Consortia May be Used

INCORPORATED CONSORTIA

Incorporated consortia, which may include domestic and/or foreign entities, are eligible to apply for funding as a prime recipient (lead organization) or subrecipient (team member).

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

UNINCORPORATED CONSORTIA

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

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

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

Note that a consortium is applied for in one application and results in one award with subawards to consortia members. Multi-institutional teams may, if permitted under this FOA, submit collaborative applications with each institution submitting its own application with an identical research narrative, resulting in multiple awards to the collaborating institutions.

5. How to Submit Letters of Intent

Do not submit an LOI unless an FOA requires or allows their submission.

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

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

Submit Your Letter of Intent:

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

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

WARNING: The PAMS website at https://pamspublic.science.energy.gov/ will permit you to edit a previously submitted LOI in the time between your submission and the deadline. If you choose to edit, doing so will remove your previously submitted version

from consideration. If you are still editing at the time of the deadline, you will not have a valid submission. Please pay attention to the deadline.

6. How to Submit a Pre-Application

Do not submit a pre-application unless an FOA requires or permits their submission.

It is important that the pre-application be a single file with extension .pdf, .docx, or .doc. The filename must not exceed 50 characters. The PI and anyone submitting on behalf of the PI must register for an account in PAMS before it will be possible to submit a pre-application. All PIs and those submitting pre-applications 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.

Submit Your Pre-Application:

- Create your pre-application (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 / Respond to Funding Opportunity Announcements" link and find the current announcement in the list. Click the "Actions/Views" link in the Options column next to this announcement to obtain a dropdown menu. Select "Submit Preproposal" from the dropdown.
- On the Submit Preproposal page, select the institution from which you are submitting this preproposal from the Institution dropdown. If you are associated with only one institution in the system, there will only be one institution in the dropdown.
- Note that you must select one and only one PI per preproposal; to do so, click the "Select PI" button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the "Actions" link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose "Select PI."
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the "Invite PI" link at the top left of the "Select PI" screen. You can enter an optional personal message to the PI in the "Comments" box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the preproposal. Save the preproposal for later work by clicking the "Save" button at the bottom of the screen. It will be stored in "My Preproposals" for later editing.
- Enter a title for your preproposal.
- Select the appropriate technical contact from the Program Manager dropdown.
- To upload the preproposal file into PAMS, click the "Attach File" button at the far right side of the screen. Click the "Browse" (or "Choose File" depending on your browser) button to

search for your file. You may enter an optional description of the file you are attaching. Click the "Upload" button to upload the file.

- At the bottom of the screen, click the "Submit to DOE" button to save and submit the preproposal to DOE.
- Upon submission, the PI will receive an email from the PAMS system <\text{PAMS.Autoreply@science.doe.gov} acknowledging receipt of the preproposal.

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

WARNING: The PAMS website at https://pamspublic.science.energy.gov will permit you to edit a previously submitted pre-application 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.

7. How to Register and Submit an Application in Grants.gov

This section provides the application submission and receipt instructions for applications to SC. Please read the following instructions carefully and completely.

ELECTRONIC DELIVERY

SC is participating in the Grants.gov initiative to provide the grant community with a single site to find and apply for grant funding opportunities. SC requires applicants to submit their applications online through Grants.gov.

HOW TO REGISTER TO APPLY THROUGH GRANTS.GOV

a. Instructions: Read the instructions below about registering to apply for SC funds. Applicants should read the registration instructions carefully and prepare the information requested before beginning the registration process. Reviewing and assembling the required information before beginning the registration process will alleviate last-minute searches for required information.

Organizations must have a Data Universal Numbering System (DUNS) Number, active System for Award Management (SAM) registration, and Grants.gov account to apply for grants. If individual applicants are eligible to apply for this FOA, then you may begin with step 3, Create a Grants.gov Account, listed below.

Creating a Grants.gov account can be completed online in minutes, but DUNS and SAM registrations may take several weeks. Therefore, an organization's registration should be done in sufficient time to ensure it does not impact the entity's ability to meet required application submission deadlines.

Complete organization registration instructions can be found on Grants.gov here: https://www.Grants.gov/web/grants/applicants/organization-registration.html

- 1) *Obtain a DUNS Number*: All entities applying for funding, including renewal funding, must have a DUNS Number from Dun & Bradstreet (D&B). Applicants must enter the DUNS Number in the data entry field labeled "Organizational DUNS" on the SF-424 form. For more detailed instructions for obtaining a DUNS Number, refer to: https://www.Grants.gov/web/grants/applicants/organization-registration/step-1-obtain-duns-number.html
- 2) Register with SAM: All organizations applying online through Grants.gov must register with SAM at https://www.sam.gov. Failure to register with SAM will prevent your organization from applying through Grants.gov. SAM registration must be renewed annually. For more detailed instructions for registering with SAM, refer to:

 https://www.Grants.gov/web/grants/applicants/organization-registration/step-2-register-with-sam.html
- 3) *Create a Grants.gov Account*: The next step is to register an account with Grants.gov. Follow the on-screen instructions or refer to the detailed instructions here: https://www.Grants.gov/web/grants/applicants/registration.html
- 4) Add a Profile to a Grants.gov Account: A profile in Grants.gov corresponds to a single applicant organization the user represents (i.e., an applicant) or an individual applicant. If you work for or consult with multiple organizations and have a profile for each, you may log in to one Grants.gov account to access all of your grant applications. To add an organizational profile to your Grants.gov account, enter the DUNS Number for the organization in the DUNS field while adding a profile. For more detailed instructions about creating a profile on Grants.gov, refer to: https://www.Grants.gov/web/grants/applicants/registration/add-profile.html
- 5) EBiz POC Authorized Profile Roles: After you register with Grants.gov and create an Organization Applicant Profile, the organization applicant's request for Grants.gov roles and access is sent to the Electronic Business Point of Contact (EBiz POC). The EBiz POC will then log in to Grants.gov and authorize the appropriate roles, which may include the Authorized Organization Representative (AOR) role, thereby giving you permission to complete and submit applications on behalf of the organization. You will be able to submit your application online any time after you have been assigned the AOR role. For more detailed instructions about creating a profile on Grants.gov, refer to: https://www.Grants.gov/web/grants/applicants/registration/authorize-roles.html
- 6) *Track Role Status*: To track your role request, refer to: https://www.Grants.gov/web/grants/applicants/registration/track-role-status.html
- b. *Electronic Signature*: When applications are submitted through Grants.gov, the name of the organization applicant with the AOR role that submitted the application is inserted into the

signature line of the application, serving as the electronic signature. The EBiz POC must authorize people who are able to make legally binding commitments on behalf of the organization as a user with the AOR role; this step is often missed and it is crucial for valid and timely submissions.

HOW TO SUBMIT AN APPLICATION TO SC VIA GRANTS.GOV

Grants.gov applicants can apply online using Workspace. Workspace is a shared, online environment where members of a grant team may simultaneously access and edit different webforms within an application. For each FOA, you can create individual instances of a workspace.

Below is an overview of applying on Grants.gov. For access to complete instructions on how to apply for opportunities, refer to:

 $\underline{https://www.Grants.gov/web/grants/applicants/apply-for-grants.html}$

- 1) Create a Workspace: Creating a workspace allows you to complete it online and route it through your organization for review before submitting.
- 2) Complete a Workspace: Add participants to the workspace, complete all the required forms, and check for errors before submission.
 - a. Adobe Reader: If you decide not to apply by filling out webforms you can download individual PDF forms in Workspace so that they will appear similar to other Standard forms. The individual PDF forms can be downloaded and saved to your local device storage, network drive(s), or external drives, then accessed through Adobe Reader.

NOTE: Visit the Adobe Software Compatibility page on Grants.gov to download the appropriate version of the software at: https://www.Grants.gov/web/grants/applicants/adobe-software-compatibility.html

- b. Mandatory Fields in Forms: In the forms, you will note fields marked with an asterisk and a different background color. These fields are mandatory fields that must be completed to successfully submit your application.
- c. Complete SF-424 Fields First: The forms are designed to fill in common required fields across other forms, such as the applicant name, address, and DUNS number. To trigger this feature, an applicant must complete the SF-424 information first. Once it is completed, the information will transfer to the other forms.
- 3) Submit a Workspace: An application may be submitted through workspace by clicking the Sign and Submit button on the Manage Workspace page, under the Forms tab. Grants.gov recommends submitting your application package *at least 24-48 hours prior to the close date* to provide you with time to correct any potential technical issues that may disrupt the application submission.

4) Track a Workspace: After successfully submitting a workspace package, a Grants.gov Tracking Number (GRANTXXXXXXXX) is automatically assigned to the package. The number will be listed on the Confirmation page that is generated after submission.

For additional training resources, including video tutorials, refer to: https://www.Grants.gov/web/grants/applicants/applicant-training.html

Applicant Support: Grants.gov provides applicants 24/7 support via the toll-free number 1-800-518-4726 and email at support@Grants.gov. For questions related to the specific grant opportunity, contact the number listed in the application package of the grant you are applying for.

If you are experiencing difficulties with your submission, it is best to call the Grants.gov Support Center and get a ticket number. The Support Center ticket number will assist SC with tracking your issue and understanding background information on the issue.

TIMELY RECEIPT REQUIREMENTS AND PROOF OF TIMELY SUBMISSION

Proof of timely submission is automatically recorded by Grants.gov. An electronic date/time stamp is generated within the system when the application is successfully received by Grants.gov. The applicant AOR will receive an acknowledgement of receipt and a tracking number (GRANTXXXXXXXX) from Grants.gov with the successful transmission of their application. Applicant AORs will also receive the official date/time stamp and Grants.gov Tracking number in an email serving as proof of their timely submission.

When SC successfully retrieves the application from Grants.gov, and acknowledges the download of submissions, Grants.gov will provide an electronic acknowledgment of receipt of the application to the email address of the applicant with the AOR role. Again, proof of timely submission shall be the official date and time that Grants.gov receives your application. Applications received by Grants.gov after the established due date for the program will be considered late and may not be considered for funding by SC.

Applicants using slow internet, such as dial-up connections, should be aware that transmission can take some time before Grants.gov receives your application. Again, Grants.gov will provide either an error or a successfully received transmission in the form of an email sent to the applicant with the AOR role. The Grants.gov Support Center reports that some applicants end the transmission because they think that nothing is occurring during the transmission process. Please be patient and give the system time to process the application.

8. How to Prepare an Application

APPLICATION PREPARATION

You must submit the application through Grants.gov at https://www.Grants.gov/, using either the online webforms or downloaded forms. (Additional instructions are provided in 7., above.)

You are required to use the compatible version of Adobe Reader software to complete a <u>Grants.gov</u> Adobe application package. To ensure you have the <u>Grants.gov</u> compatible version of Adobe Reader, visit the software compatibility page at https://www.Grants.gov/web/grants/applicants/adobe-software-compatibility.html.

You must complete the mandatory forms and any applicable optional forms (e.g., Disclosure of Lobbying Activities (SF-LLL)) in accordance with the instructions on the forms and the additional instructions below.

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

Please note the following restrictions that apply to the names of all files attached to your application:

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

RENEWAL APPLICATIONS

For renewal applications only, the PI is required to submit a Renewal Proposal Products section through the PAMS website at https://pamspublic.science.energy.gov. The PI must enter into PAMS each product created during the course of the previous project period. Types of products include publications, intellectual property, technologies or techniques, and other products such as databases or software. As soon as the renewal application is assigned to a DOE Program Manager, the PI will receive an automated email from PAMS

(<PAMS.Autoreply@science.doe.gov>) instructing him or her to navigate to the PAMS Task tab to complete and submit the Renewal Proposal Products. The submitted product list will be sent for merit review as part of the application. The application will not be considered complete and cannot be sent for review until the product list has been submitted.

RESUBMISSION OF APPLICATIONS

Applications submitted under this FOA may be withdrawn from consideration by using the PAMS website at https://pamspublic.science.energy.gov. Applications may be withdrawn at any time between when the applicant submits the application and when DOE makes the application available to merit reviewers. Such withdrawals take effect immediately and cannot be reversed.

Please exercise due caution. After the application is made available to merit reviewers, the applicant may contact the DOE program office identified in this FOA to request that it be withdrawn.

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

Note that there may be a delay between the application's submission in Grants.gov and when it is available to be withdrawn in PAMS. SC will usually consider the last submission, according to its Grants.gov timestamp, to be the intended version. Please consult with your program manager to resolve any confusion about which version of an application should be considered.

IMPROPER CONTENTS OF APPLICATIONS

Applications submitted under this FOA will be stored in controlled-access systems, but they may be made publicly available if an award is made. As such, it is critical that applicants follow these guidelines:

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

CHANGE OF AWARDEE INSTITUTION

If an awardee chooses to relinquish an award made under this FOA to permit the transfer of the award to a new institution, the new institution must submit an application under the then-available SC "annual" or "open" FOA.

9. How to Prepare a Biosketch

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

SC requires the use of the format approved by the National Science Foundation (NSF), which may be generated by the Science Experts Network Curriculum Vita (SciENcv), a cooperative

venture maintained at https://www.ncbi.nlm.nih.gov/sciencv/, and is also available at https://nsf.gov/bfa/dias/policy/nsfapprovedformats/biosketch.pdf. The use of a format required by another agency is intended to reduce the administrative burden to researchers by promoting the use of common formats.

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

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

Requested information may be appended to a biosketch, whether produced from a fillable PDF or in SciENcv.

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

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.

10. How to Prepare a List of Individuals Who Should Not Serve as Reviewers

To assist in identifying individuals who should not serve as merit reviews, provide the following information for each and every senior/key person who is planned to be or is identified in Section A of the R&R Budget for the applicant and any proposed subrecipients:

- Advisees (graduate students or postdocs) of the senior/key person
- Advisors of the senior/key person while a graduate student or a postdoc
- Close associates of the senior/key person over the past 48 months
- Co-authors of the senior/key person over the past 48 months
- Co-editors of the senior/key person over the past 48 months
- Co-investigators of the senior/key person over the past 48 months
- Collaborators of the senior/key person over the past 48 months

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

Large collaborations of 50 or more researchers do not require that all collaborators be identified: rather, only list the researchers with whom the senior/key person actually collaborated.

For all identified individuals, provide the following information:

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

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

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

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

For your convenience, a template is available at https://science.osti.gov/grants/Policy-and-Guidance/Agreement-Forms. The template may also be posted with this FOA in Grants.gov.

11. How to Prepare Current and Pending Support

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

Current and Pending support is intended to allow the identification of potential duplication, overcommitment, potential conflicts of interest or commitment, and all other sources of support. The PI and each senior/key person at the prime applicant and any proposed subaward must provide a list of all sponsored activities, awards, and appointments, whether paid or unpaid; provided as a gift with terms or conditions or provided as a gift without terms or conditions; full-time, part-time, or voluntary; faculty, visiting, adjunct, or honorary; cash or in-kind; foreign or domestic; governmental or private-sector; directly supporting the individual's research or indirectly supporting the individual by supporting students, research staff, space, equipment, or other research expenses. All foreign government-sponsored talent recruitment programs must be

identified in current and pending support.

SC requires the use of the format approved by the National Science Foundation (NSF), which may be generated by the Science Experts Network Curriculum Vita (SciENcv), a cooperative venture maintained at https://www.ncbi.nlm.nih.gov/sciencv/, and is also available at https://www.nsf.gov/bfa/dias/policy/nsfapprovedformats/cps.pdf. The use of a format required by another agency is intended to reduce the administrative burden to researchers by promoting the use of common formats.

For every activity, list the following items:

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

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

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

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

12. How to Prepare a Data Management Plan

In general, a DMP should address the following requirements:

- 1. DMPs should describe whether and how data generated in the course of the proposed research will be shared and preserved. If the plan is not to share and/or preserve certain data, then the plan must explain the basis of the decision (for example, cost/benefit considerations, other parameters of feasibility, scientific appropriateness, or limitations discussed in #4). At a minimum, DMPs must describe how data sharing and preservation will enable validation of results, or how results could be validated if data are not shared or preserved.
- 2. DMPs should provide a plan for making all research data displayed in publications resulting from the proposed research open, machine readable, and digitally accessible to the public at the time of publication. This includes data that are displayed in charts, figures, images, etc. In addition, the underlying digital research data used to generate the displayed data should be made as accessible as possible to the public in accordance with the principles stated in the

- Office of Science Statement on Digital Data Management (https://science.osti.gov/funding-opportunities/digital-data-management. This requirement could be met by including the data as supplementary information to the published article, or through other means. The published article should indicate how these data can be accessed.
- 3. DMPs should consult and reference available information about data management resources to be used in the course of the proposed research. In particular, DMPs that explicitly or implicitly commit data management resources at a facility beyond what is conventionally made available to approved users should be accompanied by written approval from that facility. In determining the resources available for data management at Office of Science User Facilities, researchers should consult the published description of data management resources and practices at that facility and reference it in the DMP. Information about other Office of Science facilities can be found at https://science.osti.gov/user-facilities/.
- 4. DMPs must protect confidentiality, personal privacy, Personally Identifiable Information, and U.S. national, homeland, and economic security; recognize proprietary interests, business confidential information, and intellectual property rights; avoid significant negative impact on innovation, and U.S. competitiveness; and otherwise be consistent with all applicable laws, and regulations. There is no requirement to share proprietary data.

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

13. How to Prepare a Research and Related Budget and Justification

The following advice will improve the accuracy of your budget request:

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

If you are proposing indirect costs and do not already have an Indirect Cost Rate Agreement with your Cognizant Federal Agency or documentation of rates accepted for estimating purposes by DOE or another Federal agency, it is recommended that you begin preparing an Indirect Cost Rate Proposal to be submitted, upon request, to the DOE contract specialist/grants management specialist who will evaluate your application if you are selected for award.

For your convenience in preparing an Indirect Cost Rate proposal, a link to applicant resources, including indirect rate model templates, has been provided below: https://science.osti.gov/sbir/applicant-resources/grant-application/.

Budget Fields

Senior/Key Person personnel, base salary, the number of months that person will be allocated to the project, requested salary, fringe benefits, and the total funds requested for each person. The requested salary must be the product of the base salary and the effort. Include a written narrative in the budget justification that justifies the need for requested personnel. Within the justification, explain the fringe benefit rate used if it is not the standard faculty rate. Section B Other Personnel List personnel, the number of months that person will be allocated to the project, requested salary fringe benefits, and the total funds requested for each person. Include a written narrative in the budget justification that fully justification the need for requested personnel. Within the justification, provide the number of positions being filled in each category of other personnel. Section C Equipment For the purpose of this budget, equipment is designated as an item of property that has an acquisition cost of \$5,000 or more and an expect service life of more than one year, unless a different threshold is
funds requested for each person. The requested salary must be the product of the base salary and the effort. Include a written narrative in the budget justification that justifies the need for requested personnel. Within the justification, explain the fringe benefit rate used if it is not the standard faculty rate. Section B Other Personnel List personnel, the number of months that person will be allocated to the project, requested salary fringe benefits, and the total funds requested for each person. Include a written narrative in the budget justification that fully justification the number of positions being filled in each category of other personnel. Section C 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 expect
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specified in a negotiated Facilities and Administrative Cost Rate. (No
that this designation applies for proposal budgeting only and differs
from the DOE definition of capital equipment.) List each item of
equipment separately and justify each in the budget justification
section. Do not aggregate items of equipment. Allowable items
ordinarily will be limited to research equipment and apparatus not
already available for the conduct of the work. General-purpose office
equipment is not eligible for support unless primarily or exclusively
used in the actual conduct of scientific research.
Section D For purposes of this section only, travel to Canada or to Mexico is
Travel considered domestic travel. In the budget justification, list each trip's
destination, dates, estimated costs including transportation and
subsistence, number of staff traveling, the purpose of the travel, and
how it relates to the project. Indicate the basis for the cost estimate
(quotes from vendors or suppliers, past experience of similar items, or
some other basis). To qualify for support, attendance at meetings or
conferences must enhance the investigator's capability to perform the
research, plan extensions of it, or disseminate its results. Domestic
travel is to be justified separately from foreign travel. Within the
budget justification, detail the number of personnel planning to trave
and the estimated per-traveler cost for each trip.

Section E
Participant/Trainee
Support Costs

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

Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).

Section F Other Direct Costs

- Materials and Supplies: Enter total funds requested for materials and supplies in the appropriate fields. In the budget justification, indicate general categories such as glassware, and chemicals, including an amount for each category (items not identified under "Equipment"). Categories less than \$1,000 are not required to be itemized. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).
- **Publication Costs:** Enter the total publication funds requested. The proposal budget may request funds for the costs of documenting, preparing, publishing or otherwise making available to others the findings and products of the work conducted under the award. In the budget justification, include supporting information. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).
- Consultant Services: Enter total funds requested for all consultant services. In the budget justification, identify each consultant, the services he/she will perform, total number of days, travel costs, and total estimated costs. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).
- ADP/Computer Services: Enter total funds requested for ADP/Computer Services. Cloud computing costs must be included under this item. The cost of computer services, including computer-based retrieval of scientific, technical and education information may be requested. In the budget justification, include the established computer service rates at the proposing organization if applicable. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis).
- Subawards/Consortium/Contractual Costs: Enter total costs

	for all subawards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details. • Equipment or Facility Rental/User Fees: Enter total funds requested for Equipment or Facility Rental/User Fees. In the budget justification, identify each rental/user fee and justify. Indicate the basis for the cost estimate (quotes from vendors or suppliers, past experience of similar items, or some other basis). • Alterations and Renovations: Enter total funds requested for Alterations and Renovations. In the budget justification, itemize by category and justify the costs of alterations and renovations, including repairs, painting, removal or installation of partitions, shielding, or air conditioning. Where applicable, provide the square footage and costs. • Other: Add text to describe any other Direct Costs not requested above. Enter costs associated with "Other" item(s). Use the budget justification to further itemize and justify.
Section G	This represents Total Direct Costs (Sections A through F)
Direct Costs	,
Section H	Enter the Indirect Cost information, including the rates and bases being
Other Indirect Costs	used, for each field. Only four general categories of indirect costs are
	allowed/requested on this form, so please consolidate if needed.
	Include the cognizant Federal agency and contact information if using a
	negotiated rate agreement. Within the budget justification, explain the
~	use of multiple rates, if multiple rates are used.
Section I	This is the total of Sections G and H
Total Direct and	
Indirect Costs	

14. How to Register in PAMS

After you submit your application through Grants.gov, the application will automatically transfer into the Portfolio Analysis and Management System (PAMS) for processing by the DOE SC. Many functions for grants and cooperative agreements can be done in PAMS, which is available at https://pamspublic.science.energy.gov.

You will want to "register to" your application: a process of linking yourself to the application after it has been submitted through Grants.gov and processed by DOE.

You must register in PAMS to submit a pre-application or a LOI.

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

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.

CREATE PAMS ACCOUNT:

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

- Click the "No, I have never had an account" link and then the "Create Account" button.
- You will be prompted to enter your name and email address, create a username and password, and select a security question and answer. Once you have done this, click the "Save and Continue" button.
- On the next page, enter the required information (at least one phone number and your mailing address) and any optional information you wish to provide (e.g., FAX number, website, mailstop code, additional email addresses or phone numbers, Division/Department). Click the "Create Account" button.
- Read the user agreement and click the "Accept" button to indicate that you understand your responsibilities and agree to comply with the rules of behavior for PAMS.
- PAMS will take you to the "Having Trouble Logging In?" page. (If you have been an SC merit reviewer or if you have previously submitted an application, you may already be linked to an institution in PAMS. If this happens, you will be taken to the PAMS home page.)

REGISTER TO YOUR INSTITUTION:

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

- If you do not see your institution in the initial search results, you can search again by clicking the "Cancel" button, clicking the Option 2 link, and repeating the search.
- If, after searching, you think your institution is not currently in the database, click the "Cannot Find My Institution" button and enter the requested institution information into PAMS. Click the "Create Institution" button. PAMS will add the institution to the system, associate your profile with the new institution, and return you to the "Institutions List" page when you are finished.

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

15. How to View Applications in PAMS

Each Grants.gov application submitted to the DOE SC automatically transfers into PAMS and is subsequently assigned to a program manager. At the time of program manager assignment, the three people listed on the SF-424 (R&R) cover page will receive an email with the subject line, "Receipt of Proposal 0000xxxxxxx by the DOE Office of Science." These three people are the PI (Block 14), Authorized Representative (Block 19), and Point of Contact (Block 5). In PAMS notation, applications are known as proposals, the PI is known as the PI, the Authorized Representative is known as the Sponsored Research Officer/Business Officer/Administrative Officer (SRO/BO/AO), and the Point of Contact is known as the POC.

There will be a period of time between the application's receipt at Grants.gov and its assignment to a DOE SC program manager. Program managers are typically assigned two weeks after applications are due at Grants.gov: please refrain from attempting to view the proposal in PAMS until you receive an email providing the assignment of a program manager.

Once the email is sent, the PI, SRO/BO/PO, and POC will each be able to view the submitted proposal in PAMS. Viewing the proposal is optional.

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

Following are two sets of instructions for viewing the submitted proposal, one for individuals who already have PAMS accounts and one for those who do not.

If you already have a PAMS account, follow these instructions:

- 1. Log in to PAMS at https://pamspublic.science.energy.gov/.
- 2. Click the "Proposals" tab and click "Access Previously Submitted Grants.gov Proposal."
- 3. Enter the following information:
 - Proposal ID: Enter the ten-digit PAMS proposal ID, including the leading zeros (e.g.,

- 00002xxxxx). Do not use the Grants.gov proposal number. Use the PAMS number previously sent to you in the email with subject line, "Receipt of Proposal ...".
- Email (as entered in Grants.gov application): Enter your email address as it appears on the SF424(R&R) Cover Page.
- Choose Role: Select the radio button in front of the role corresponding to the SF-424 (R&R) cover page. If your name appears in block 19 of the SF-424 (R&R) cover page as the authorizing representative, select "SRO/BO/AO (Sponsored Research Officer/Business Officer/Administrative Officer)." If your name appears in block 14 of the SF424 R&R cover page as the PI, select "Principal Investigator (PI)." If your name appears in block 5 of the SF424 R&R as the point of contact, select "Other (POC)."
- 4. Click the "Save and Continue" button. You will be taken to your "My Proposals" page. The Grants.gov proposal will now appear in your list of proposals. Click the "Actions/Views" link in the options column next to this proposal to obtain a dropdown list. Select "Proposal" from the dropdown to see the proposal. Note that the steps above will work only for proposals submitted to the DOE SC since May 2012.

If you do not already have a PAMS account, follow these instructions:

- 1. To register, click the "Create New PAMS Account" link on the website https://pamspublic.science.energy.gov/.
- 2. Click the "No, I have never had an account" link and then the "Create Account" button.
- 3. 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.
- 4. 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.
- 5. 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.
- 6. You will be taken to the Register to Institution page. Select the link labeled, "Option 1: My institution has submitted a proposal in Grants.gov. I am here to register as an SRO, PI, or POC (Sponsored Research Officer, Principal Investigator, or Point of Contact)."
- 7. Enter the following information:
 - Proposal ID: Enter the ten-digit PAMS proposal ID, including the leading zeros (e.g., 00002xxxxx). Do not use the Grants.gov proposal number. Use the PAMS number previously sent to you in the email with subject line, "Receipt of Proposal ...".
 - Email (as entered in Grants.gov proposal): Enter your email address as it appears on the SF424(R&R) Cover Page.
 - Choose Role: Select the radio button in front of the role corresponding to the SF-424 (R&R) cover page. If your name appears in block 19 of the SF-424 (R&R) cover page as the authorizing representative, select "SRO/BO/AO (Sponsored Research Officer/Business Officer/Administrative Officer)." If your name appears in block 14 of the SF424 R&R cover page as the PI, select "Principal Investigator (PI)." If your name appears in block 5 of the SF424 R&R as the point of contact, select "Other (POC)."

8. Click the "Save and Continue" button. You will be taken to your "My Proposals" page. The Grants.gov proposal will now appear in your list of proposals. Click the "Actions/Views" link in the options column next to this proposal to obtain a dropdown list. Select "Proposal" from the dropdown to see the proposal.

If you were listed as the PI on a prior submission but you have not previously created an account, you may already be listed in PAMS. If this is the case, you will be taken to the PAMS home page after agreeing to the Rules of Behavior. If that happens, follow the instructions listed above under "If you already have a PAMS account…" to access your Grants.gov proposal.

16. How to Register in Other Systems Before Submitting an Application

SYSTEMS TO REGISTER IN

Applicants must complete a series of registrations and enrollments to submit applications in response to this FOA. Applicants not currently registered with SAM and Grants.gov should allow **at least four weeks** to complete these requirements.

You should start the process as soon as possible.

You may not be able to use your preferred Internet browser: Each system has its own requirements.

Applicants must obtain a DUNS number at https://fedgov.dnb.com/webform.

Applicants must register with SAM at https://www.sam.gov/. More information about SAM registration for applicants is found at

https://www.sam.gov/SAM/transcript/Quick_Guide_for_Grants_Registrations.pdf. SAM maintains a complete user guide at

https://www.sam.gov/SAM/transcript/SAM Non Federal User Guide.pdf.

Applicants must provide a Taxpayer Identification Number (TIN) to complete their registration in www.SAM.gov. An applicant's TIN is an EIN assigned by the Internal Revenue Service (IRS). In limited circumstances, a Social Security Number (SSN) assigned by the Social Security Administration (SSA) may be used as a TIN. You may obtain an EIN from the IRS at https://www.irs.gov/businesses/small-businesses-self-employed/apply-for-an-employer-identification-number-ein-online.

Do not use a SSN as a TIN.

Obtain a TIN from the IRS using the website listed above.

Applicants must register with FedConnect at www.FedConnect.net. The full, binding version of assistance agreements will be posted to FedConnect.

Recipients must register with the Federal Funding Accountability and Transparency Act Subaward Reporting System at https://www.fsrs.gov. This registration must be completed before an award may be made: you are advised to register while preparing your application.

REGISTERING IN GRANTS.GOV

Applicants must register with Grants.gov, following the instructions at https://www.Grants.gov/web/grants/applicants/registration.html and described above.

WHERE TO SUBMIT AN APPLICATION

You must submit the application through Grants.gov at <u>www.Grants.gov</u>, using either the online webforms or downloaded forms, or a system-to-system service

Submit electronic applications through the "Apply for Grants" function at www.Grants.gov. If you have problems completing the registration process or submitting your application, call Grants.gov at 1-800-518-4726 or send an email to support@Grants.gov.

Please ensure that you have read the applicable instructions, guides, help notices, frequently asked questions, and other forms of technical support on Grants.gov.

DOE SC PORTFOLIO ANALYSIS AND MANAGEMENT SYSTEM (PAMS)

Applicants must register in the Portfolio Analysis and Management System (PAMS) to submit letters of intent and pre-applications, to view merit reviewer comments, or to take a number of post-award actions.

B. POLICY PROVISIONS

1. 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 application, consents to the use of non-Federal reviewers/administrators. Non-Federal reviewers must sign a conflict of interest agreement and a certificate of confidentiality prior to reviewing an application. Non-Federal personnel conducting administrative activities must sign a non-disclosure agreement.

2. Government Right to Reject or Negotiate

DOE reserves the right, without qualification, to reject any or all applications received in response to this FOA and to select any application, in whole or in part, as a basis for negotiation and/or award.

3. Intergovernmental Review

This program is not subject to Executive Order 12372 Intergovernmental Review of Federal Programs.

4. Modifications

Notices of any modifications to this FOA will be posted on Grants.gov and the FedConnect portal. You can receive an email when a modification or an FOA message is posted by registering with FedConnect as an interested party for this FOA. It is recommended that you register as soon after release of the FOA as possible to ensure you receive timely notice of any modifications or other FOAs. More information is available at www.FedConnect.net.

C. ADMINISTRATIVE AND NATIONAL POLICY REQUIREMENTS

1. Administrative Requirements

The administrative requirements for DOE grants and cooperative agreements are contained in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulations).

2. 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 DOE Contracting Officer for this award and until the awardee receives notice of such availability, to be confirmed in writing by the DOE Contracting Officer.

3. Conference Spending (February 2015)

The recipient shall not expend any funds on a conference not directly and programmatically related to the purpose for which the grant or cooperative agreement was awarded that would defray the cost to the United States Government of a conference held by any Executive branch department, agency, board, commission, or office for which the cost to the United States Government would otherwise exceed \$20,000, thereby circumventing the required notification by the head of any such Executive Branch department, agency, board, commission, or office to the Inspector General (or senior ethics official for any entity without an Inspector General), of the date, location, and number of employees attending such conference.

4. Commitment of Public Funds

(a) A DOE financial assistance award is valid only if it is in writing and is signed, either in writing or electronically, by a DOE Contracting Officer.

(b) Recipients are free to accept or reject the award. A request to draw down DOE funds constitutes the Recipient's acceptance of the terms and conditions of this Award.

5. Corporate Felony Conviction and Federal Tax Liability Representations (March 2014)

In submitting an application in response to this FOA the Applicant represents that:

- It is **not** a corporation that has been convicted of a felony criminal violation under any Federal law within the preceding 24 months,
- It is **not** a corporation that has any unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or have lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability.

For purposes of these representations the following definitions apply:

• A Corporation includes any entity that has filed articles of incorporation in any of the 50 states, the District of Columbia, or the various territories of the United States [but not foreign corporations]. It includes both for-profit and non-profit organizations.

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

With respect to the performance of any portion of the work under this award which is performed at a DOE-owned or controlled site, the recipient agrees to comply with all state and Federal ES&H regulations, and with all other ES&H requirements of the operator of such site.

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

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

7. Federal, State, and Local Requirements

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

8. Funding Restrictions

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

Cost Principles: Costs must be allowable, allocable and reasonable in accordance with the applicable Federal cost principles referenced in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation).

Pre-award Costs: Recipients may charge to an award resulting from this FOA pre-award costs that were incurred within the ninety (90) calendar day period immediately preceding the effective date of the award, if the costs are allowable in accordance with the applicable Federal cost principles referenced in 2 CFR 200 as modified by 2 CFR 910 (DOE Financial Assistance Regulation). Recipients must obtain the prior approval of the DOE Contracting Officer for any pre-award costs that are for periods greater than this 90-day calendar period.

Pre-award costs are incurred at the applicant's risk. DOE is under no obligation to reimburse such costs if for any reason the applicant does not receive an award or if the award is made for a lesser amount than the applicant expected.

9. National Environmental Policy Act (NEPA) Compliance

If question 4.a. on the "Research and Related Other Project Information" document indicates "potential impact on the environment", or if DOE's own review indicates it, DOE may ask the applicant to provide additional information on those impacts in order to prepare an environmental critique/synopsis per 10 CFR 1021.216. Note that this pre-award environmental critique/synopsis process would be separate from the preparation of a NEPA document such as an environmental impact statement (EIS) or an environmental assessment (EA). If DOE determines the latter documentation is necessary, this process would need to be completed, funded by and with the participation of the awardee, prior to them taking any action on the proposed project that could have adverse environmental effects or that could limit the choice of reasonable alternatives. Note that in most cases, even when "Potential Impact to the Environment" is checked "Yes," preparation of such NEPA documents is rarely necessary, but DOE has the expectation that the Applicant will disclose the potential, which would serve to initiate dialog with DOE if necessary. The inability to satisfy the NEPA requirements after an award would result in cancellation of the award.

10. Nondisclosure and Confidentiality Agreements Representations (June 2015)

In submitting an application in response to this FOA the Applicant represents that:

- (1) It **does not and will not** require its employees or contractors to sign internal nondisclosure or confidentiality agreements or statements prohibiting or otherwise restricting its employees or contactors from lawfully reporting waste, fraud, or abuse to a designated investigative or law enforcement representative of a Federal department or agency authorized to receive such information.
- (2) It **does not and will not** use any Federal funds to implement or enforce any nondisclosure and/or confidentiality policy, form, or agreement it uses unless it contains the following provisions:
 - a. "These provisions are consistent with and do not supersede, conflict with, or otherwise alter the employee obligations, rights, or liabilities created by existing statute or Executive order relating to (1) classified information, (2) communications to Congress, (3) the reporting to an Inspector General of a violation of any law, rule, or regulation, or mismanagement, a gross waste of funds, an abuse of authority, or a substantial and

specific danger to public health or safety, or (4) any other whistleblower protection. The definitions, requirements, obligations, rights, sanctions, and liabilities created by controlling Executive orders and statutory provisions are incorporated into this agreement and are controlling.'

- b. The limitation above shall not contravene requirements applicable to Standard Form 312, Form 4414, or any other form issued by a Federal department or agency governing the nondisclosure of classified information.
- c. Notwithstanding provision listed in paragraph (a), a nondisclosure or confidentiality policy form or agreement that is to be executed by a person connected with the conduct of an intelligence or intelligence-related activity, other than an employee or officer of the United States Government, may contain provisions appropriate to the particular activity for which such document is to be used. Such form or agreement shall, at a minimum, require that the person will not disclose any classified information received in the course of such activity unless specifically authorized to do so by the United States Government. Such nondisclosure or confidentiality forms shall also make it clear that they do not bar disclosures to Congress, or to an authorized official of an executive agency or the Department of Justice, that are essential to reporting a substantial violation of law.

11. Notice Regarding Eligible/Ineligible Activities

Eligible activities under this program include those which describe and promote the understanding of scientific and technical aspects of specific energy technologies, but not those which encourage or support political activities such as the collection and dissemination of information related to potential, planned or pending legislation.

12. Prohibition on Discrimination and Harassment

All people conducting, supporting, or participating in scientific research under this award must be able to do so on the basis of their abilities and without any unnecessary barriers. Recipients of awards resulting from this FOA are prohibited from engaging in discrimination on any basis prohibited by law, including harassment (sexual or non-sexual) as contained in 10 CFR 1040, 1041, and 1042.

Recipients may contact the DOE's Office of Civil Rights for technical assistance in meeting their institutional requirements under these regulations, including assistance in addressing complaints of discrimination or harassment (https://www.energy.gov/diversity/title-ix). The United States Equal Employment Opportunity Commission also makes a number of resources available at https://www.eeoc.gov/eeoc/publications/index.cfm to ensure that employees may perform their work without hindrance. Graduate students and post-doctoral researchers are understood to have a dual role as both trainees and employees, in accordance with 2 CFR 200.400 (f).

13. Prohibition on Lobbying Activity

By accepting funds under this award, you agree that none of the funds obligated on the award shall be expended, directly or indirectly, to influence congressional action on any legislation or

appropriation matters pending before Congress, other than to communicate to Members of Congress as described in 18 USC 1913. This restriction is in addition to those prescribed elsewhere in statute and regulation.

14. Proprietary Application Information

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

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

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

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

15. Publications

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

16. Registration Requirements

Additional administrative requirements for DOE grants and cooperative agreements are contained in 2 CFR 25 (See: www.eCFR.gov). Prime awardees must keep their data in SAM current at www.SAM.gov. Subrecipients at all tiers must obtain DUNS numbers and provide the DUNS to the prime awardee before the subaward can be issued.

17. Research Misconduct

Scientific discoveries can only take place when scientific research is conducted in a fair, transparent, and honestly reported manner. Any form of dishonesty—whether plagiarism, falsifying results, or misrepresenting conditions—makes it impossible to advance our understanding of the physical universe.

Recipients are "responsible for maintaining the integrity of research of any kind under an award from DOE including the prevention, detection, and remediation of research misconduct, and the conduct of inquiries, investigations, and adjudication of allegations of research misconduct," and conducting appropriate administrative processes in response to allegations of research misconduct in accordance with 2 CFR 910.132. Allegations of any misconduct under an award resulting from this FOA must be reported to the appropriate institutional officials in accordance with institutional policies against misconduct. Additional information on DOE research misconduct policies can be found at: https://science.osti.gov/grants/Policy-and-Guidance/Research-Misconduct.

18. Rights in Technical Data

Normally, the government has unlimited rights in technical data created under a DOE agreement, including the right to distribute to the public. Delivery or third-party licensing of proprietary software or data developed solely at private expense ("Limited Rights Data") will not normally be required except as specifically negotiated in a particular agreement to satisfy DOE's own needs or to ensure the commercialization of technology developed under a DOE agreement.

If software is specified for delivery to DOE, or if other special circumstances exist, e.g., DOE specifying "open-source" treatment of software, then the DOE Contracting Officer, after negotiation with the recipient, may include in the award special provisions requiring the recipient to obtain written approval of the DOE Contracting Officer prior to asserting copyright in the software, modifying the retained Government license, and/or otherwise altering the copyright provisions.

19. Subaward and Executive Reporting

Additional administrative requirements necessary for DOE grants and cooperative agreements to comply with the Federal Funding and Transparency Act of 2006 (FFATA) are contained in 2 CFR 170. (See: www.eCFR.gov). Prime awardees must register with the new FSRS database at https://www.fsrs.gov and report the required data on their first tier subrecipients. Prime awardees must report the executive compensation for their own executives as part of their registration profile in SAM.

20. Title to Subject Inventions

A primary objective of DOE's multi-billion dollar research, development and demonstration investments is to cultivate new research and development ecosystems, manufacturing

capabilities, and supply chains for and by U.S. industry and labor. Therefore, in exchange for receiving taxpayer dollars to support an applicant's project, the applicant must agree to the following U.S. Competitiveness Provision as part of an award under this FOA.

U.S. Competitiveness

The Recipient agrees that any products embodying any subject invention or produced through the use of any subject invention will be manufactured substantially in the United States unless the Recipient can show to the satisfaction of DOE that it is not commercially feasible. In the event DOE agrees to foreign manufacture, there will be a requirement that the Government's support of the technology be recognized in some appropriate manner, e.g., alternative binding commitments to provide an overall net benefit to the U.S. economy. The Recipient agrees that it will not license, assign or otherwise transfer any subject invention to any entity, at any tier, unless that entity agrees to these same requirements. Should the Recipient or other such entity receiving rights in the invention(s): (1) undergo a change in ownership amounting to a controlling interest, or (2) sell, assign, or otherwise transfer title or exclusive rights in the invention(s), then the assignment, license, or other transfer of rights in the subject invention(s) is/are suspended until approved in writing by DOE. The Recipient and any successor assignee will convey to DOE, upon written request from DOE, title to any subject invention, upon a breach of this paragraph. The Recipient will include this paragraph in all subawards/contracts, regardless of tier, for experimental, developmental or research work.

Please note that a subject invention is any invention conceived or first actually reduced in performance of work under an award. An invention is any invention or discovery which is or may be patentable. The contractor includes any awardee, recipient, sub-awardee, or subrecipient.

As noted in the U.S. Competitiveness Provision, at any time in which an entity cannot meet the requirements of the U.S. Competitiveness Provision, the entity may request a modification or waiver of the U.S. Competitiveness Provision. For example, the entity may propose modifying the language of the U.S. Competitiveness Provision in order to change the scope of the requirements or to provide more specifics on the application of the requirements for a particular technology. As another example, the entity may request that the U.S. Competitiveness Provision be waived in lieu of a net benefits statement or U.S. manufacturing plan. The statement or plan would contain specific and enforceable commitments that would be beneficial to the U.S. economy and competitiveness. Examples of such commitments could include manufacturing specific products in the U.S., making a specific investment in a new or existing U.S. manufacturing facility, keeping certain activities based in the U.S. or supporting a certain number of jobs in the U.S. related to the technology. DOE may, in its sole discretion, determine that the proposed modification or waiver promotes commercialization and provides sufficient U.S. economic benefits, and grant the request. If granted, DOE will modify the award terms and conditions for the requesting entity accordingly.

The U.S. Competitiveness Provision is implemented by DOE pursuant to a Determination of Exceptional Circumstances (DEC) under the Bayh-Dole Act and DOE Patent Waivers.

- Determination of Exceptional Circumstances (DEC): On June 07, 2021, DOE approved a
 DETERMINATION OF EXCEPTIONAL CIRCUMSTANCES (DEC) UNDER THE
 BAYH-DOLE ACT TO FURTHER PROMOTE DOMESTIC MANUFACTURE OF DOE
 SCIENCE AND ENERGY TECHNOLOGIES. In accordance with this DEC, all awards,
 including sub-awards, under this FOA shall include the U.S. Competitiveness Provision
 above. A copy of the DEC can be found at https://www.energy.gov/gc/determination-exceptional-circumstances-decs.
- Pursuant to 37 CFR § 401.4, any nonprofit organization or small business firm as defined by 35 U.S.C. 201 affected by any DEC has the right to appeal it by providing written notice to DOE within 30 working days from the time it receives a copy of the determination.
- DOE may require additional submissions or requirements as authorized by any applicable DEC.
- DEC: DOE has issued the DEC entitled, "DETERMINATION OF EXCEPTIONAL CIRCUMSTANCES UNDER THE BAYH-DOLE ACT FOR QUANTUM INFORMATION SCIENCE TECHNOLOGIES", dated August 28, 2020, pursuant to 37 CFR 401.3(a)(2), which applies to agreements issued under this FOA requiring each applicant to agree to a U.S. Competitiveness Provision. DOE has determined that exceptional circumstances exist that warrant the modification of the standard patent rights clause for small businesses and non-profit awardees under the Bayh-Dole Act, 35 U.S.C. 200 et seq., to the extent necessary to ensure that DOE "obtains sufficient rights in the federally supported inventions to meet the needs of [DOE]" and "to promote the commercialization and public availability of inventions made in the United States by United States industry and labor" and/or further promote other purposes of the Bayh-Dole Act. 35 U.S.C. § 200.

D. REFERENCE MATERIAL

Glossary of Useful Grants and Cooperative Agreement terms

Acquisition cost	Acquisition cost means the cost of the asset including the cost to ready the asset for its intended use. Acquisition cost for equipment, for example, means the net invoice price of the equipment, including the cost of any modifications, attachments, accessories, or auxiliary apparatus necessary to make it usable for the purpose for which it is acquired. Acquisition costs for software includes those development costs capitalized in accordance with generally accepted accounting principles (GAAP). Ancillary charges, such as taxes, duty, protective in transit insurance, freight, and installation may be included in or excluded from the acquisition cost in accordance with the non-Federal entity's regular accounting practices.
Administrative requirements	Administrative requirements means the general business management practices that are common to the administration of all grants, such as financial accountability, reporting, equipment management, and retention of records.
Advance payment	Advance payment means a payment that a Federal awarding agency or pass- through entity makes by any appropriate payment mechanism, including a predetermined payment schedule, before the non-Federal entity disburses the

	funds for program purposes.
Allocation	Allocation means the process of assigning a cost, or a group of costs, to one or more cost objective(s), in reasonable proportion to the benefit provided or other equitable relationship. The process may entail assigning a cost(s) directly to a final cost objective or through one or more intermediate cost objectives.
Allocability	Allocability means the principle which requires that an expense or service charged must directly benefit and be necessary for the performance of the project; when multiple projects are benefited reasonable proportions must be able to be assigned. See 2 CFR 200.405.
Allowable cost	Allowable cost means a cost incurred by a recipient that is: (1) reasonable for the performance of the award; (2) allocable; (3) in conformance with any limitations or exclusions set forth in the Federal cost principles applicable to the organization incurring the cost or in the award documents as to the type or amount of cost; (4) consistent with regulations, policies, and procedures of the recipient that are applied uniformly to both federally supported and other activities of the organization; (5) accorded consistent treatment as a direct or indirect cost; (6) determined in accordance with generally accepted accounting principles; and (7) not included as a cost in any other federally supported award (unless specifically authorized by statute). See 2 CFR 200.403.
Application	Application means a request for financial support of a project or activity submitted to DOE on specified forms and in accordance with DOE instructions. Also known as a proposal.
Appropriation Act	Appropriation act means the statute that provides the authority for Federal agencies to incur obligations to and make payments out of the U.S. treasury for specified purposes.
Approved budget	The approved budget for the Federal award summarizes the financial aspects of the project or program as approved during the Federal award process. It may include either the Federal and non-Federal share or only the Federal share, depending upon Federal awarding agency requirements. It must be related to performance for program evaluation purposes whenever appropriate. See 2 CFR 200.308(a).
Assurance	Assurance means a certification by an applicant, normally included with the application or State plan, indicating that the entity is in compliance with, or that it will abide by, a particular requirement if awarded a Federal grant.
Authorized organizational representative	Authorized organizational representative means the individual, named by the applicant organization, who is authorized to act for the applicant and to assume the obligations imposed by the Federal laws, regulations, requirements, and conditions that apply to grant applications or grant awards.
Award	Award means the provision of funds by DOE, based on an approved application and budget or progress report, to an organizational entity or an individual to carry out a project or activity.
Award documents	 Award documents means the entirety of the documents describing the legal relationship between DOE and an awardee or recipient. The award documents include an Assistance Agreement and other documents which may be incorporated by reference or as attachments to the Assistance Agreement. The award documents are the official, legally binding document, signed (or the electronic equivalent of signature) by a Contracting Officer that: notifies the recipient of the award of a grant; contains or references all the terms and conditions of the grant and Federal funding limits and obligations; and, provides the documentary basis for recording the obligation of Federal

	funds in the DOE accounting system.
Bayh-Dole Act	Bayh-Dole Act means a law which encourages universities and researchers to develop their inventions into marketable products; formal citation is Section 6
Budget	of the Patent and Trademark Amendment of 1980, Pub. L 96-517 as amended. Budget means the financial plan for the project or program that the Federal awarding agency or pass-through entity approves during the Federal award process or in subsequent amendments to the Federal award. It may include the Federal and non-Federal share or only the Federal share, as determined by the Federal awarding agency or pass-through entity.
Budget period	Budget period means the intervals of time (usually 12 months each) into which a project period is divided for budgetary and funding purposes.
Business officer	Business officer means the financial official of the grantee who has primary fiscal responsibility for the grant. Also known as authorized organizational representative.
Capital assets	Capital assets means tangible or intangible assets used in operations having a useful life of more than one year which are capitalized in accordance with GAAP. Capital assets include: (a) Land, buildings (facilities), equipment, and intellectual property (including software) whether acquired by purchase, construction, manufacture, lease-purchase, exchange, or through capital leases; and (b) Additions, improvements, modifications, replacements, rearrangements, reinstallations, renovations or alterations to capital assets that materially increase their value or useful life (not ordinary repairs and maintenance).
Carryover	Carryover means unobligated Federal funds remaining at the end of any budget period that may be carried forward to another budget period to cover allowable costs of that budget period (whether as an offset or additional authorization). Obligated, but unliquidated, funds are not considered carryover.
Change in scope	Change in scope means an activity whereby the objectives or specific aims identified in the approved grant application are significantly changed by the grantee after award. Contracting Officer prior approval is required for a change in scope to be allowable under an award.
Closeout	Closeout means the process by which a Federal awarding agency determines that all applicable administrative actions and all required work under an award have been completed by the grantee and the Federal awarding agency.
Competitive segment	Competitive segment means the initial project period recommended for support or each extension of a project period resulting from a renewal award.
Conference (domestic or international)	Conference (domestic or international) means a symposium, seminar, workshop, or any other organized and formal meeting, whether conducted face-to-face or via the Internet, where individuals assemble (or meet virtually) to exchange information and views or explore or clarify a defined subject, problem, or area of knowledge, whether or not a published report results from such meeting.
Consortium or sub-award agreement	Consortium or sub-award agreement means a formalized agreement whereby a research project is carried out by the grantee and one or more other organizations that are separate legal entities. Under the agreement, the grantee must perform a substantive role in the conduct of the planned research and not merely serve as a conduit of funds to another party or parties. These agreements typically involve a specific level of effort from the consortium organization's PD/PI and a categorical breakdown of costs, such as personnel, supplies, and other allowable expenses, including F&A costs. The relationship between the recipient and the collaborating organizations is considered a sub-award relationship.

Consultant	Consultant means an individual who provides professional advice or services for a fee, but not as an employee of the engaging party. To prevent apparent or actual conflicts of interest, grantees and consultants must establish written guidelines indicating the conditions of payment of consulting fees. Consultants also include firms that provide professional advice or services. See 2 CFR 200.459.
Continuation application/award	Continuation application/award means a financial assistance request (in the form of an application or progress report) or resulting award for a subsequent budget period within a previously approved project period for which a recipient does not have to compete with other applicants.
Contract	Contract means a legal instrument by which a non-Federal entity purchases property or services needed to carry out the project or program under a Federal award. The term as used in this part does not include a legal instrument, even if the non-Federal entity considers it a contract, when the substance of the transaction meets the definition of a Federal award or sub-award (see 2 CFR 200.1 Subaward).
Contractor	<i>Contractor</i> means an entity that receives a contract as defined in 2 CFR 200.1 Contract.
Contracting (or Grants) Officer	Contracting (or Grants) Officer means a DOE official responsible for the business management aspects of grants and cooperative agreements, including review, negotiation, award, and administration, and for the interpretation of grants administration policies and provisions. COs and GOs are delegated the authority to obligate DOE to the expenditure of funds and permit changes to approved projects on behalf of DOE.
Contracting (or Grants Management) specialist	Contracting (or Grants Management) specialist means a DOE staff member who works with a Contracting or Grants Officer and is assigned the day-to-day management of a portfolio of grants and/or cooperative agreements. These activities include, but are not limited to, evaluating grant applications for administrative content and compliance with statutes, regulations, and guidelines; negotiating grants; providing consultation and technical assistance to grantees; and administering grants after award.
Cooperative agreement	Cooperative agreement means a type of financial assistance used when there will be substantial Federal scientific or programmatic involvement. Substantial involvement means that, after award, scientific or program staff will assist, guide, coordinate, or participate in project activities.
Cost principles	Cost principles means the government-wide principles, 2 CFR 200 Subpart E (or, in the case of commercial organizations, the Federal Acquisition Regulation [48 CFR 31], or, in the case of hospitals, see Appendix IX to Part 200—Hospital Cost Principles, Appendix E, "Principles For Determining Costs Applicable to Research and Development Under Grants and Contracts with Hospitals"), on allowability and unallowability of costs under federally sponsored agreements.
Cost sharing or matching	Cost sharing or matching means the portion of project costs not paid by Federal funds (unless otherwise authorized by Federal statute). See also 2 CFR 200.306 Cost sharing or matching.
Deadline	Deadline means the published date and/or time that a grant application is to be submitted to the funding agency.
Debarment and suspension	Debarment and suspension means the actions taken by a debarring official in accordance with OMB guidance at 2 CFR 180, "Non-procurement Debarment and Suspension," to exclude a person or organization from participating in grants and other non-procurement awards government-wide. If debarred or suspended, the person or organization may not receive financial assistance (under a grant, cooperative agreement, or sub-award, or contract under a grant)

	for a specified period of time. Debarments and suspensions carried out pursuant to 2 CFR 376 are distinct from post-award suspension action by an awarding agency. See 2 CFR 901 for DOE implementation.
Direct costs	Direct costs means costs that can be identified specifically with a particular sponsored project, an instructional activity, or any other institutional activity, or that can be directly assigned to such activities relatively easily with a high degree of accuracy. See 2 CFR 200.413.
Disallowed costs	Disallowed costs means those charges to a Federal award that the Federal awarding agency or pass-through entity determines to be unallowable, in accordance with the applicable Federal statutes, regulations, or the terms and conditions of the Federal award.
Domestic organization	Domestic organization means a public (including a State or other governmental agency) or private non-profit or for-profit organization that is located in the United States or its territories, is subject to U.S. laws, and assumes legal and financial accountability for awarded funds and for the performance of the grant-supported activities.
DUNS number	DUNS number means a nine-digit number established and assigned by Dun and Bradstreet to uniquely identify a business entity.
Effort	Effort means the amount of time, usually expressed as a percentage of the total, which a faculty member or other employee spends on a sponsored project. No one is allowed to spend more than 100% total commitment on all academic activities, including grant-sponsored research, university-sponsored research, teaching, administration, advising and other contracted duties. Effort is indicated on the budget in units of person-months.
Equipment	Equipment means tangible personal property (including information technology systems) having a useful life of more than one year and a per-unit acquisition cost which equals or exceeds the lesser of the capitalization level established by the non-Federal entity for financial statement purposes, or \$5,000. See also 2 CFR 200.1 Capital assets, Computing devices, General purpose equipment, Information technology systems, Special purpose equipment, and Supplies.
Expanded authorities	Expanded authorities means authorization to grantees under certain research grant mechanisms which waives the requirement for prior agency approval for specified actions related to awards. Example: 90-day pre-award spending authority, no cost extensions for up to one additional year, and automatic carryover of unobligated funds from one budget period to the next. The expanded authorities are now contained in the standard terms and conditions for most research grants.
Expiration date	Expiration date means generally, the date signifying the end of the current project period, after which the grantee is not authorized to obligate grant funds.
Facilities and administrative costs	Facilities and administrative costs means costs that are incurred by a grantee for common or joint objectives and that, therefore, cannot be identified specifically with a particular project or program. These costs also are known as indirect costs.
Federal financial report	Federal financial report means submitted on Standard Form (SF) 425, to indicate the status of awarded funds for the period covered. Frequency of reporting is specified in the Reporting Checklist provided as part of the award documents.
Financial assistance	Financial assistance means transfer by DOE of money or property to an eligible entity to support or stimulate a public purpose authorized by statute.
Financial status report	Financial status report means see Federal Financial Report.
Foreign travel	Foreign travel is meant to include travel outside of North America (Canada, Mexico, and the United States) and U.S. territories and possessions (Guam,

	American Samoa, Puerto Rico, the U.S. Virgin Islands. A trip is considered foreign travel for all legs of the itinerary if the traveler does not return to his or her post prior to departure for a foreign destination. Costs for foreign travel may be restricted by the language of a Funding Opportunity Announcement.
Funding opportunity announcement (FOA)	Funding opportunity announcement (FOA) means A publicly available document by which a Federal Agency makes known its intentions to award discretionary grants or cooperative agreements, usually as a result of competition for funds. Funding opportunity announcements may be known as program announcements, requests for applications, notices of funding availability, solicitations, or other names depending on the Agency and type of program. Funding opportunity announcements can be found at www.Grants.gov . An FOA may also be known as a solicitation.
Grant agreement	Grant agreement means a legal instrument of financial assistance between a Federal awarding agency or pass-through entity and a non-Federal entity that, consistent with 31 USC 6302, 6304: (a) Is used to enter into a relationship the principal purpose of which is to transfer anything of value from the Federal awarding agency or pass-through entity to the non-Federal entity to carry out a public purpose authorized by a law of the United States (see 31 USC 6101(3)); and not to acquire property or services for the Federal awarding agency or pass-through entity's direct benefit or use; (b) Is distinguished from a cooperative agreement in that it does not provide for substantial involvement between the Federal awarding agency or pass-through entity and the non-Federal entity in carrying out the activity contemplated by the Federal award. (c) Does not include an agreement that provides only: (1) Direct United States Government cash assistance to an individual; (2) A subsidy; (3) A loan; (4) A loan guarantee; or (5) Insurance.
Grant-supported project or activity	Grant-supported project or activity means those activities specified or described in a grant application or in a subsequent submission that are approved by DOE for funding, regardless of whether Federal funding constitutes all or only a portion of the financial support necessary to carry them out.
Grantee	Grantee means the organization or individual awarded a grant or cooperative agreement by DOE that is responsible and accountable for the use of the funds provided and for the performance of the grant-supported project or activity. The grantee is the entire legal entity even if a particular component is designated in award documents. The grantee is legally responsible and accountable to DOE for the performance and financial aspects of the grant-supported project or activity. Also known as awardee or recipient.
Grants.gov	Grants.gov (https://www.Grants.gov/) has been designated by the Office of Management and Budget as the single access point for all grant programs offered by 26 Federal grant-making agencies. It provides a single interface for agencies to announce their grant opportunities and for all applicants to find and apply for those opportunities.
Indirect costs (facilities & administrative)	Indirect (F&A) costs means those costs incurred for a common or joint purpose benefitting more than one cost objective, and not readily assignable to the cost objectives specifically benefitted, without effort disproportionate to the results achieved. To facilitate equitable distribution of indirect expenses to the cost objectives served, it may be necessary to establish a number of pools

	of indirect (F&A) costs. Indirect (F&A) cost pools must be distributed to
	benefitted cost objectives on bases that will produce an equitable result in consideration of relative benefits derived.
Institutional base salary	Institutional base salary means the annual compensation paid by an organization for an employee's appointment, whether that individual's time is spent on research, teaching, patient care, or other activities. Base salary excludes any income that an individual may be permitted to earn outside of duties for the applicant/grantee organization. Base salary may not be increased as a result of replacing organizational salary funds with grant funds.
Matching or cost sharing	Matching or cost sharing means the value of third-party in-kind contributions and the portion of the costs of a federally assisted project or program not borne by the Federal government. Matching or cost sharing may be required by statute or program regulation. Costs used to satisfy matching or cost-sharing requirements are subject to the same policies governing allowability as other costs under the approved budget.
Merit (or peer) review	Merit (or peer) review means the process that involves the consistent application of standards and procedures that produce fair, equitable, and objective examinations of applications based on an evaluation of scientific or technical merit or other relevant aspects of the application. The review is performed by experts (reviewers) in the field of endeavor for which support is requested. Merit review is intended to provide guidance and to the DOE individuals responsible for making award decisions.
Monitoring	Monitoring means a process whereby the programmatic and business management performance aspects of a grant are assessed by reviewing information gathered from various required reports, audits, site visits, and other sources.
NEPA	NEPA means the National Environmental Policy Act (NEPA), Public Law 91-190, as amended. NEPA requires Federal agencies to assess the environmental effects of proposed major Federal actions prior to making decisions.
No-cost extension	<i>No-cost extension</i> means an extension of time to a project period and/or budget period to complete the work of the grant under that period, without additional Federal funds or competition.
Non-Federal share	Non-Federal share means when cost sharing or matching is required as a condition of an award, the portion of allowable project/program costs not borne by the Federal government.
Obligations	Obligations when used in connection with a non-Federal entity's utilization of funds under a Federal award, <i>obligations</i> means orders placed for property and services, contracts and sub-awards made, and similar transactions during a given period that require payment by the non-Federal entity during the same or a future period.
OMB circulars	OMB circulars means government-wide guidance issued to Heads of Federal agencies by the Director of the Office of Management and Budget.
Other significant contributors	Other significant contributors means individuals who have committed to contribute to the scientific development or execution of the project, but are not committing any specified measurable effort (i.e., person months) to the project. These individuals are typically presented at "effort of zero person months" or "as needed." Individuals with measurable effort may not be listed as Other Significant Contributors (OSCs). Consultants should be included if they meet this definition.
Program participant	Program participants are the recipients of service or training provided at a workshop, conference, seminar, symposium or other short-term instructional or information-sharing activity funded by an external grant or award, or the training beneficiaries of the project or program funded by an external grant or

	award. A participant is not involved in providing any deliverable to the grantee
Participant support costs	or a third party or would not be terminated or replaced for failure to perform. Participant support costs means direct costs for items such as stipends or subsistence allowances, travel allowances, and registration fees paid to or on behalf of participants or trainees (but not employees) in connection with conferences, or training projects.
Person months	Person months is the metric for expressing the effort (amount of time) PD/PI(s), faculty and other senior/key personnel devote to a specific project. The effort is based on the type of appointment of the individual with the organization; e.g., calendar year, academic year, and/or summer term; and the organization's definition of such. For instance, some institutions define the academic year as a 9-month appointment while others define it as a 10-month appointment.
Pre-application or pre- proposal	 Pre-application or pre-proposal means a brief outline or narrative of proposed work and sometimes budget, for informal review by a sponsor to determine whether an application should be submitted. Three predominant reasons for requiring submission of a preliminary pre-application are: Reduce the applicant's unnecessary effort in proposal preparation when the chance of success is very small. This is particularly true of exploratory initiatives where the community senses that a major new direction is being identified, or competitions that will result in a small number of actual awards. Increase the overall quality of the submission. Distill the number of applications that will be submitted to the agency and the number of anticipated reviewers needed to review.
Pre-award costs	<i>Pre-award costs</i> means any cost incurred prior to the beginning date of the project period or the initial budget period of a competitive segment (under a multi-year award), in anticipation of the award and at the applicant's own risk, for otherwise allowable costs.
Prior approval	<i>Prior approval</i> means written approval from the designated Contracting Officer.
Program Director/ Principal Investigator	Program Director/ Principal Investigator means the individual(s) designated by the applicant organization to have the appropriate level of authority and responsibility to direct the project or program to be supported by the award. The applicant organization may designate multiple individuals as program directors/principal investigators (PD/PIs) who share the authority and responsibility for leading and directing the project, intellectually and logistically. When multiple PD/PIs are named, each is responsible and accountable to the applicant organization, or as appropriate, to a collaborating organization for the proper conduct of the project or program including the submission of all required reports. The presence of more than one PD/PI on an application or award diminishes neither the responsibility nor the accountability of any individual PD/PI.
Program income	Program income means gross income earned by the non-Federal entity that is directly generated by a supported activity or earned as a result of the Federal award during the period of performance except as provided in 2 CFR 200.307 paragraph (f). (See 2 CFR 200.1 Period of performance.) Program income includes but is not limited to income from fees for services performed, the use or rental or real or personal property acquired under Federal awards, the sale of commodities or items fabricated under a Federal award, license fees and royalties on patents and copyrights, and principal and interest on loans made with Federal award funds. Interest earned on advances of Federal funds is not program income. Except as otherwise provided in Federal statutes, regulations,

	or the terms and conditions of the Federal award, program income does not include rebates, credits, discounts, and interest earned on any of them. See also
	2 CFR 200.407 Prior written approval (prior approval). See also 35 USC 200-
	212 "Disposition of Rights in Educational Awards" for inventions made under
	Federal awards.
Program Manager	Program Manager means the DOE official responsible for the programmatic,
	scientific, and/or technical aspects of a grant. The same role is filled by
	Program Directors, Program Officers, or Project Directors at other Federal
	agencies.
Progress report	Progress report means periodic, frequently annual, report submitted by the
	grantee and used by DOE to assess progress and to determine whether to
Project/performance site	provide funding for the budget period subsequent to that covered by the report. Project/ performance site means location(s) of where the work described in the
Project/performance site	research plan will be conducted.
Project period	Project period means the total time for which Federal support of a project has
1 Toject period	been programmatically approved as shown in the award documents; however,
	it does not constitute a commitment by the Federal government to fund the
	entire period. The total award period comprises the initial competitive
	segment, any subsequent competitive segments resulting from a renewal
	award(s), and extensions.
Proposal	See application.
Re-budgeting	Re-budgeting means reallocation of funds available for spending between
	approved budget categories to allow best use of funds to accomplish the
Destated	project goals.
Recipient	<i>Recipient</i> means the organizational entity or individual receiving a grant or cooperative agreement.
Renewal application	Renewal application means an application requesting additional funding for a
renewai application	period subsequent to that provided by a current award. Renewal applications
	compete for funds with all other peer reviewed applications and must be
	developed as fully as though the applicant is applying for the first time.
Research	Research is defined as a systematic study directed toward fuller scientific
	knowledge or understanding of the subject studied. See 2 CFR 200.1 Research
	and Development (R&D).
Research misconduct	Research misconduct means fabrication, falsification, or plagiarism in
	proposing, performing, or reviewing research, or in reporting research results,
SAM gov	but does not include honest error or differences of opinion. See 10 CFR 733. SAM.gov is the System for Award Management (SAM) a consolidated service
SAM.gov	that includes Entity Registration, Assistance Listings, and other services for
	making, managing, and receiving Federal awards.
Scope of work	Scope of work means the aims, objectives, and purposes of a grant; as well as
<u>*</u> *	the methodology, approach, analyses or other activities; and the tools,
	technologies, and timeframes needed to meet the grant's objectives. This
	includes the research or training plan included with the original grant
	application, along with any approved modifications.
Senior/Key Personnel	Senior/Key personnel means the PD/PI and other individuals who contribute to
	the scientific development or execution of a project in a substantive,
	measurable way, whether or not they receive salaries or compensation under
	the grant. Typically, these individuals have doctoral or other professional
	degrees, although individuals at the masters or baccalaureate level may be
	considered senior/key personnel if their involvement meets this definition. Consultants and those with a postdoctoral role also may be considered
	senior/key personnel if they meet this definition. "Zero percent" effort or "as
	needed" is not an acceptable level of involvement for Senior/Key Personnel.
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Significant re-budgeting	Significant re-budgeting means a threshold that is reached when expenditures in a single direct cost budget category deviate (increase or decrease) from the
	categorical commitment level established for the budget period by more than
	25 percent of the total costs awarded. Significant re-budgeting is one indicator
	of change in scope.
Small business concern	Small business concern means a business that meets the regulatory and size
	requirements established by the SBA at 13 CFR part 121.
Solicitation	See Funding Opportunity Announcement.
Subaward	Subaward means a legal instrument by which a recipient provides funds (or
	property in lieu of funds) to an eligible subrecipient (or a lower-tier
	transaction) to perform a substantive portion of the grant-supported program or
	project. The term includes such financial assistance when provided by any
	legal agreement (even if the agreement is called a contract) but does not
	include any form of assistance which is excluded from the definition of a
	grant, including the recipient's procurement of property or services needed to
	carry out the project or program. The term includes consortium agreements.
Subrecipient	Subrecipient means a non-Federal entity that receives a subaward from a pass-
	through entity to carry out part of a Federal program; but does not include an
	individual that is a beneficiary of such program. A sub-recipient may also be a
	recipient of other Federal awards directly from a Federal awarding agency.
Supplement	Supplement means a request for an increase in support during a current budget
	period for expansion of the project's scope or to meet increased costs
	unforeseen at the time of the new or renewal application. A supplement may
	increase support for future years in addition to the current year. Supplements
	require applications and are subject to administrative and merit review.
Terms and conditions of	Terms and conditions of award means all legal requirements imposed on a
award	grant by DOE, whether based on statute, regulation, policy, or other document
	referenced in the grant award, or specified by the grant award document itself.
	The award documents may include both standard and special conditions that
	are considered necessary to attain the grant's objectives, facilitate post-award
	administration of the grant, conserve grant funds, or otherwise protect the
	Federal government's interests.
Unallowable costs	<i>Unallowable costs</i> means costs that cannot be charged, directly or indirectly,
	to Federal awards because the costs are prohibited by law, regulation
	(including applicable cost principles), or the terms and conditions of award.
	Costs that are not allowable, allocable, or reasonable are unallowable.
Unliquidated obligation	Unliquidated obligations means, for financial reports prepared on a cash basis,
	obligations incurred by the non-Federal entity that have not been paid
	(liquidated). For reports prepared on an accrual expenditure basis, these are
	obligations incurred by the non-Federal entity for which an expenditure has not been recorded.
Unobligated balance	Unobligated balance means the amount of funds under a Federal award that
Unobligated balance	the non-Federal entity has not obligated. The amount is computed by
	subtracting the cumulative amount of the non-Federal entity's unliquidated
	obligations and expenditures of funds under the Federal award from the
	cumulative amount of the funds that the Federal awarding agency or pass-
	pass-
	through entity authorized the non-Federal entity to obligate
Validate	In the context of the data management plan requirements, <i>validate</i> means to
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Validate	In the context of the data management plan requirements, <i>validate</i> means to support, corroborate, verify, or otherwise determine the legitimacy of the
Validate	In the context of the data management plan requirements, <i>validate</i> means to support, corroborate, verify, or otherwise determine the legitimacy of the research findings. Validation of research findings could be accomplished by
Validate	In the context of the data management plan requirements, <i>validate</i> means to support, corroborate, verify, or otherwise determine the legitimacy of the