U.S. Department of Energy

Small Business Innovation Research (SBIR) and
Small Business Technology Transfer (STTR) Programs

Topics
FY 2021
Phase I
Release 1

Version 3, August 17, 2020

Office of Advanced Scientific Computing Research
Office of Basic Energy Sciences
Office of Biological and Environmental Research
Office of Nuclear Physics

Schedule

Event	Dates
Topics Released:	Monday, July 13, 2020
Funding Opportunity Announcement Issued:	Monday, August 24, 2020
Letter of Intent Due Date:	Tuesday, September 08, 2020 5:00pm ET
Application Due Date:	Monday, October 19, 2020 11:59pm ET
Award Notification Date:	Monday, January 11, 2021*
Start of Grant Budget Period:	Tuesday, February 22, 2021

*** Date Subject to Change**

Table of Changes		
Version	**Date**	**Change**
Ver. 1	July 13, 2020	Original
Ver. 2	Aug. 10, 2020	• Topic 30: Updated Topic Description • Topic 30, subtopic a: Updated Subtopic Description • Topic 30, references: Added Reference 11
Ver. 3	Aug. 17, 2020	• Updated Schedule

INTRODUCTION TO DOE SBIR/STTR TOPICS

This SBIR/STTR topics document is issued in advance of the FY 2020 DOE SBIR/STTR Phase I Release 1 Funding Opportunity Announcement scheduled to be issued in on August 12, 2019. The purpose of the early release of the topics is to allow applicants an opportunity to identify technology areas of interest and to begin formulating innovative responses and partnerships. Applicants new to the DOE SBIR/STTR programs are encouraged to attend upcoming topic and Funding Opportunity Announcement webinars. Dates for these webinars are listed on our website: https://science.osti.gov/sbir/Funding-Opportunities.

Topics may be modified in the future. Applicants are encouraged to check for future updates to this document, particularly when the Funding Opportunity Announcement is issued. Any changes to topics will be listed at the beginning of this document.

General introductory information about the DOE SBIR/STTR programs can be found online here: https://science.osti.gov/SBIRLearning. Please check out the tutorials--a series of short videos designed to get you up to speed quickly.

COMMERCIALIZATION

Federal statutes governing the SBIR/STTR programs require federal agencies to evaluate the commercial potential of innovations proposed by small business applicants. To address this requirement, the DOE SBIR/STTR programs require applicants to submit commercialization plans as part of their Phase I and II applications. DOE understands that commercialization plans will evolve, sometimes significantly, during the course of the research and development, but investing time in commercialization planning demonstrates a commitment to meeting objectives of the SBIR/STTR programs. During Phase I and II awards, DOE provides small businesses with commercialization assistance through a DOE-funded contractor.

The responsibility for commercialization lies with the small business. DOE's SBIR/STTR topics are drafted by DOE program managers seeking to advance the DOE mission. Therefore, while topics may define important scientific and technical challenges, we look to our small business applicants to define how they will bring commercially viable products or services to market. In cases where applicants are able identify a viable technical solution, but unable to identify a successful commercialization strategy, we recommend that they do not submit an SBIR/STTR application.

TECHNOLOGY TRANSFER OPPORTUNITIES

Selected topic and subtopics contained in this document are designated as **Technology Transfer Opportunities (TTOs)**. The questions and answers below will assist you in understanding how TTO topics and subtopics differ from our regular topics.

What is a TTO?

A TTO is an opportunity to leverage technology that has been developed at a university or DOE National Laboratory. Each TTO will be described in a particular subtopic and additional information may be obtained by using the link in the subtopic to the university or National Lab that has developed the technology. Typically the technology was developed with DOE funding of either basic or applied research and is available for transfer to the private sector. The level of technology maturity will vary and applicants are encouraged to contact the appropriate university or Laboratory prior to submitting an application.

How would I draft an appropriate project description for a TTO?
For Phase I, you would write a project plan that describes the research or development that you would perform to establish the feasibility of the TTO for a commercial application. The major difference from a regular subtopic is that you will be able to leverage the prior R&D carried out by the university or National Lab and your project plan should reflect this.

Am I required to show I have a subaward with the university or National Lab that developed the TTO in my grant application?
No. Your project plan should reflect the most fruitful path forward for developing the technology. In some cases, leveraging expertise or facilities of a university or National Lab via a subaward may help to accelerate the research or development effort. In those cases, the small business may wish to negotiate with the university or National Lab to become a subawardee on the application.

Is the university or National Lab required to become a subawardee if requested by the applicant?
No. Collaborations with universities or National Labs must be negotiated between the applicant small business and the research organization. The ability of a university or National Lab to act as a subcontractor may be affected by existing or anticipated commitments of the research staff and its facilities.

Are there patents associated with the TTO?
The TTO will be associated with one or in some cases multiple patent applications or issued patents.

Will the rights to the TTO be exclusive or non-exclusive?
Each TTO will describe whether the license rights will be exclusive or non-exclusive. Licenses are typically limited to a specific field of use.

If selected for award, what rights will I receive to the technology?
Those selected for award under a TTO subtopic, will be assigned rights to perform research and development of the technology during their Phase I or Phase II grants. Please note that these are NOT commercial rights which allow you to license, manufacture, or sell, but only rights to perform research and development. In addition, an awardee will be provided, at the start of its Phase I grant, with a no-cost, six month option to license the technology. It will be the responsibility of the small business to demonstrate adequate progress towards commercialization and negotiate an extension to the option or convert the option to a license. A copy of an option agreement template will be available at the university or National Lab which owns the TTO.

How many awards will be made to a TTO subtopic?
We anticipate making a maximum of one award per TTO subtopic. If we receive applications to a TTO that address different fields of use, it is possible that more than one award will be made per TTO.

How will applying for an SBIR or STTR grant associated with a TTO benefit me?
By leveraging prior research and patents from a National Lab you will have a significant “head start” on bringing a new technology to market. To make greatest use of this advantage it will help for you to have prior knowledge of the application or market for the TTO.

Is the review and selection process for TTO topics different from other topics?
No. Your application will undergo the same review and selection process as other applications.

PROGRAM AREA OVERVIEW: OFFICE OF SCIENCE

The Office of Science's mission is to deliver scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic and national security of the United States. The Office of Science 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. For more information on the Office of Science mission please visit https://science.osti.gov/. The topic below is a collaborative topic among multiple programs in the Office of Science.

1. TECHNOLOGIES FOR MANAGING AND ANALYZING COMPLEX DATA IN SCIENCE AND ENGINEERING

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

There is only one subtopic for this Topic, which has four application areas of focus. Proposals and Letters of Intent should explicitly state which application areas are relevant to the proposal. Priority will be given to grant applications that propose a single solution to address more than one of the application areas detailed below or that draw on complex data from the domain sciences of the DOE programs participating in this solicitation.

a. Complex Data

The offices of Advanced Scientific Computing Research (ASCR), Biological and Environmental Research (BER), and Basic Energy Sciences (BES) in the Office of Science at the US Department of Energy (DOE) are soliciting grant applications for managing and analyzing complex scientific and engineering data sets. The challenge of managing and analyzing complex data is impacting every sector of modern society from energy, defense, healthcare, and transportation to science and engineering. Unlike traditional structured data sets, complex data are characterized by multi-dimensional features including the hallmark characteristics of Big Data: large data volumes, variety, velocity, and veracity. Despite the ubiquitous data challenges faced by the scientific and engineering communities there is still a lack of cost-effective and easy-to-use tools and services that facilitate and accelerate the analysis, organization, retrieval, sharing, and modeling of complex data. The focus of this topic is on the development of commercializable data technology products and services that reduce bottlenecks and increase efficiency in the management and analysis of complex data for science and engineering. Potential grant applicants should focus on the development of innovative data products in the form of turnkey subsystems, cloud-based services, and complete toolkits that can be packaged as standalone or value-added commercial products and services. Companies should develop generic solutions that can be used by many different science communities. The Application Areas listed below may provide exemplars to demonstrate the effectiveness of the proposed product or service. The proposed tools or technology should address at least one of the following capability areas of interest, listed here as sub-bullets:

- Management of complex, scientific data, including data from simulation, experiment, and observation
  - Integrating new results with reference data in real time
  - Managing unstructured metadata and provenance
  - Methods for hosting, archiving, indexing, registration, and support for sharing and reuse of data
  - Return to Table of Contents
  - Automated Quality Assurance/Quality Control (QA/QC) of data
  - Managing data across distributed environments and/or heterogeneous architectures

- Effective use of federated data – facilitating data access and analysis across distributed platforms and logical domains
  - Efficient and cost-effective retention of complex data, taking advantage of a variety of memory and storage options
  - Managing and curating data for Artificial Intelligence / Machine Learning applications – making data "AI-ready"
- Analysis of complex data in databases and/or streams
  - Tools for reasoning about and making sense of large, multi-dimensional, multi-modal data through, for example, feature extraction, machine learning, dimensional reduction, compression, and knowledge representation. This includes tools to reduce dimensionality of complex data and identify fundamental descriptors of physical behavior.
  - Visualization tools, especially those that take advantage of new computing hardware and/or that reduce the scale of computing resources needed
  - Tools to integrate data with mathematical models and simulation for enhanced understanding
  - Tools that identify knowledge gaps in highly specific topics. Gaps can be identified through a combined analysis of datasets and published literature. Topics of interest to BES include, for example, synthesis-characterization-functionality relationships for specific families of chemicals or materials
  - Tools that identify experimental best practices, protocols, benchmarks, and candidate standards for the characterization of complex physical behavior (e.g., chemical kinetics, multiple phase changes, etc.)
  - Tools that facilitate artificial or machine learning on data and/or improve access to learned models for broader use.

Grant applications that focus exclusively on the following topics will be considered nonresponsive and will not undergo merit review: a) data analytics algorithms that are not packaged as complete commercial products or services, and b) improvements or extensions of data analytics and open software source stacks that do not lead to commercializable products or services.

Grant applications will be considered nonresponsive and will not undergo merit review if they do not clearly address one or more of the application areas below and state which application areas are being addressed. Priority will be given to grant applications that propose a single solution to address more than one of the application areas detailed below or that draw on complex data from the domain sciences of the DOE programs participating in this solicitation.

Successful grant applications will be required to satisfy the following two important criteria: a) a clear plan to develop innovative data analytics or data management techniques and b) the use of appropriate data sets that represent complex data, namely, data sets that are not easily analyzed by current tools and can include characteristics of Big Data.

Office of Biological and Environmental Research (BER)

Application Area 1: Advanced Data Analytic Technologies for Systems Biology and Bioenergy
BER's Biological Systems Science Division programs integrate multidisciplinary discovery and hypothesis driven science with technology development to understand plant and microbial systems relevant to national priorities in sustainable energy and innovation in life sciences. These programs generate very large and complex data sets that have all of the characteristics of Big Data. Technology improvements in biological instruments from sequencers to advanced imaging devices are continuing to advance at exponential rates, with data volumes in petabytes today and expected to grow to exabytes in the future.

These data are highly complex ranging from high-throughput "omics" data, experimental and contextual environmental data across multiple scales of observations, from the molecular to cellular to the multicellular scale (plants and microbial communities), and multiscale 3D and 4D images for conceptualizing and visualizing the spatiotemporal expression and function of biomolecules, intracellular structures, and the flux of materials across cellular compartments. Currently, the ability to generate complex multi-"omic" environmental data and associated meta-datasets greatly exceeds the ability to interpret these data. Innovative solutions and frameworks for management and analysis of large-scale, multimodal and multiscale data, that enhance effectiveness and efficiency of data processing for investigations across spatial scales and scientific disciplines are needed. New data integration approaches, software tools and modelling frameworks for managing and analyzing 'big data' will be considered.

Grant applications that focus on novel data analytic methods and algorithms for COVID-19 data analyses to facilitate improved modeling and understanding of natural viral populations and persistence in the environment, as well as predictive modeling for viral stability and evolution in changing environmental conditions; understanding virus-microbiome community composition, function, and evolution will also be considered.

Questions – Contact: Ramana Madupu, Ramana.Madupu@Science.doe.gov

Application Area 2: Technologies and Tools to Integrate and Analyze Data from Multiple User Facilities, Community Resources, Instruments and Data Systems

A 2017 workshop report on Grand Challenges from BER's Advisory Committee[1] (BERAC) identifies the need for technologies and tools to integrate and analyze data being generated through BER-funded research and at BER's EMSL[2] and JGI[3] user facilities, as well as data being hosted at other BER-supported community resources such as, but not exclusive to, ESS-DIVE[4], KBase[5], the AmeriFlux network[6], the WHONDRS network[7] and the AQUA-MER database[8].

In addition, the 2018 CESD Strategic Plan[9] identifies scientific grand challenges in biogeochemistry and the integrated water cycle to advance a systems-level understanding of earth and environmental sciences. Both grand challenges rely on analyses that require integrating a wide variety of physical and chemical process data with biological process data. The Plan also identifies data-model integration and the development of interconnected capabilities and tools as an infrastructure grand challenge.

Beyond the databases, systems and networks identified in the preceding paragraph, data on physical, chemical and biological processes are also being generated by many different types of advanced instruments, including new bioimaging capabilities that are being developed with BER support[10] as well as projects supported by the joint EMSL/JGI FICUS program[11] and those supported by the Subsurface Biogeochemical Research (SBR)[12] and Terrestrial Ecosystem Science (TES)[13] programs.
However, progress has been slow in capturing the data from all these different facilities, community resources, and research programs/efforts and making them collectively available to the scientific community. For example, scientists can access data generated by multiple EMSL instruments[14], but technologies and tools to integrate EMSL-generated data with data generated from other user facilities (e.g., JGI) or hosted by community resources (e.g., KBase, ESS-DIVE, WHONDRS) are not readily available. Similarly, technologies and tools to integrate data from research activities (SBR SFAs and TES field projects – SPRUCE, NGEE-Arctic and NGEE-Tropics) and other community resources with each other are not readily available. There is a clear need for improved technologies and tools to extract, integrate and analyze those types of data/data sets collectively.

BER and BERAC have identified the need to better integrate data from microbial, plant and fungal research efforts (both individual cells and communities of microbes) with physical and chemical data from the surrounding soil/rhizosphere/aqueous/subsurface environment in part of the BERAC Grand Challenges report[15] and several other recent reports[16-19]. To address the biogeochemistry and integrated water cycle grand challenges in the CESD Strategic Plan, the SBR and TES communities generate heterogeneous spatial and temporal data from experiments and observations from watersheds and terrestrial ecosystems; these data are then used to test and further advance predictive models of the structure, functioning/dynamics and evolution of these watersheds and terrestrial ecosystems. Innovations in technologies and tools to integrate and analyze data from multiple user facilities, community resources, instruments and data systems are needed to enhance the effectiveness and efficiency of data processing for investigations across spatial and temporal scales and across scientific disciplines.

Questions – Contact: Paul Bayer, Paul.Bayer@science.doe.gov

Office of Basic Energy Sciences (BES)

Application Area 3: Capabilities for Structuring, Mining and Extracting Knowledge from Chemical and Geochemical Data

The Chemical Sciences, Geosciences, and Biosciences (CSGB) Division supports theoretical, computational and experimental research to attain fundamental understanding of chemical transformations and mass and energy transport in systems relevant to DOE missions. This knowledge serves as a basis for the development of new processes for the extraction, generation, storage, separation, and use of chemicals and energy and for mitigation of the environmental impacts of these processes. Circular use of resources and replacement of critical ones by more abundant ones are motivations to explore and discover new pathways.

The DOE-BES science community has identified priority research directions and published them in a series of Basic Research Needs workshop reports – refer to those mentioned in **Application Area 3 ref. 2**. Measurement and computation-based inquiries in these areas create large complex unstructured and distributed collections of data. Mechanisms are needed to generate open repositories of physico-chemical structure-behavior data that abide by the FAIR principles and that are AI-ready. Ideally, those databases should be suitable for scientific inference and knowledge extraction relevant to chemical and geochemical processes. Existing data structures and pipelines to integrate data of varied provenance, as for example, synthetic protocols, compositional, structural, reactivity, and spectroscopic information, are not general enough to encourage data sharing beyond small groups of researchers.

Although physico-chemical data pockets abound worldwide, only a handful can be mined to generalize chemical structure-behavior properties beyond the original use case that motivated the data collection. One example is molecular recognition phenomena, which are the bases for synthesis and separation of compounds, selective conversion of chemicals, waste reduction, crystalline and isotopic differentiation during mineral growth, and many biological processes; although the principles of molecular recognition are the same, the theoretical/experimental data and data models for each of these use cases are not transferable.

In Chemical and Geochemical sciences there is also a strong need to develop tools that facilitate hybrid data-physical models either for extrapolation to data-poor regions, or to extend fundamental theory to complex multicomponent systems, or ideally to lead to novel chemical concepts based on previously undetected correlations. For example, more efficient pipelines are needed to mine heterogeneous multidimensional databases that contain kinetics and thermodynamics of chemical syntheses and reactions, reaction selectivity, phase transformations, transport in complex fluid mixtures, etc., to derive lower order scaling relations or features that can be used to refine existing separation, reaction, and transport theories. Teams that include both data scientists and chemical domain experts are preferred for this research.

Questions – Contact: Raul Miranda, Raul.Miranda@science.doe.gov

Application Area 4: Capabilities for Management, Mining and Knowledge Extraction from Materials Databases

The Materials Sciences and Engineering (MSE) Division supports fundamental experimental, theoretical, and computational research to provide the knowledge base for the discovery and design of new materials with novel structures, functions, and properties. This knowledge serves as a basis for the development of new materials for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use. Crosscutting problems within MSE include the need for knowledge creation, manipulation, and extraction tools for materials discovery, materials design, and functional materials for energy-relevant technologies.

In these and other areas, the DOE-BES science community has identified priority research directions that are published in a series of Basic Research Needs workshop reports – for example, see the list below for Application Area 4. Applications should focus on identifying and closing the knowledge gaps of functional and topological materials through artificial intelligence and neural network learning techniques, for example, but not limited to natural language processing of the literature and technical reports.

Another focus is how to make effective use of federated data distributed over many independent materials repositories. Providing a cloud or web based solution for facilitating data access and analysis across distributed heterogeneous platforms, repositories, and logical domains through a single materials portal with the full suite of complex data analysis tools, including cross-checking and validation or uncertainty quantification of data entries.

Questions – Contact: Matthias Graf, Matthias.Graf@science.doe.gov

References: General:

1. U.S. Department of Energy. (2020). *DOE Exascale Requirements Review Workshop Reports,* Exascale Age. http://exascaleage.org/

References: Application Area 1:

1. U.S. Department of Energy. (2018). *Genomic Science Program,* Systems Biology for Energy and Environment, Office of Science. http://genomicscience.energy.gov/index.shtml
2. U.S. Department of Energy. (2016). *Biological and Environmental Research, Exascale Requirements Review,* Advanced Science Computing Research, Biological and Environmental Research, p. 366. https://www.osti.gov/servlets/purl/1375720/
3. U.S. Department of Energy. (2015). *Biological Systems Science Division*, Strategic Plan, Office of Biological and Environmental Research, p. 18. http://genomicscience.energy.gov/pubs/BSSDStrategicPlan.pdf

References: Application Area 2:

1. U.S. Department of Energy. (2017). *Grand Challenges for Biological and Environmental Research: Progress and Future Vision report*, Biological and Environmental Research Advisory Committee, p. 71- 94. https://genomicscience.energy.gov/BERfiles/BERAC-2017-Grand-Challenges-Report.pdf

2. U.S. Department of Energy. (2020). *Environmental Molecular Sciences Laboratory (EMSL)*, User Facility, U.S. Department of Energy, Office of Science. https://science.osti.gov/ber/Facilities/User-Facilities/EMSL
3. U.S. Department of Energy. (2020). *Joint Genome Institute User Facility*, U.S. Department of Energy, Office of Science. https://science.osti.gov/ber/Facilities/User-Facilities/JGI
4. U.S. Department of Energy. (2020). *Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE)*, U.S. Department of Energy, Office of Science. http://ess-dive.lbl.gov/
5. U.S. Department of Energy. (2020). *Systems Biology Knowledgebase (KBase),* U.S. Department of Energy, Office of Science. http://kbase.us/
6. U.S. Department of Energy, AmeriFlux Network, Biological and Environmental Research (BER), Climate and Environmental Sciences Division, p. 2. https://tes.science.energy.gov/research/ameriflux.shtml
7. U.S. Department of Energy. (2020). *Worldwide Hydrobiogeochemical Observation Network for Dynamic River Systems (WHONDRS) Network*, U.S. Department of Energy, Pacific Northwest National Library. https://sbrsfa.pnnl.gov/whondrs.stm
8. AQUA-MER Database, U.S. Department of Energy, Biological and Environmental Research (BER), Climate and Environmental Sciences Division. https://pubmed.ncbi.nlm.nih.gov/31603259/
9. U.S. Department of Energy. (2018). *Climate and Environmental Sciences Division Strategic Plan,* DOE/SC-0192, Office of Biological and Environmental Research, p. 19-20. https://science.osti.gov/~/media/ber/pdf/workshop%20reports/2018_CESD_Strategic_Plan.pdf
10. U.S. Department of Energy, Office of Biological and Environmental Research. (2019). *Bioimaging Science Program,* 2019 PI Meeting Proceedings https://science.osti.gov/-/media/ber/pdf/community-resources/2019/Bioimaging_Science_Program_PI_Meeting.pdf?la=en&hash=6CE5F09925A4399D4CCE1CB68228F8644139DABF
11. U.S. Department of Energy. (2020). *Facilities Integrating Collaborations for User Science (FICUS)*, U.S. Department of Energy, Office of Biological and Environmental Research, Environmental Molecular Sciences Laboratory. https://www.emsl.pnnl.gov/emslweb/facilities-integrating-collaborations-user-science-ficus
12. U.S. Department of Energy. (2020). *National Laboratory Scientific Focus Areas*, Subsurface Biogeochemical Research Program, Biological and Environmental Research (BER), Climate and Environmental Sciences Division. https://doesbr.org/research/sfa/index.shtml
13. U.S. Department of Energy, Terrestrial Ecosystem Science Program. (2020). *Terrestrial Ecosystem Science Program,* Biological and Environmental Research (BER), Climate and Environmental Sciences Division. https://tes.science.energy.gov/
14. U.S. Department of Energy, Office of Biological and Environmental Research. (2020). *Environmental Molecular Sciences Laboratory Data Management Policy*. https://www.emsl.pnnl.gov/emslweb/emsl-data-management-policy.
15. BERAC. (2017). Grand Challenges for Biological and Environmental Research: Progress and Future Vision report, Biological and Environmental Research Advisory Committee, DOE/SC-0190, p. 43- 56. https://genomicscience.energy.gov/BERfiles/BERAC-2017-Grand-Challenges-Report.pdf
16. U.S. Department of Energy, Office of Biological and Environmental Research. (2015). *Molecular Science Challenges Workshop Report*, p. 24-34. https://science.osti.gov/-/media/ber/pdf/workshop-reports/MolecularScienceChallenges-April-9-2015Final.pdf?la=en&hash=23D955DBD29539EDECC7F4ED968768530BFD53E1
17. U.S. Department of Energy. (2017). *Technologies for Characterizing Molecular and Cellular Systems Relevant to Bioenergy and Environment*, DOE/SC-0189, Office of Biological and Environmental Research, p. 15-27 and 29-36. https://science.osti.gov/-/media/ber/pdf/community-resources/Technologies_for_Characterizing_Molecular_and_Cellular_Systems.pdf?la=en&hash=E1E5BBA3761132641342AF80BC92AB9EDACB4B72
18. U.S. Department of Energy. (2016). *Biological and Environmental Research, Exascale Requirements Review Workshop Report*, Advanced Scientific Computing Research, Biological and Environmental Research, p. 44-49. https://www.osti.gov/servlets/purl/1375720

19. U.S. Department of Energy. (2015). *Biological System Sciences Division Strategic Plan*, Office of Biological and Environmental Research, p. 8-9 and 11. https://genomicscience.energy.gov/pubs/BSSDStrategicPlanOct2015.pdf

References: Application Area 3:

(See https://science.osti.gov/bes/Community-Resources/Reports)

1. U.S. Department of Energy. (2015). Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science, A Report from the Basic Energy Sciences Advisory Committee. https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#CFME
2. U.S. Department of Energy. (2007). *Basic Research Needs: Catalysis for Energy*, Basic Energy Sciences Workshop. https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#CAT
3. U.S. Department of Energy. (2016). Basic Research Needs For Synthesis Science. https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#SS
4. U.S. Department of Energy. (2015*). Basic Research Needs for Environmental Management*, Report of the Office of Science Workshop on Environmental Management, July 8-11. https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#BRNEM
5. U.S. Department of Energy. (2020). *Basic Research Needs for Transformative Manufacturing.* https://science.osti.gov/-/media/bes/pdf/reports/2020/Transformative_Mfg_Brochure.pdf

References: Application Area 4:

(See https://science.osti.gov/bes/Community-Resources/Reports)

1. U.S. Department of Energy. (2015). *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science*, A Report from the Basic Energy Sciences Advisory Committee. https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#CFME
2. U.S. Department of Energy. (2010). Computational Materials Science and Chemistry – Accelerating Discovery and Innovation through Simulation-Based Engineering and Science, Report of the Department of Energy Workshop. https://www.osti.gov/biblio/1294275
3. U.S. Department of Energy. (2016). *Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology*, Report of the Department of Energy Workshop. https://science.osti.gov/bes/Community-Resources/Reports/Abstracts#BRNQM

PROGRAM AREA OVERVIEW: OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

The primary mission of the Advanced Scientific Computing Research (ASCR) program is to discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to the Department of Energy. A particular challenge of this program is fulfilling the science potential of emerging computing systems and other novel computing architectures, which will require numerous significant modifications to today's tools and techniques to deliver on the promise of exascale science. To accomplish this mission, ASCR funds research at public and private institutions and at DOE laboratories to foster and support fundamental research in applied mathematics, computer science, and high-performance networks. In addition, ASCR supports multidisciplinary science activities under a computational science partnership program involving technical programs within the Office of Science and throughout the Department of Energy.

ASCR supports research on applied computational sciences in the following areas:

1. Applied and Computational Mathematics to develop the mathematical algorithms, tools, and libraries to model complex physical and biological systems.
2. High-performance Computing Science to develop scalable systems software and programming models, and to enable computational scientists to effectively utilize petascale computers to advance science in areas important to the DOE mission.
3. Distributed Network Environment to develop integrated software tools and advanced network services to enable large-scale scientific collaboration and make effective use of distributed computing and science facilities in support of the DOE science mission.
4. Applied Computational Sciences Partnership to achieve breakthroughs in scientific advances via computer simulation technologies that are impossible without interdisciplinary effort.

ASCR also operates high-performance computing (HPC) centers and maintains a high-speed network infrastructure (ESnet) at Lawrence Berkeley National Laboratory (LBNL) to support computational science research activities. The HPC facilities include the Oak Ridge Leadership Computing Facility (OLCF) at Oak Ridge National Laboratory (ORNL), the Argonne Leadership Computing Facility (ALCF) at Argonne National Laboratory (ANL), and the National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory (LBNL).

For additional information regarding the Office of Advanced Scientific Computing Research priorities, click here.

Please note that all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use DOE NERSC resources. See more info and how to apply: https://science.osti.gov/sbir/Applicant-Resources/National-Labs-Profiles-and-Contacts/National-Energy-Research-Scientific-Computing-Center

Proprietary work may be done at the ALCF and OLCF facilities using a cost recovery model.

References:

1. U.S. Department of Energy. (2020). Apply For Your First NERSC Allocation, NERSC. http://www.nersc.gov/users/accounts/allocations/first-allocation/ (Questions – Contact: Richard Gerber, ragerber@lbl.gov)

2. HPC CODE AND SOFTWARE TOOLS

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The Office of Science (SC) Office of Advanced Scientific Computing Research (ASCR) has invested millions of dollars in the development of HPC software in the areas of modeling and simulation, solvers, and tools, including software for managing, analyzing and visualizing scientific data. Many of these tools are open source, but are complex "expert" level tools. The expertise required to install, utilize and run these assets poses a significant barrier to many organizations due to the levels of complexity built into them to facilitate scientific discovery and research, but such complexity may not necessarily be required for industrial applications. Grant applications are sought to harden codes and software tools developed exclusively by the Scientific Discovery through Advanced Computing (SciDAC) program and/or ASCR Computer Science and Applied Mathematics programs. All other codes are deemed out of scope.

a. Hardening of R&D Code or Software Tools

This topic solicits proposals that will take a component or components of codes developed via Scientific Discovery through Advanced Computing (SciDAC) program and/or ASCR Computer Science and Applied Mathematics programs, and "shrink wrap" them into tools that require a lower level of expertise to utilize. This may include design, implementation and usability testing of Graphical User Interfaces (GUIs) or web interfaces, simplification of user input, decreasing complexity of a code by stripping out components not required, user support tools/services, or other ways that make the code more widely useable to the industrial applications. In addition, applicants may choose to strip out code components, harden them and join them with already mature code tools and/or suites of tools to increase the overall toolset and scalability of commercial software. Proposals should include a reference (webpage or other citation) to show that the relevant code has been supported by ASCR. See the references for a partial listing of available codes.

Questions – Contact: Ceren Susut, Ceren.Susut-Bennett@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above within the context of HPC.

Questions – Contact: Ceren Susut, Ceren.Susut-Bennett@science.doe.gov

References:

1. U.S. Department of Energy. (2020). *Software*, Scientific Discovery through Advanced Computing (SciDAC), U.S. Department of Energy. https://www.scidac.gov/software-list.html
2. U.S. Department of Energy. (2020). *SciDAC Feature*, Scientific Discovery through Advanced Computing (SciDAC), U.S. Department of Energy. http://www.scidac.gov
3. U.S. Department of Energy. (2020). *DOE CODE*, U.S. Department of Energy, Office of Scientific and Technical Information. https://www.osti.gov/doecode/

3. HPC CYBERSECURITY

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Large scale computationally intensive platforms, systems, facilities relying on High Performance Computing (HPC) systems to enable large scale information processing for a multitude of areas such as business, utility, financial, scientific, and national infrastructure systems that form the backbone of our nation's economy, security, and health. HPC facilities, centers, infrastructure, or resources are designed to be easily accessible by users over a worldwide network, and ensuring effective cybersecurity monitoring, situational awareness, logging, reporting, preventions, remediation, etc, is an increasingly important task. A proposal submitted to this topic area must be unclassified and clearly address solutions for state-of-the-art HPC systems. Applications or proposals that do not address the range of desired products mentioned in this specific topic or are primarily focused on: Single node/host-, handheld-, mobile-, cloud-, cryptography-, statistical-, grid-, desktop-, and/or wireless-based solutions; internet; networking; internet-of-things; internet-of-everything; cyber-physical; data centers; database; basic research; natural language processing; computing clusters; distributed computing; human factors; computer human interactions; not focused specifically on state-of-the-art HPC systems; visualization; social media; data analytics; web applications; social networks; authentication; firewall; hardware; edge computing; cryptanalysis; encryption; or propose to change, modify, and/or alter application's code, will be considered nonresponsive and will not undergo merit review.

Grant applications are sought in the following subtopics:

a. Cybersecurity Technologies

This topic solicits unclassified proposals that will deliver and market commercial products ensuring effective and practical cybersecurity for HPC systems, centers, and/or user facilities. The proposal must clearly address solutions for state-of-the-art HPC systems in particular. These tools will have the capability to detect, prevent, or analyze attempts to compromise or degrade systems or applications consequently increasing their cybersecurity. Any submitted proposal must be unclassified.
Relevant evaluation metrics may include delivery of potential solutions involving minimizing the overall security overhead required to deal with data parallelism, concurrency, storage and retrieval, hardware heterogeneity, and how to monitor, visualize, categorize, or report cybersecurity challenges effectively. Current cybersecurity tools and products could potentially be enhanced or transitioned to help secure HPC systems. However, any proposal idea must specifically and clearly address solutions geared for state-of-the-art HPC systems.

Questions – Contact: Robinson Pino, robinson.pino@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above within the context of HPC.

Questions – Contact: Robinson Pino, robinson.pino@science.doe.gov

References:

1. U.S. Department of Energy. (2015). *ASCR Cybersecurity for Scientific Computing Integrity - Research Pathways and Ideas Workshop*, DOE Workshop Report, June 2-3. https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/ASCR_Cybersecurity_20_Research_Pathways_and_Ideas_Workshop.pdf?la=en&hash=3C580BB860E9A59ABDF11DA555D36E9EB0B574F7
2. U.S. Department of Energy. (2015). *ASCR Cybersecurity for Scientific Computing Integrity Workshop*, DOE Workshop Report. http://science.osti.gov/~/media/ascr/pdf/programdocuments/docs/ASCR_Cybersecurity_For_Scientific_Computing_Integrity_Report_2015.pdf

3. Campbell, S., and Mellander, J. (2011). *Experiences with Intrusion Detection in High Performance Computing.* https://cug.org/5-publications/proceedings_attendee_lists/CUG11CD/pages/1-program/final_program/Monday/03B-Mellander-Paper.pdf
4. Malin, A. B., and Van Heule, G. K. (2013). *Continuous Monitoring and Cyber Security for High Performance Computing*, Report LA-UR-13-21921 http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-13-21921

4. INCREASING ADOPTION OF HPC

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Over the past decades, The Department of Energy's (DOE) supercomputing program has played an increasingly important role in the scientific discovery process by allowing scientists to create more accurate models of complex systems, simulate problems once thought to be impossible, and analyze the increasing amount of data generated by experiments. Despite the great potential of HPC to increase understanding of a variety of important challenges, modeling, simulation and data analytics using HPC has been underutilized in some areas such as microelectronic device design, manufacturing, engineering and environmental clean-up.

Application complexity, in both the development and execution phase requires a substantial in-house expertise to fully realize the benefits of the software tool or service. High capital equipment and labor costs can severely limit a company's ability to incorporate HPC into their development process. It should also be recognized that significant advances in HPC hardware including many-core, multi-core processors, GPU-based and other accelerators, multi-tiered memory subsystems, and extreme bandwidths have made a significant impact on the HPC systems' performance and usability. Programming tools and services that can hide this hardware complexity without impacting performance are required. Methods that ease adding parallel performance while minimizing development phase costs and expertise are encouraged.

This topic is specifically focused on bringing HPC solutions and capabilities to the new applications sectors. Applications that address areas where HPC has a robust code base will be deemed out of scope and include materials, chemistry, nuclear engineering, biotechnology, oil and gas exploration, and finance.

Grant applications are sought in the following subtopics:

a. Turnkey HPC Solutions

HPC modeling and simulation applications are utilized by many industries in their product development cycle, but hurdles remain for wider adoption especially for small and medium sized firms. Some of the hurdles are: overly complex applications, lack of hardware resources, inability to run proof of concept simulations on desktop workstations, solutions that have well developed user interfaces, but are difficult to scale to higher end systems, solutions that are scalable but have poorly developed user interfaces, etc. While many advances have been made in making HPC applications easier to use they are still mostly written with an expert level user in mind.

Grant applications that are sought for this subtopic are limited in the description below. All other applications will be deemed nonresponsive and will not undergo merit review.

HPC applications that address challenges in microelectronic device design, manufacturing, engineering and environmental clean-up. Issues to be addressed include, but are not limited to: Developing turn-key HPC application solutions, porting open source HPC software to platforms that have a more reasonable cost vs.

current high end systems (this could also include porting to high performance workstations (CPU/GPU) which would provide justification for the procurement of HPC assets, small scale clusters, hybrid platforms or to a high performance "cloud" type environment or service), HPC software or hardware as a service (hosted locally or in the "cloud"), near real time modeling and simulation tools, etc. Preference will be given to porting codes to utilize GPUs and/or scaling GPU ready codes.

Questions – Contact: Christine Chalk, christine.chalk@science.doe.gov

b. Enhancements to Support HPC-driven Data Analytic Workflows

Data analytics on HPC requires supporting software which facilitates data interfaces and interaction. Linkages between HPC and Department of Energy experimental and observational scientific data often require software for high bandwidth transfers, orchestration of computing resources with low latency, and other user facing controls. In-operando spectroscopies, imaging and other advanced sensors may benefit from timely data analysis on remotely located HPC resources. Lowering barriers to automation in HPC-driven data analytic workflows for high-throughput and high-content screening techniques is sought through reusable software solutions. Some of the hurdles involve data transport, formatting and interaction which are unique to a single instrument or few experimental teams. Beamlines, telescopes, microscopes, and other instruments of unique design are operationally enhanced by software systems that allow reuse of data logistic and analytics techniques.

Grant applications that are sought for this subtopic are limited in the description below. All other applications will be deemed nonresponsive and will not undergo merit review.

Using software and technologies from existing Department of Energy scientific data analytic pipelines, high-throughput and high-content screening methods and related technologies to make software packages usable by domain scientists and engineers that are not HPC experts. Developing integrated software packages that support a wide range of data analysis methods while allowing the user to focus on the science and engineering work rather than data logistics. Preference will be given to projects with a defined user community and demonstrated community need.

Questions – Contact: Christine Chalk, christine.chalk@science.doe.gov

c. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Christine Chalk, christine.chalk@science.doe.gov

References:

1. U.S. Department of Energy, Oak Ridge National Laboratory. (2017). Accelerated Computing Guide. https://www.olcf.ornl.gov/tutorials/accelerated-computing-guide/2
2. Siegel, A., Draeger, E., Deslippe, J., Dubey, A., Evans, T., Germann, T., and Hart, W. (2020). *Early Application Results on Pre-exascale Architecture with Analysis of Performance Challenges and Projections*, WBS 2.2, Milestone PM-AD-1080. https://www.exascaleproject.org/wp-content/uploads/2020/03/ECP_AD_Milestone-Early-Application-Results_v1.0_20200325_FINAL.pdf
3. Heroux, M. A., Carter, J., Thakur, R., Vetter, J. S., McInnes, L. C., Ahrens, J., Munson, T., and Neely, J. R. (2020). *ECP Software Technology Capability Assessment Report-Public*, ECP-RPT-ST-0002-2020-Public. https://www.exascaleproject.org/wp-content/uploads/2020/02/ECP-ST-CAR-V20-1.pdf

4. Ross, R., Ward, L., Carns, P., Grider, G., Klasky, S., Koziol, Q., Lockwood, G. K., Mohror, K., Settlemyer, B., and Wolf, M. (2018). *Storage Systems and Input/Output: Organizing, Storing, and Accessing Data for Scientific Discovery*, Report for the DOE ASCR Workshop on Storage Systems and I/O. https://www.osti.gov/servlets/purl/1491994
5. U.S. Department of Energy. (2017). *Basic Research Needs For Energy and Water*, Report of the Office of Basic Energy Sciences. https://science.osti.gov/-/media/bes/pdf/reports/2017/BRN_Energy_Water_rpt.pdf
6. U.S. Department of Energy. (2018). *Basic Research Needs for Microelectronics*, Report of the Office of Science Workshop, October 23-25. https://science.osti.gov/-/media/bes/pdf/reports/2019/BRN_Microelectronics_rpt.pdf

5. TECHNOLOGIES FOR SHARING NETWORK PERFORMANCE DATA

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Network devices (e.g., hosts, servers, switches, and routers) generate a huge amount of health and performance data during normal operations. Switches and routers may be configured to capture basic health data (e.g., interface up/down status, bytes sent/received, errors encountered). They may also save aggregate flow data (i.e., netflow, sflow) recording the length and size of each individual flow as it crosses this device. Hosts and servers typically record basic interface health data and capture higher level details in log files that record what actions were taken (e.g., file being transferred, web content downloaded). Network flow and packet header data has proven useful to network operators to understand how their infrastructure is operating. The log file data has proven useful to system administrators to understand how hosts/servers are operating.

However, it has proven difficult to share any of this data with the broader network research community due to privacy and security concerns. This topic solicits proposal that would make it possible to share this type of data publicly while preserving all privacy concerns and meeting all security constraints.

a. Anonymization Tools and Services

Network data that is useful to network researchers primarily comes from packet or frame headers. This would be any combination of the transport (TCP/UDP), network (IPv4 or IPv6), and data link (Ethernet, Wifi) layer headers. Typically the payload data is not useful to network researchers. Full packet trace data techniques are typically used to capture packet header data. Flow data typically contains a limited subset data from the Transport (TCP/UDP) and Network (IPv4 or IPv6) header fields. TSTAT data is typically collected on instrumented hosts or servers.

Due to the design of the Internet, IP addresses are associated with an individual interface on a host, server, or router. In addition, unique Ethernet addresses are assigned to network interface cards by manufactures. Privacy concerns make it imperative that publicly releasable data anonymize any header fields that would allow someone to identify the individual or host/server that was generating, receiving, or handling these packets. This subtopic solicits proposals to develop tools or service that can anonymize packet header data, flow data, or TSTAT data in a manner that allows those datasets to be publicly released while preserving the scientific content the data they contain. Consideration should also be given to methods that can correlate data that is collected at multiple points in the network (e.g., packet header data collected on the source host and flow data collected by the first hop switch).

Questions – Contact: Richard Carlson, Richard.Carlson@Science.doe.gov

b. Correlate Log Data and or Host Sensor Data with Network Trace Data

Log data collected by hosts and servers provides a high level view of how these systems are being used. For example; GridFTP server logs provide details on what files were moved and how the service decided to perform the transfer task (e.g.; parallel or sequential processing) of files. This data contains local and remote host names, which trivially translate into IP addresses. While the same anonymization concerns expressed above exist, it is also important that this log data be correlated with the network trace data. Without this correlation it is difficult or impossible to fully explain why transfer times vary as much as they are observed to. Many other network services (e.g., http/https, Luster file system, ssh access, workflow engines) create log files that contain similar information highlighting the need for a correlation service.

In addition, when looking at end-to-end performance it is necessary to understand everything that the source and destination hosts are doing. A server with a low performing disk I/O subsystem can significantly impact the throughput of a network file transfer. A server that is performing a heavy computational task (e.g., compiling a program) will also impact the throughput of a network file transfer. Therefore, tools and services that can also correlate data from host sensors (e.g., CPU load, Disk I/O rate) with log files and network traces are of interest.

This subtopic solicits proposals to develop tools or services that can correlate host/server log data and/or sensor data with network trace data that may be captured at a different point in the network.

Questions – Contact: Richard Carlson, Richard.Carlson@Science.doe.gov

c. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Richard Carlson, Richard.Carlson@Science.doe.gov

References:

1. Dijkhuizen, N. V., Der Ham, J. V. (2018). *A Survey of Network Traffic Anonymisation Techniques and Implementations*, Article No.: 52. https://dl.acm.org/doi/10.1145/3182660
2. Liu, Z., Kettimuthu, R., Leyffer, S., Palkar, P., and Foster, I. (2018). *A Mathematical Programming- and Simulation-Based Framework to Evaluate Cyberinfrastructure Design Choices*, IEEE 13th International Conference on e-Science (e-Science), Auckland, 2017, pp. 148-157. https://ieeexplore.ieee.org/document/8109132
3. Chung, J., Liu, Z., Kettimuthu, R., and Foster, I. (2019). *Elastic Data Transfer Infrastructure for a Dynamic Science DMZ*, 15th IEEE International Conference on eScience (eScience 2019), San Diego, CA, Sep. 2019 https://www.mcs.anl.gov/~kettimut/publications/elasticDTN.pdf
4. Liu, Z., Kettimuthu, R., Balaprakash, P., Rao, N. S., Foster, I. (2018). *Building a Wide-area File Transfer Performance Predictor: An Empirical Study*, International Conference on Machine Learning for Networking, (MLN2018), November 27-29, Paris, France. https://www.ornl.gov/publication/building-wide-area-file-transfer-performance-predictor-empirical-study

References: Subtopic a:

1. Liu, Z., Balaprakash, P., Kettimuthu, R., and Foster, I. (2017). *Explaining Wide Area Data Transfer Performance*, In Proceedings of the 26th International Symposium on High-Performance Parallel and Distributed Computing (HPDC ’17). Association for Computing Machinery, New York, NY, USA, 167–178. https://doi.org/10.1145/3078597.3078605

2. Liu, Z., Kettimuthu, R., Foster, I., and Liu, Y. (2018). *A Comprehensive Study of Wide Area Data Movement at a Scientific Computing Facility*, 2018 IEEE 38th International Conference on Distributed Computing Systems (ICDCS), Vienna, 2018, pp. 1604-1611. https://www.researchgate.net/publication/328353101_A_comprehensive_study_of_wide_area_data_movement_at_a_scientific_computing_facility
3. Rao, N. S., Liu, Q., Sen, S., Hanley, J., Foster, I., Kettimuthu, R., Wu, C. Q., Yun, D., Towsley, D., and Vardoyan, G. (2017). *Experiments and Analyses of Data Transfers Over Wide-area Dedicated Connections*, The 26th International Conference on Computer Communications and Networks (ICCCN 2017), July 31-August 3, 2017, Vancouver, Canada. https://www.ornl.gov/publication/experiments-and-analyses-data-transfers-over-wide-area-dedicated-connections
4. Lu, Z., Kettimut, R., Foster, I., and Beckman, P. H. (2018). *Toward a Smart Data Transfer Node*, Future Generation Computing Systems, 2018. https://www.sciencedirect.com/science/article/abs/pii/S0167739X18302346?via%3Dihub

References: Subtopic b:

1. Allcock, W. (2003). *GridFTP: Protocol Extensions to FTP for the Grid*. Global Grid ForumGFD-R-P.020, 2003. https://www.ogf.org/documents/GFD.20.pdf
2. Allcock, W., Bresnahan, J., Kettimuthu, R., Link, M., Dumitrescu, C., Raicu, I., and Foster, I. (2005). *The Globus Striped GridFTP Framework and Server*, SC '05: Proceedings of the 2005 ACM/IEEE Conference on Supercomputing, Seattle, WA, USA, 2005, pp. 54-54, https://dl.acm.org/doi/10.1109/SC.2005.72
3. Kiran, M., Wang, C., Papadimitriou, A. Mandal, E. Deelman. (2020). *Detecting Anomalous Packets in Network Transfers: Investigations Using PCA, Autoencoder and Isolation Forest in TCP*, Machine Learning 109, 1127–1143 (2020). https://doi.org/10.1007/s10994-020-05870-y
4. Papadimitriou, G., Kiran, M., Wang, C., Mandal, A., and Deelman, E. (2019). *Training Classifiers to Identify TCP Signatures in Scientific Workflows*, 2019 IEEE/ACM Innovating the Network for Data Intensive Science (INDIS), Nov 2019. https://ieeexplore.ieee.org/document/8940199
5. Kiran, M., Mohammed, B., and Krishnaswamy, N. (2020). *DeepRoute: Herding Elephant and Mice Flows with Reinforcement Learning*, International Conference on Machine Learning for Networkin. https://www.researchgate.net/publication/340785610_DeepRoute_Herding_Elephant_and_Mice_Flows_with_Reinforcement_Learning
6. Dijkhuizen, N. V., and Der Ham, J. V. (2018). A Survey of Network Traffic Anonymisation Techniques and Implementations, ACM Computing Surveys No. 52. https://doi.org/10.1145/3182660

6. EMERGING NETWORK TECHNOLOGIES

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The Office of Advanced Scientific Computing Research (ASCR) at the US- Department of Energy would like to solicit applications focusing on the development of commercial-grade quantum optical communication networks infrastructures. The current interest for this topic is on photonic quantum networks that coexist with classical networks on a shared optical fiber transmission systems. Specific technologies and devices of interest are limited to the following:

a. Transparent Optical Quantum Network Devices

The current interest for this topic is on photonic quantum networks that coexist with classical networks on a shared optical fiber transmission systems. Specific technologies and devices of interest are limited to the following:

1. Quantum frequency converters – which allows quantum states of two light beams of different frequencies can be interchanged in response to classical wavelength conversion or other quantum operations;
2. Quantum optical MUX/DeMUX aggregating quantum states for different users on a shared quantum link;
3. Quantum Buffers – Limited capacity memory to temporally delay quantum photons in transparent optical quantum communication networks components such as quantum repeaters, routers, and switches;
4. Homodyne detectors for processing single as applicable to classical light and to new kinds of quantum states of light include squeezed states of light;
5. Narrow linewidth (<150 kHz) frequency stabilized lasers (>25 mW average power);
6. Shot-noise limited high efficiency homodyne detectors with 45 dB of common mode rejection, as well as low-loss high-extinction phase and amplitude modulators for C-band telecom optical signals;
7. Superconducting qubits and circuits--individual qubits as well as small connected arrays with microwave inputs and outputs

Quantum devices in scope for this subtopics are limited to the specific devices listed above. All grant applications must clearly state how the proposed devices or technologies fit in the long-distance quantum networks by specifying the network functions being addressed. Proposals that fail to do this or focus other types of quantum devices will be considered out of scope and will not be reviewed. There is a clear distinction between Quantum Key Distribution system and transparent optical quantum networks. Quantum devices and technologies that focus on QKD networks are also considered out of scope. Applicants are encouraged to get a good description of transparent optical quantum networks in reference [5]

Questions – Contact: Thomas Ndousse-Fetter, Thomas.Ndousse-Fetter@science.doe.gov

b. Embedded Software-Defined (SDN) Controller for Quantum Networks and Intelligent Internet of Things (IoT)

The goal of this subtopic is on intelligent embedded SDN-enabled controllers realized with Machine Learning (ML) and Deep Learning to support dynamic control of quantum network subsystems and Network Internet of Things (N-IoT) in scientific environment such supercomputers, scientific instruments, and observatories.

SDN controllers designed for general IoT and consumer environment will be considered out of scope and will not be reviewed. Additionally, controllers with no onboard ML/DL capabilities and with a form factor greater than 12inch x 6in x 4 inches will not considered an intelligent embedded controller and will not be reviewed as well.

Questions – Contact: Thomas Ndousse-Fetter, Thomas.Ndousse-Fetter@science.doe.gov

c. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Thomas Ndousse-Fetter, Thomas.Ndousse-Fetter@science.doe.gov

References: Subtopic a:

1. U.S. Department of Energy. (2018). *Quantum Networks for Open Science Workshop*, Office of Advanced Scientific Computing Research, p. 41. https://info.ornl.gov/sites/publications/Files/Pub124247.pdf
2. Dias, J. and Ralph, T.C. (2016). *Quantum Repeaters using Continuous-variable Teleportation*, Physical Review A, Vol. 95, 022312, p. 11. https://arxiv.org/pdf/1611.02794.pdf
3. Takeda, S., and Furusawa, A. (2014). *Optical Hybrid Quantum Information Processing*, https://www.researchgate.net/publication/261512563_Optical_Hybrid_Quantum_Information_Processing
4. Takeda, S., Fuwa, M., Van Loock, P., and Furusawa, A. (2018). *Entanglement Swapping between Discrete and Continuous Variables*, Physical Review Letters, Vol. 114, 100501, p. 9. https://arxiv.org/pdf/1411.1310.pdf
5. U.S. Department of Energy. (2018). *Quantum Networks for Open Science Workshop*, Office of Advanced Scientific Computing Research, p. 41. https://info.ornl.gov/sites/publications/Files/Pub124247.pdf

References: Subtopic b:

1. Latah, M., and Toker, L. (2018). *Artificial Intelligence Enabled Software Defined Networking: A Comprehensive Overview.* https://arxiv.org/abs/1803.06818
2. Ramel, D. (2019). *Survey Report Details AI Influence on New-Age Networking*, Pure AI. https://pureai.com/articles/2019/06/07/sdn-survey.aspx
3. Lewis, B. (2015). *Software-Defined Networking - A view from the top,* Embedded Computing Design. https://www.embedded-computing.com/embedded-computing-design/software-defined-networking-a-view-from-the-top.
4. Ellinidou, S., Sharma, G., Dricot, J. M., and Markowitch, O. (2018). A SDN Solution For System-On-Chip World, 2018 Fifth International Conference on Software Defined Systems (SDS). https://ieeexplore.ieee.org/document/8370416/authors#authors

7. TECHNOLOGIES FOR EXTREME-SCALE COMPUTING

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Extreme-scale computing that is 50 to 100 times faster than the fastest systems of today is planned to be available in the 2021-23 timeframe. Computing at this scale will enable significant advances in many scientific domains, such as discovery of new materials, accurate prediction of severe weather events, reducing pollution, investigating new treatments for cancer, and enabling faster and more accurate engineering designs. Furthermore, the architectural makeup of these systems will form the basis for the next generation of widely deployed systems in data centers in the commercial and academic sectors.

DOE has supported research of software technologies for Exascale computing since the beginning of this decade. AI/ML methods were included in research prototypes for compilers, programming environments, and runtime systems. AI/ML methods have been applied to performance portability solutions, supporting models and tools for implementing and optimizing science and engineering codes on new architectures. The research community has been working on software for analysis, machine learning, and visualization of data that allows low-latency access, rapid data migration, and integration across multiple sites and platforms, including seamless, fully integrated access between experimental and extreme-scale supercomputing facilities.

In algorithms, researchers have been working on statistical machine learning methods and dimension reduction methods for extremely high-dimension, molecular-scale data. They have also recognized that a key capability for their scientific code would be the combination of less-structured, machine learning approaches with deterministic models based on rigorous physical theory.

A number of challenges remain to be addressed, such as expressing and managing billion-way concurrency, the need for improved time to solution, quality of solution, minimized resource consumption at Exascale, parallel debugging at large scale, performance evaluation, verification of correctness, and code transformation, complexity of node, memory, and storage architectures, and resiliency and reliability of the system. These challenges are significantly increased by the rapid introduction of heterogeneous processing components to the HPC ecosystem. AI/ML approaches are promising in tackling some of these challenges.

Proposals submitted to this topic may include hardening/combining/integrating research prototypes in order to create commercializable products and services which fully exploit AI/ML methods.

This topic solicits proposals that address issues related to extreme-scale computing in the following areas:

a. Algorithms for Scientific Applications

Development of new algorithms, both AI/ML and statistically based, are required to accelerate scientific simulation as well as data-intensive applications that improve time to solution, quality of solution, and minimize resource consumption on extreme-scale systems. All algorithms must be scalable to large-scale parallel systems or clusters with hundreds or thousands of nodes, each node comprising any combination of manycore CPUs and heterogeneous accelerators. Application development areas in scope include: Chemistry and Materials, Energy, Earth and Space Sciences, Data Analytics and Optimization, and Co-design projects aimed at developing crosscutting capabilities.

Questions – Contact: Sonia R. Sachs, Sonia.Sachs@Science.doe.gov

b. Software Technologies

Performance improvements and/or hardening of existing software technologies essential for extreme-scale computing in the areas of: programming models and runtime systems; AI/ML or statistically based development tools (e.g., parallel debugging, performance evaluation, verifying correctness, code transformation for performance portability); mathematical libraries; and data and visualization. The scope of a proposed technology must extend to large-scale parallel systems and/or complex nodes consisting of manycore CPUs, GPUs, FPGAs, or other accelerators, as appropriate. Of high interest are solutions for performance portability across heterogeneous hardware architectures.

Questions – Contact: Sonia R. Sachs, Sonia.Sachs@Science.doe.gov

c. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above. Applicants to this subtopic are strongly encouraged to confirm the responsiveness of their proposed innovation with the contact provided below before submitting an application.

Questions – Contact: Sonia R. Sachs, Sonia.Sachs@Science.doe.gov

References:

1. U.S. Department of Energy. (2020). *Exascale Computing Project Website*, U.S. Department of Energy. https://exascaleproject.org/
2. Wallace, T. (2018). *U.S. Should Regain Lead In Supercomputing*, Albuquerque Journal. https://www.abqjournal.com/1164689/us-should-regain-lead-in-supercomputing.html

3. Sarrao, J. (2018). *Exascale Computing Project: Status and Next Steps*, Exascale Computing Project, U.S. Department of Energy, p. 29. https://science.osti.gov/~/media/ascr/ascac/pdf/meetings/201804/ECP_Update_ASCAC_20180417.pdf
4. Kothe, D.B. and Lee, S. (2017). *Exascale Computing Project Update*, Exascale Computing Project, U.S. Department of Energy, p. 32. https://science.osti.gov/~/media/ascr/ascac/pdf/meetings/201712/ECP_Update_ASCAC_20171220.pdf
5. Larzelere, A.R. (2018). *Momentum Builds for US Exascale*, HPC Wire. https://www.hpcwire.com/2018/01/09/momentum-builds-us-exascale/
6. U.S. Department of Energy, *DOE Exascale Requirements Review Workshop Reports*, Exascale Age. http://exascaleage.org/

8. TECHNOLOGY TO FACILITATE THE USE OF NEAR-TERM QUANTUM COMPUTING HARDWARE

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic is focused on specific technologies to facilitate effective implementation of gate-based quantum computing methods on quantum processors available or expected to be available within the next five years. Grant applications focused on quantum annealing, analog simulation, or other non-gate-based approaches to quantum computing will be considered out of scope.

Grant applications are sought in the following subtopics:

a. Ultra-low Vibration, Ultra-high Vacuum Cryostat for Trapped Ions

Arrays of trapped ions offer unique capabilities for quantum information processing; however, broad utilization of ion traps is limited by the complexity of equipment needed to maintain a favorable operating environment for the ions. Ions must be trapped in an ultra-high vacuum (UHV) enclosure and mounted on an ultra-low-vibration (ULV) platform to ensure that the laser beams used to manipulate the ions do not move with respect to the ion chain. To obtain the best noise performance, the ions should be trapped in a cryogenic environment to reduce collisions with background gas that limit qubit coherence. We therefore seek grant applications to develop a closed-cycle cryostat suitable for trapped ion quantum computing.

Such a cryostat would have a cooling power of at least 2W at 15K, vibrations no greater than 10 nm peak-to-peak, and allow the ions to be trapped at a pressure no greater than 10-12 Torr. In addition, such a system requires 100+ DC signals as well as RF (~50 MHz) and microwave (~12 GHz) signals routed to the ion trap. Multi-port optical access is also necessary because trapped ions rely on several laser frequencies at various angles of incidence. Typical applications require a port for a beam perpendicular to the surface as well as several ports for beams parallel to the surface from 6+ angles. Additionally, the system should allow optical elements to be mounted and manipulated inside the cryostat in a manner that ensures that the optical elements satisfy the ULV requirement with respect to the ion trapping chamber.

Integration of a compact integrated ion trap package that incorporates technical advances already demonstrated in a laboratory setting is desirable but not required. Integrated designs should include sufficient flexibility for existing and future ion chip trap designs, maintain ultrahigh vacuum in a miniature vacuum system, provide a high degree of optical access at wavelengths ranging from near-ultraviolet to near-infrared, incorporate an atomic source and delivery mechanism for loading the ion species of interest, and provide a sufficient number of different types of feedthroughs (e.g, low voltage, low power, RF, fiber optic).

Questions – Contact: Claire Cramer, Claire.Cramer@science.doe.gov

b. Software for Calibration, Characterization, and Control of Quantum Processors

Effective use of near-term quantum processors requires device-specific optimization of individual operations ranging from state preparation and measurement through gate implementation and compilation. Specialized techniques and tailored pulse sequences will be necessary to suppress noise, mitigate crosstalk and control errors, and maintain optimally high-fidelity operations in the absence of formal error correction. In many cases, regular calibration and device characterization are necessary to ensure optimal performance. As algorithmic complexity and the size of qubit arrays grow, it will become increasingly important to develop software that combines knowledge of noise processes in specific quantum information processing architectures, quantum algorithms, and pulse shaping with high-efficiency optimization techniques. Grant applications are sought to develop and validate software tools for automated processor tune-up, characterization, calibration, and optimization of universal quantum gates; implementation of techniques for suppressing decoherence such as dynamical decoupling; and automation of benchmarking and compiling protocols. Open source software solutions are strongly encouraged, as is testing the software solutions on fully transparent quantum computing platforms available in research laboratories.

Questions – Contact: Claire Cramer, Claire.Cramer@science.doe.gov

References:

1. U.S. Department of Energy, 2017, ASCR Report on a Quantum Computing Testbed for Science, Office of Advanced Scientific Computing Research, p. 46. https://science.osti.gov/~/media/ascr/pdf/programdocuments/docs/2017/QTSWReport.pdf

PROGRAM AREA OVERVIEW: OFFICE OF BASIC ENERGY SCIENCES

The Office of Basic Energy Sciences (BES) supports 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 results of BES-supported research are routinely published in the open literature.

A key function of the program is to plan, construct, and operate premier scientific user facilities for the development of novel nanomaterials and for materials and chemical characterization through x-ray and neutron scattering; the former is accomplished through five Nanoscale Science Research Centers and the latter is accomplished through the world's largest suite of light source and neutron scattering facilities. These national resources are available free of charge to all researchers based on the quality and importance of proposed nonproprietary experiments.

A major objective of the BES program is to promote the transfer of the results of our basic research to advance and create technologies important to Department of Energy (DOE) missions in areas of energy efficiency, renewable energy resources, improved use of fossil fuels, the mitigation of the adverse impacts of energy production and use, and future nuclear energy sources. The following set of technical topics represents one important mechanism by which the BES program augments its system of university and laboratory research programs and integrates basic science, applied research, and development activities within the DOE.
For additional information regarding the Office of Basic Energy Sciences priorities, click here.

9. ADVANCED MICROFLUIDICS FOR X-RAY AND ELECTRON BEAMS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Within this topic, proposals are sought for the development of microfluidic devices and interfaces for use at x-ray, electron beam, and high-power laser facilities. A wide range of characterization applications requiring an ultra-high vacuum environment will benefit from the possibility of hosting the samples in high-pressure conditions that still permit the photons and electrons to be transmitted from the source to the sample and from the sample to the analyzers. Direct probing and real-time monitoring of high-pressure phenomena and processes could be achieved through incorporation of the high-pressure membrane cell system into advanced characterization instruments, able to operate at up to 300 bar. Standardized high-pressure chip interfaces and microfluidic chip interfaces, conforming to the recently released ISO guidelines, may enable the development of universal connectors for plug-and-play devices. Both multiport connectors and high-pressure connectors to 100 bar are desired for the next generation of DOE facilities' beamlines.

Grant applications are sought in the following subtopics:

a. Thin Membranes and Multiport Microfluidic Connectors for High-pressure or High-density Applications

Grant applications are sought for technology development of thin membranes and of multiport microfluidic chip interfaces and device connectors, for high-pressure or high-density fluid-handling applications. The technology, developed at Lawrence Berkeley National Laboratory, features a thin Si_3N_4 membrane window, with thickness below 200 nm and size smaller than 200 µm, that could operate under high pressure (10 - 300 bar) while still allowing transmission of ultraviolet, soft x-rays and electrons. It has been demonstrated that the high pressure of about 300 bar could be achieved using this membrane cell system. Commercial implementation of this technology could benefit a wide range of potential applications, from x-rays to Transmission Electron Microscopes. Chip interfaces based on the ISO chip guidelines with a 1.50 mm or 0.75 mm pitch that can operate at pressure up to 30 bar and with a minimum of 8 fluid ports and 2 electrical connections are needed to connect micro-devices to the macroscopic world of fluid-handling hardware. High-pressure interfaces, up to 100 bar, are also sought. They must be based on a 3mm pitch as described in ISO guidelines, with a minimum of 6 fluid ports and 2 electrical connections.

Questions – Contact: Peter Lee, peter.lee@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Peter Lee, peter.lee@science.doe.gov

References:

1. Velasco-Velez, J.J., Wu, C.H., Pascal, T.A., Wan, L. F., Guo, J., Prendergast, D. and Salmeron, M. (2014). *The Structure of Interfacial Water on Gold Electrodes Studied by X-ray Absorption Spectroscopy*, Science 346, 831 (2014). http://dx.doi.org/10.1126/science.1259437
2. Qiao R. *et al*. (2018). *Soft X-ray Spectroscopy of High Pressure Liquid*, Review of Scientific Instruments 89, 013114 (2018). https://doi.org/10.1063/1.5008444
3. Smit, E. D., Swart, I., F.C. J, Hoveling, G. H., Gilles, M. K., Tyliszczak, T., Kooyman, P. J., Zandbergen, H. W., Morin, C., Weckhuysen, B. M., and de Groot, F. M. F. (2008). *Nanoscale Chemical Imaging of a Working Catalyst by Scanning Transmission X-ray Microscopy,* Nature 456, 222 (2008). https://www.nature.com/articles/nature07516.pdf
4. ISO. (2016). *Interoperability of Microfluidic devices - Guidelines for Pitch Spacing Dimensions and Initial Device Classification*, IWA 23:2016 ISO ICS > 71 > 71.040 > 71.040.10. https://www.iso.org/standard/70603.html
5. Reyes D.R. and van Heeren H. (2019). *Proceedings of the First Workshop on Standards for Microfluidics*, J Res Natl Inst Stan 124,124001 (2019).
6. https://doi.org/10.6028/jres.124.001

10. SAMPLE ENVIRONMENT MEETING STRICT MOTION STABILITY REQUIREMENTS AT CRYOGENIC TEMPERATURES FOR SYNCHROTRON AND FREE-ELECTRON LASER X-RAY APPLICATIONS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Next-generation synchrotron and free-electron sources will begin mid-decade to deliver highly coherent intense x-ray beams with sub-micron size to many experimental stations around the globe as standard performance specifications. These stations' x-ray scattering capabilities, employing multi-circle diffractometers for the fields of condensed matter physics, materials science, device physics, and in particular quantum information science, will require low-temperature sample environments. In order to take advantage of small coherent x-ray beams, a paradigm shift of possible experiments will depend on the ability to both stabilize and control the relative position of the x-ray beam on the sample, while maintaining the experimental configurations and parameters that make such next-generation science experimentation possible.

Grant applications are sought in the following subtopics:

a. Low Vibration Cryostat for Low and Medium Energy X-ray Scattering for Synchrotron-based Multiple Circle Diffractometers

This topic seeks the development of low vibration closed cycle He cryostats, achieving high thermal stability between 5 K and 300 K with high spatial sample stability (<50 nm) and positional control with large angular x-ray access. The system needs to be versatile enough to tilt up to 45° from vertical, accommodating a large range of configurable scattering geometries while maintaining sample position stability. This call requires the provision of a prototype cryostat with unitized arrangement to be suitable for mounting on a four- or six-circle goniometer and to have three in-situ nano-positioning stages of translation at the sample mount. In a typical mechanically driven cryocooler, the cooling engine in the cryostat has vibrations in the 10 - 100 μm range, depending on the particular product. The vibrations for this call must be managed to the nanometer regime, a reduction by a factor of 1000. Closed cycle cryostats are preferred for long-term experiments because they do not require liquid helium for refrigeration. Liquid helium is a non-renewable resource of increasing cost and scarcity; its availability and cost in the future is highly uncertain.

Questions - Contact: Peter Lee, peter.lee@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions - Contact: Peter Lee, peter.lee@science.doe.gov

References:

1. Hackley, J., Kislitsyn, D. A., Beaman, D. K., Ulrich, S., and Nazin, G. (2014). *High-Stability Cryogenic Scanning Tunneling Microscope Based on a Closed-Cycle Cryostat*, Review of Scientific Instruments 85, 103704 (2014). https://doi.org/10.1063/1.4897139
2. Juska, G., Dimastrodonato, V., Mereni, L. O., Gocalinska, A., and Pelucchi, E. (2013). *Towards Quantum-Dot Arrays of Entangled Photon Emitters*, Nature Photonics 7, 527-531 (2013). https://www.nature.com/articles/nphoton.2013.128

11. IMPROVEMENTS IN OPTICAL METROLOGY FOR HIGH-PERFORMANCE X-RAY MIRRORS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

In support of high-brightness x-ray light sources, development of dedicated metrology instrumentation and analysis methods enables production and verification of the quality of reflective optics pushing toward the diffraction limit. Not only do instruments need to possess the required sensitivity, but also the interpretation of metrology data relies critically on a quantitative understanding of instrument characteristics (e.g., instrument transfer function, ITF).

Grant applications are sought in the following subtopics:

a. High-precision Interferometric Stitching and Data Reconstruction

Proposals are sought in the areas of both hardware and software supporting high-performance metrology for x-ray optics. In particular, mechanical instrumentation is needed which provides stability and precision sufficient to enable 2D interferometric stitching with sub-nm accuracy over one meter or more flat or curved mirror length. Such an accurate stitching system is expected to bridge the gap with foreign vendors in terms of metrology quality for mirrors, and coupled with deterministic polishing will support the advancements in manufacturing of high-precision optics that are mandatory for preserving brightness and wavefront quality of the newest light sources. Likewise, user-friendly software for analysis of 1D and 2D metrology data is needed which deconvolutes or otherwise explicitly accounts for a measured instrumental function in order to achieve the most accurate surface topography information possible. By accounting for data perturbation caused by limited performance of metrology tools, significant improvements in the reliability, accuracy, and effectiveness of ex-situ optical metrology are expected, which will simultaneously enable improvements in optics production and more accurately forecast beamline performance.

Questions - Contact: Peter Lee, peter.lee@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions - Contact: Peter Lee, peter.lee@science.doe.gov

References:

1. Huang, L., Wang, T., Tayabaly, K., Kuhne, D., Xu, W., Xu, W., Vescovi, M., and Idir, M. (2020) *Stitching Interferometry for Synchrotron Mirror Metrology at National Synchrotron Light Source II (NSLS-II),* Optics and Lasers in Engineering 124, 105795 (2020). https://doi.org/10.1016/j.optlaseng.2019.105795
2. Vivo, A., Barrett, R., and Perrin, F. (2019). *Stitching Techniques for Measuring X-ray Synchrotron Mirror Topography*, Review of Scientific Instruments 90, 021710 (2019). https://doi.org/10.1063/1.5063339
3. Yamauchi, K., Mimura, H., Kimura, T., Yumoto, H., Handa, S., Matsuyama, S., Arima, K., Sano, Y., Yamamura, K., and Inagaki, K. (2011). *Single-Nanometer Focusing of Hard X-rays By Kirkpatrick–Baez Mirrors*, Journal of Physics: Condensed Matter 23(39), 394206 (2011). https://doi.org/10.1088/0953-8984/23/39/394206
4. Yashchuk, V., Lacey, I., Arnold, T., Paetzelt, H., Rochester, S., Siewert, F., and Takacs, P. (2019). *Investigation On Lateral Resolution of Surface Slope Profilers*, Proc. SPIE 111090M (2019). https://doi.org/10.1117/12.2539527
5. Siewert, F., Zeschke, T., Arnold, T., Paetzold, H., and Yashchuk, V. (2016). *Linear Chirped Slope Profile for Spatial Calibration In Slope Measuring Deflectometry*, Rev. Sci. Instrum. 87(5), 051907 (2016). https://doi.org/10.1063/1.4950737

12. DEVELOPMENT OF ULTRAVIOLET LASER SYSTEMS FOR GENERATING ULTRA-BRIGHT ELECTRON BEAMS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The main limiting factor to the brightness of Free-Electron Lasers (FELs) is the brightness of the electron source (photoinjector) itself1, where microbunching and space-charge effects may contribute significantly to energy spread and emittance growth. The phase-space distribution of an electron beam from a photoinjector is contingent on the spatiotemporal distribution of the photoexcitation laser. It is well understood that longitudinally tailored charge distributions can yield significantly lower emittances from the photoinjector. For example, uniformly filled ellipsoidal charge distributions can best mitigate space-charge-induced phase-space dilution because they produce space-charge fields with linear dependence on position within the distribution2. In the case of the Linac Coherent Light Source-II, for instance, the gun is designed to yield best results with a longitudinal charge distribution provided by a flat-top ultraviolet (UV) pulse at up to 1 MHz repetition rate3. Spatiotemporally shaping and characterizing the photoexcitation lasers suitable for high-brightness photoinjectors - particularly in the UV as is the case in conventional photocathode materials - is a complex task that requires careful investigation. What is more, the new generation of high-average-power XFELs requires photoinjector systems that are able to handle multiwatt-level UV powers, which are unprecedented for these machines. These high powers are difficult to generate and deliver to the photocathode because of severe thermal load in optics and UV damage from solarization and color centers. As a result, the performance of the photoinjector laser systems is severely hampered with low-spatial-quality beams and very low throughput.

Grant applications are sought in the following subtopics:

a. UV Gratings for Spectrometers and High-resolution (< 2 pm) Ultraviolet (UV) Spectrometers

Because high-fidelity control of the photoemission process via UV generation, shaping, and characterization is central to the production of high-brightness beams, we seek development in the nonlinear optics, shaping, and characterization methods that emphasize high peak and average power operation, including

1. The development of high-efficiency high-damage-threshold UV optics, such as diffractive and volumetric gratings.
2. The development of high-resolution (< 2 pm) UV spectrometers and spatiotemporal characterization techniques.
3. Novel methods of nonlinear optical conversion.

Questions - Contact: Eliane Lessner, eliane.lessner@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions - Contact: Eliane Lessner, eliane.lessner@science.doe.gov

References:

1. Ferrario, M. et al. (2010). *Experimental Demonstration of Emittance Compensation with Velocity Bunching*. Phys. Rev. Lett. 104, 54801 (2010). https://www.researchgate.net/publication/43021829_Experimental_Demonstration_of_Emittance_Compensation_with_Velocity_Bunching
2. Kellogg, O. D. (1929). *Foundations of Potential Theory,* 31. https://archive.org/details/foundationsofpot033485mbp
3. Alverson, S., Anderson, D., and Gilevich, S. (2017). *The LCLS-II Injector Laser System*, 16th Int. Conf. on Acclerator and Large Experimental Control Systems, THPHA025, (2017). http://icalepcs2017.vrws.de/posters/thpha025_poster.pdf

13. HIGH PERFORMANCE DETECTION ELECTRONICS, X-RAY SCINTILLATORS, AND TIMING DIODES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The synchrotron and Free-Electron Laser (FEL) x-ray sources in the United States and around the world are constantly being improved and upgraded, providing ever-increasing source brightness and new capabilities. As such, high-performance x-ray instrumentation is highly desired to best take advantage of the augmented source properties, including but not limited to the measurement of the intensity, profile, and timing of the x-ray beam/pulse.

Grant applications are sought in the following subtopics:

a. Fast Detection Electronics, High-resolution High-thermal-conductivity X-ray Scintillators, and X-ray and Optical Photodiodes for Picosecond Timing

As x-ray beam intensities continue to go up even for third-generation synchrotron sources, techniques such as the Rapid Scan and Quick Scan X-ray Absorption Spectroscopy (XAS) are becoming popular for tracking in-situ chemical changes over short times and for looking at short-lived samples, whether it be from chemistry or from x-ray damage[1]. The development of a fast detection system is urgently needed for this class of techniques, for which it is critically important for the intensity monitors both before and after the sample to measure ratios linearly. Conventional ion chambers are the best choice in linearity but are too slow. Gridded ion chambers are faster but have some tradeoffs[2]. A complete electronics package with modern electronics and interfaces to work with a gridded ion chamber and a fast transimpedance amplifier is needed. The amplifier should have a rise time of 2 - 3 μs and be able to achieve the equivalent to or an order of magnitude better performance than a Keithely 428 transimpedance amplifier, which is no longer in production.

Secondly, the newly upgraded Linac Coherent Light Source-II (LCLS-II) will have a superconducting accelerator and will produce FEL pulses at a very high repetition rate up to 1 MHz in the near future, generating very high x-ray power density on beam-intercepting components and raising damage concerns on FEL imaging materials like the widely used YAG:Ce single crystal. YAG:Ce-based scintillators offer excellent imaging quality with resolutions approaching 1 μm when coupled with appropriate optics, but they have very poor thermal conduction properties due to the low thermal conductivity in the range of 10 W/m·K. For low-repetition FELs at around 100 Hz, the time between pulses is sufficiently long to allow the absorbed energy in the scintillator to dissipate. As the repetition rate increases, x-ray scintillators with sufficiently high thermal conductivity are required to continue to provide FEL imaging capability, which is essential for beamline alignment and other diagnostic measurements. The scintillator should have a thermal conductivity greater than 200 W/m·K, and provide similar performance to that of YAG:Ce in image resolution, emission wavelength, light output (photons per eV) and decay time[3].

Finally, the development of a picosecond response x-ray/optical laser photodetector is needed for coarse timing in FEL applications. This photodetector will be used for cross-correlation diagnostics[4] for pump-probe measurements where ultrafast x-ray and optical pulses need to be precisely placed or even overlapped in time. The photodetector should have a rise/fall time of 30 picoseconds or less and should be sensitive to both optical and x-ray pulses (typically requiring operation without a protective coating). This photodetector should realize the performance, and similar form factor/packaging, of the Hamamatsu G4176-03 Ultrafast Metal-Semiconductor-Metal (MSM) photodetector, which was recently discontinued.

Questions - Contact: Eliane Lessner, eliane.lessner@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions - Contact: Eliane Lessner, eliane.lessner@science.doe.gov

References:

1. Müller, O., Nachtegaal, M., Just, J., Lützenkirchen-Hecht, D., and Frahm, R. (2016). *Quick-EXAFS Setup at The SuperXAS Beamline for In Situ X-ray Absorption Spectroscopy with 10 ms Time Resolution*, J. of Synchrotron Rad., 23, 26. (2016). https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4733929/
2. Müller, O., Stotzel, J., Lützenkirchen-Hecht, D., and Frahm, R. (2013). *Gridded Ionization Chambers for Time Resolved X-Ray Absorption Spectroscopy*, J. Phys.: Conf. Ser. 425, 092010 (2013). https://www.crystals.saint-gobain.com/sites/imdf.crystals.com/files/documents/yag-material-data-sheet_69775.pdf
3. C. Gahl et al. (2008). A Femtosecond X-ray/Optical Cross-Correlator, Nature Photonics 2, 165 (2008). https://www.nature.com/articles/nphoton.2007.298.pdf

14. MULTI-MEGAWATT RF VACUUM WINDOW FOR HIGH DUTY-FACTOR RF ACCELERATING CAVITIES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic targets the development of large-size waveguide radiofrequency (RF) vacuum windows for UHF frequencies and for use with high-peak and high-average-power pulsed RF particle accelerators. Typical vacuum windows are designed to have good impedance matching for RF transmission but still have power dissipations inside. Over time, the surface condition of the windows can degrade, which further increases this loss. Historically, high-purity Alumina ceramic dielectric has been used in RF vacuum windows for accelerating cavities. Vacuum windows experience high electrical and mechanical stresses. Substantial optimization processes are required to ensure a desired RF performance and mechanical integrity. Most often, the window ceramic material is brazed to a metal flange. The ceramic-to-metal brazing process for this frequency range is of particular concern due to its large size. In addition, electron activity such as multipacting and arcing near the ceramic disk and surrounding metal surfaces must be suppressed. Typical manufacturing processes suppress multipacting by coating the ceramic with a low-secondary-emission-yield material such as TiN. While TiN is effective, in existing manufacturing processes it is difficult to control uniform deposition of TiN on the ceramic surface. The operating condition sought here is for low-band UHF frequencies (300 - 1000 MHz) with > 3-MW pulsed peak power at > 10% duty factor with well-controlled multipacting suppression. Consistently manufacturing an RF window for this frequency range and for high-power applications has proven challenging throughout the industry. Developing a novel design and manufacturing process meeting these specifications would greatly benefit the accelerator community and potentially fill a void that is critical to high-power accelerators.

a. Development of High-Average-Power RF Waveguide Vacuum Window for Pulsed RF Accelerating Cavities

Grant applications are wanted to develop the RF vacuum windows for the high-power RF accelerator applications as described above. Specifically, control of deposition thickness and adhesion of the TiN material must be repeatable and verifiable. The main aspect of the development is to have minimized electric field strength in the structure vacuum and improved repeatability and uniformity of the multipacting suppression material deposition with reliable quality control.

The window should be constructed to satisfy the following specifications for continuous operation:

1. Preferred operating RF frequency: 402.5 MHz
2. Bandwidth, 1 dB: > 4 MHz
3. Forward power: > 3 MW pulsed peak at > 10 % duty cycle and pulse length > 1.5 ms
4. Peak E-field, simulated estimate: < 300 kV/m at 3 MW
5. Insertion loss: < 0.005 dB
6. Return loss: > 35 dB, matched load
7. Input VSWR: 3.00 sustainable if mismatched, any phase

The structure should be compatible with ultra-high vacuum conditions typical for normal conducting accelerator cavities. Main vacuum pumping for operation is provided externally. The window structure needs properly designed and positioned ports for reliable vacuum and RF breakdown protection with the associated sensors properly mounted.

Questions - Contact: Eliane Lessner, eliane.lessner@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions - Contact: Eliane Lessner, eliane.lessner@science.doe.gov

References:

1. Neubauer, M., Fant, K., Hodgson, J., Judkins, J., Schwarz, H., and Rimmer, R. A. (1996). *High-Power RF Window and Coupler Development for the PEP-II B Factory*, Proceedings of the PAC 1995. https://accelconf.web.cern.ch/p95/ARTICLES/WPR/WPR08.PDF
2. Tamura, J., Kondo, Y., Morishita, T., Ao, H., Naito, F., Otani, M., and Nemoto, Y. (2018). *Low-Reflection RF Window for ACS Cavity In J-Parc Linac*, 9th International Particle Accelerator Conference IPAC2018, Vancouver, BC, Canada. http://accelconf.web.cern.ch/ipac2018/papers/tupal022.pdf
3. Bousonville, M., and Choroba, S. (2018). *Multipacting in an RF Window: Simulations and Measurements,* 9th International Particle Accelerator Conference IPAC2018, Vancouver, BC, Canada. http://accelconf.web.cern.ch/ipac2018/papers/wepmf051.pdf
4. Neubauer, M. (2012). *Rugged Ceramic Window for RF Applications*, Report No. DE-FG02 08ER85171. https://www.osti.gov/servlets/purl/1053988

15. SINGLE-PHOTON DETECTOR FOR SOFT X-RAY REGIME

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

In support of high-brightness x-ray light sources time-resolved experiments, development of detectors that can register a single photon with time stamping, to be used in the soft x-ray regime, benefits a wide variety of techniques. High-resolution photon-counting detection systems based on Microchannel plate amplification and subsequent event encoding will be very useful for many photoemission applications like X-ray Photon Correlation Spectroscopy or Time Resolved Photoemission at synchrotron or Free-Electron Laser facilities.

Grant applications are sought in the following subtopics:

a. Microchannel Plate Single-photon Detector

This topic seeks the development of detectors that enable single-photon counting with time stamping in the soft x-ray regime using microchannel plate and fast event-encoding readout (e.g. Timepix-like readout). The detector shall work in the UHV regime providing arrival time and photon counting measurements with sub-50 ns resolution. This detector can, potentially, benefit a large number of beamlines in the DOE complex, enabling high-impact time-resolved experiments not currently possible worldwide.

Questions - Contact: Eliane Lessner, eliane.lessner@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions - Contact: Eliane Lessner, eliane.lessner@science.doe.gov

References:

1. Ballabriga, R., Campbell, M., Llopart, X. (2020). *An introduction to The Medipix Family ASICs,* Radiation Measurements, 106271 (2020). https://doi.org/10.1016/j.radmeas.2020.106271
2. Llopart, X., Ballabriga, R., Campbell, M., Tlustos, L., and Wong, W. (2007*). Timepix, A 65k Programmable Pixel Readout Chip For Arrival Time, Energy and/or Photon Counting Measurements*, Nucl. Instrum. Meth. A. Vol. 581, 485 (2007). https://doi.org/10.1016/j.nima.2007.08.079
3. Tremsin, A. S., Vallerga, J. V., and Siegmund, O. H. W. (2020). *Overview Of Spatial and Timing Resolution of Event Counting Detectors with Microchannel Plates*, Nucl. Instrum. Meth. A Vol. 949, 162768 (2020). https://doi.org/10.1016/j.nima.2019.162768

16. CRYOGENIC SPECTROSCOPY FOR QUANTUM INFORMATION SYSTEMS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Accelerating the design and discovery of quantum materials with desired properties and functionality is a scientific challenge and opportunity identified in the recent Basic Energy Sciences workshop report on Basic Research Needs on Quantum Materials for Energy Relevant Technology [1]. While combinatorial theory and materials synthesis approaches have been rapidly developing, so far pairing these advances with equally high-throughput measurement techniques that interrogate the quantum properties of choice is still lacking. A primary challenge is that many quantum phenomena manifest themselves at cryogenic temperatures, and measurements that involve cooling down to liquid helium temperatures and beyond are intrinsically time-consuming and low-throughput. Furthermore, performing correlated measurements across multiple experimental platforms to get a comprehensive characterization of structural, optical, magnetic, and electronic properties is currently time-consuming. Finally, automation of sample position, temperature, and pressure together with seamless interfacing with a final characterization tool will be crucial for achieving the goals of high-throughput characterization of emergent quantum materials. Specifically, in the area of next-generation color centers for quantum information science there is a need to screen new materials systems for long coherence lifetimes and high brightness for incorporation into quantum communication and sensing networks [2].

Additionally, the development of ultra-low-temperature scanning microwave near-field microscopy will help systematically advance superconducting qubits and provide unprecedented insights into collective quantum phase transitions in solid-state systems. The ability to measure the properties of such quantum systems during operation would enable a deeper level of understanding of quantum phenomena and their coupling to the macroscopic world for quantum computing, sensing, and communications applications.

Grant applications are sought in the following subtopics:

a. High-Throughput Cryogenic Optical Spectroscopy of Quantum Systems

To address this critical need, grant applications are sought for developing cryogenic optical spectroscopy systems for high-throughput screening of large arrays of potential quantum emitters for their coherence lifetimes together with their ease of performing correlated measurements across other characterization tools like atomic force and electron microscopy. Scope for automation and for measurements in a magnetic field is also encouraged. System requirements include: <1.7K base temperature with potential for dilution fridge upgrade to mK, with operation beyond room temperature; <10 nm peak-to-peak vibrations in x, y, z; <100 nm repeatability in scanning to locate positions across different measurements and characterization tools; inspection capabilities at low magnification (5x to 20x) along with high magnification and NA (60x-100x, >0.4 NA).

Questions – Contact: George Maracas, george.maracas@science.doe.gov

b. In Operando Ultra-Low-Temperature Scanning Microwave Nearfield Microscopy

Superconducting Qubits are currently the most promising quantum computing technology [1]. However, parasitic two-level systems (TLSs) create local decoherence channels [2] in the main qubit components, a) the active TLS – the Josephson Junction (JJ), and b) the resonator to read out the JJ. In superconducting resonators parasitic TLSs limit the resonator's quality factor, reducing the accessible coherence time of a qubit [3]. In JJs parasitic TLSs induce fluctuations in coherence time, making reliable sequential operations challenging, and introducing inter-qubit non-uniformity, limiting scaling to multi-qubit devices [4]. The problem: The nature, location, and density of parasitic TLSs have not yet been determined. This information is paramount to systematically advance superconducting qubits and hence quantum computing. Unfortunately, the identification of these parasitic TLSs is further complicated by the following challenges: a) not all defects are bad - atomically precise MBE-grown JJs provide shorter coherence time than sputter-evaporated JJs; hence, distinguishing coherence-enhancing versus coherence-reducing defects is critical; b) one parasitic TLS within 100 nm^2 is sufficient to degrade qubit performance; c) these scattered parasitic TLSs can only be accessed at ultra-low temperatures and low photon limit – i.e., under the operating conditions of a qubit. At 100mK and above and/or under high photon flux the few scattered parasitic TLSs will be saturated and hence invisible. There is a clear need for the development of critical instrumentation to identify parasitic two-level systems in superconducting qubits and to visualize (de-)coherence channels in next-generation quantum materials.

Superconducting qubits are excited and read out using microwaves. The readout signal integrates over all parasitic TLSs in the qubit circuitry. However, recent advancements in scanning microwave near-field microscopy demonstrated microwave impedance measurements with sub-5 nm spatial resolution at room temperature [5]. Developing a user-friendly scanning microwave near-field microscope operating at sub 100mK would allow visualizing and characterizing local decoherence channels in superconducting materials. Combined with Scanning Gate Microscopy, also operated at mK, it could identify the electronic properties of decoherence channels. Combined with microwave detectors employed by the qubit community to operate in the low photon limit, it would enable operando characterization of a superconducting qubit and would identify with sufficient resolution individual parasitic TLSs. In addition, ultra-low temperature scanning microwave near-field microscopy will be of much broader scope beyond parasitic TLS identification, and will enable the visualization of local conduction and ultimately coherence and decoherence channels in next-generation quantum materials systems. Specifically impacted will be topological systems exhibiting Majorana fermions, moiré physics, as well as both classical and high-temperature superconductors. All of these exciting quantum material phenomena lack critical insight to provide a better understanding of what causes these quantum phase transitions. Ultra-low temperature scanning microwave near-field microscopy with sub-10 nm spatial resolution would provide unprecedented insight into local conductive properties of these quantum materials.

The measurement system must combine the following three components. Applications not addressing all three will be considered unresponsive.

1. An instrument that combines a super-high-resolution scanning microwave near-field microscope and a scanning gate microscope. The microscope should have sub-10 nm spatial resolution in the microwave mode and operate at sub-100mK temperatures.
2. Detection schemes having very low noise that will enable scanning microwave near-field microscopy operation in single-photon mode while operating at sub-100mK temperatures.
3. A microwave feedthrough and manifold should be designed for ultra-low temperature scanning microwave near-field microscopy. The desire is to connect to and operate eight superconducting qubits and perform near-field optical microscopy in operando below 100mK and with sub-10nm spatial resolution.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

c. Actively Stabilized Compact Femtosecond Lasers - Nanostructured Platforms for Detection, Lasing, Quantum Optics, and Separations

Ultrafast infrared lasers with pulse lengths below a picosecond capable of high average power while operating at high electrical-to-optical efficiency are a backbone technology needed for many areas of DOE applications including advanced accelerators, the generation of electromagnetic radiation ranging from THz to gamma rays, and the generation of neutron, proton, and light ion beams. The applications of femtosecond lasers have become increasingly broadened in commercial industries, including precision fabrication, THz spectroscopy, and medical surgeries. Currently, femtosecond lasers are unstable, requiring complex schemes to operate, which increase cost and size, as well as reducing efficiency. [1] Active control of the laser cavity polarization state holds the promise to substantially simplify the femtosecond laser construction, realizing the benefits of smaller size, lower cost, shorter pulse width, and lower power consumption. [2-4] This topic area is aimed at developing technologies for actively compensating the polarization state variation of the ultrafast lasers to achieve high operational stability and reliability for fabrication and advanced additive manufacturing techniques.

Grant applications are sought to realize actively stabilized femtosecond lasers. Development of a technique is desired to perform feedback control of the polarization state of an ultrafast laser by incorporating a ferroelectric optical crystal inside the laser cavity. The goal would be to demonstrate an environmentally stabilized femtosecond laser operated at a wavelength longer than 2 micrometers for DOE applications mentioned above. A new ultrafast cavity configuration of compact size, shorter pulse, high power, and simplified configuration is desirable. The program target is a new type of femtosecond laser with pulse energy >5mJ, repetition rate >1Mhz, energy stability <0.1%, wall-plug efficiency >20%, and emission wavelength >2 micrometers.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

d. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

References:

1. U.S. Department of Energy. (2016). Basic Research Needs on Quantum Materials for Energy Relevant Technology, February 8-10, 2016. https://science.osti.gov/-/media/bes/pdf/reports/2016/BRNQM_rpt_Final_12-09-2016.pdf?la=en&hash=E7760711641883FFC9F110D70385937D6A31C64F
2. U.S. Department of Energy. (2017). Opportunities for Basic Research for Next-Generation Quantum Systems, Basic Energy Sciences Roundtable. October 30-31, 2017. https://science.osti.gov/-/media/bes/pdf/reports/2018/Quantum_systems.pdf?la=en&hash=291099097EBCCFAB99D86F60F62EA061F996424C

References: Subtopic a:

1. U.S. Department of Energy. (2017). *Opportunities for Quantum Computing in Chemical and Materials Sciences*, Report of the Basic Energy Sciences Roundtable October 31–November 1, 2017. https://science.osti.gov/-/media/bes/pdf/reports/2018/Quantum_computing.pdf?la=en&hash=C767B23CFFD250A01F846D3B6FB62143BEC258B0

References: Subtopic b:

1. Kjaergaard, M., Schwartz, M. E., Braumuller, J., Krantz, P., I-JWang, J., Gustavsson, S., and Oliver, W. D. (2020). *Superconducting Qubits: Current State of Play*, arXiv:1905.13641v3, 21 Apr 2020. https://arxiv.org/pdf/1905.13641.pdf
2. Müller, C., Cole, J. H., and Lisenfeld, J. (2018). *Towards Understanding Two-Level-Systems In Amorphous Solids -- Insights From Quantum Circuits*, arXiv:1705.01108v2 (2018). https://arxiv.org/pdf/1705.01108.pdf
3. Murch, K.W., Vool, U., Zhou, D., Weber, S. J., Girvin, S. M., and Siddiqi, I. (2012). *Cavity-Assisted Quantum Bath Engineering,* Phys. Rev. Lett. 109, 183602 (2012), DOI: 10.1103/PhysRevLett.109.183602 https://arxiv.org/abs/1207.0053
4. Klimov, P. V., Kelly, J., Chen, Z., Neeley, M., Megrant, A., Burkett, B., Barends, R., Arya, K., Chiaro, B., Chen, Y., Dunsworth, A., Fowler, A., Foxen, B., Gidney, C., Giustina, M., Graff, R., Huang, T., Jeffrey, E., Lucero, E., Mutus, J. Y., Naaman, O., Neill, C., Quintana, C., Roushan, P., Sank, D., Vainsencher, A., Wenner, J., White, T. C., Boixo, S., Babbush, R., Smelyanskiy, V. N., Neven, H., and Martinis, J. M. (2018). *Fluctuations of Energy-Relaxation Times in Superconducting Qubits*, Phys. Rev. Lett. 121, 090502 (2018), DOI: 10.1103/PhysRevLett.121.090502 https://arxiv.org/abs/1809.01043
5. Lee, K., Utama, M. I. B., Kahn, S., Samudrala, A., Leconte, N., Yang, B., Wang, S., Watanabe, K., Taniguchi, T., Zhang, G., Weber-Bargioni, A., Crommie, M., Ashby, P. D., Jung, J. I., Wang, F., and Zettl, A. (2020). *Ultra-High-Resolution Imaging Of Moiré Lattices and Superstructures Using Scanning Microwave Impedance Microscopy Under Ambient Conditions*, arXiv:2006.04000. https://arxiv.org/abs/2006.04000

References: Subtopic c:

1. Karlsson, O., Brentel, J., and Andrekson, P. A. (2000). *Long-Term Measurement of PMD and Polarization Drift In Installed Fibers*, J. Lightwave Technol. 18(7), 941–951 (2000). https://ieeexplore.ieee.org/document/850739
2. Santiago-Hernández, H., Bracamontes-Rodríguez, Y. E., Beltrán-Pérez, G., Armas-Rivera, I., RodríguezMorales, L. A., Pottiez, O., Ibarra-Escamilla, B., Durán-Sánchez, M., Hernández-Arriaga, M. V., and Kuzin, E. A. (2017). *Initial Conditions For Dissipative Solitons In a Strict Polarization-Controlled Passively Mode-Locked Er-Fiber Laser*, Opt. Express 25(21), 25036–25045 (2017). https://pubmed.ncbi.nlm.nih.gov/29041175/
3. Brunton, S.L., Fu, X., and Kutz, J. N. (2014). *Self-Tuning Fiber Lasers*, IEEE J. Sel. Top. Quantum Electron. 20(5), 1101408 (2014). http://faculty.washington.edu/sbrunton/papers/BrFuKu2014.pdf
4. Winters, D. G., Kirchner, M.S., Backus, S. J., and Kapteyn, H. C. (2017). *Electronic Initiation and Optimization of Nonlinear Polarization Evolution Mode-Locking In a Fiber Laser*, Opt. Express 25(26), 33216–33225 (2017). https://www.osapublishing.org/oe/abstract.cfm?URI=oe-25-26-33216

Additional information:
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17. ADVANCED ELECTRON MICROSCOPY - ANALYSIS TOOLS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Electron microscopy (EM) is a cornerstone technique of the materials and biological communities. It is capable of imaging the structure of materials as well as mapping their composition with atomic resolution. EM datasets are being produced in the imaging, diffraction, and spectroscopic modes at higher and higher data rates than ever before. A key component to any advanced analysis now rests as much on the quality of the data that is acquired as on the post-processing and visualization steps to arrive at the results. Open-source development of analytical capabilities for EM is providing rapid advances, but these capabilities often require extensive knowledge of advanced data science and visualization codes driven mostly by command-line interactions. An important example is the use of machine learning for image data analysis, but its reach has been limited due to the need for domain expertise and a clear set of models trained for specific applications. Data analysis in EM is becoming a complex set of tasks which makes reproducibility a major unnoticed issue. As such, the development of an extensible, repeatable, and user-friendly software program designed with speed, shareability, and repeatability would greatly benefit the community as a whole while providing access to advanced capabilities by users of all abilities.

Data analysis stacks such as the Scipy and Numpy environments combined with the Jupyter Notebook environment provide a way for coding experts to easily share their code and results simultaneously with moderate to expert users, but these environments have several limitations which need to be overcome. Data analysis in the EM community relies heavily on live feedback and parameter tweaking due to the flexibility of EM imaging techniques, the large heterogeneity of samples, and the large number of different techniques that can be applied to those samples. The future size and scale of terabyte-sized datasets will require optimized analysis and visualization routines that take advantage of modern programming languages. AI/ML will exacerbate this problem as models need to be trained and validated, adding another step which is not always saved, shared, or repeatable. Development of software that contains the capabilities of reproducible, shareable analysis pipelines with highly optimized visualization and rendering code to offer the interactivity needed by the community is paramount.

Grant applications are sought in the following subtopics:

a. Software Environment for Reproducible Data Analysis for Electron Microscopy

Grant applications are sought for open-source tools that simultaneously address the following three considerations. Applications not effectively addressing all three simultaneously will be considered non-responsive.

1. **Interactive data exploration**: A cross-platform (Windows, Mac, Linux) software program that provides the basics for graphical user interactions for EM image, diffraction, and spectroscopic datasets, is optimized for live feedback and extremely large data sets, and can be extended with user-driven modules such as scripts or plugins.
2. **Quantitative data analysis**: Development of a system for customizable, shareable and reproducible analysis and visualization pipelines. The system should be ready to utilize machine learning techniques as well as to document all training parameters and datasets utilized in the analysis of a data set.
3. **Live feedback of results**: An important part of EM data analysis is live feedback for parameter optimization, ideally as close to the data acquisition system as possible. The software should provide highly parallelized basic features that can be built upon by users and utilized during a data acquisition session. The user-facing applications should leverage edge computing, cloud, and/or HPC resources for seamless analysis and visualization on users' desktops/laptops.

Electron microscopy and cryo-EM are powerful tools to image hard and soft materials in three dimensions with atomic resolution. These tools, coupled with complementary characterization capabilities, provide insight into virus properties and their behavior in different conditions. The NSRCs have a suite of capabilities that are addressing COVID-19 issues. Grant applications that focus on novel data analytic methods and algorithms to produce EM data analysis software technology with applicability to COVID-19 research will also be considered.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

b. Open-Source Control Software for TEM

Design and develop an open-source control software platform that can support automated or autonomous workflows for transmission electron microscopes (TEMs) based on existing Open Source Control Software.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

c. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

References:

1. Minor, A. M., Denes, P., and Muller, D. A. (2019). Cryogenic Electron Cicroscopy for Quantum Science, MRS BULLETIN. vol. 44, 964 (December 2019). https://www.cambridge.org/core/journals/mrs-bulletin/article/cryogenic-electron-microscopy-for-quantum-science/D6EDDE3F2185E7C80B641C0B7A246779
2. Ren, D., Ophus, C., Chen, M., and Waller, L. (2019). *A Multiple Scattering Algorithm for Three Dimensional Phase Contrast Atomic Electron Tomography*, Ultramicroscopy 208 (2020) 112860. https://www.sciencedirect.com/science/article/pii/S030439911930052X

Additional information:

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NSRC Portal: https://nsrcportal.sandia.gov/

18. LOW-POWER, HIGH-THROUGHPUT VOLUMETRIC LITHOGRAPHY

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The structuring and miniaturization of materials has revolutionized the world, from the transistors enabling modern computing to the micromirror arrays in light projectors to the inertial measurement units in every drone, smartphone, and modern GPS. In the nanoscale and single-digit-micron scale, processing by lithography has been extremely well optimized, on the heels of massive investment from the semiconductor industry. However, these technologies are all based on planar approaches, limiting products to two dimensions or, in the case of some painstaking processes, multiple exposures to build up quasi-three-dimensional objects. There is a need for lithographic processes that can extensively pattern materials at the nanoscale in three dimensions.

One notable exception is direct laser writing approaches that can truly pattern in 3 dimensions at the nanoscale. Unfortunately, the slow printing speed of the laser (<100 mm/s), high instantaneous power requiring expensive, ultrafast lasers (~10^{12} W/cm^2), small scan fields (<1 mm) and limited working distance (<8 mm) limit practical, scalable applications of this attractive technology. There is an unmet need for scalable, rapid approaches to nano/microfabrication in three dimensions. A rapid, affordable, large-area lithography approach with volumetric capability will enable a multitude of applications ranging from microoptics, tissue scaffolding, metamaterials and other fields currently unserved by planar lithography or direct laser writing approaches.

Grant applications are sought in the following subtopics:

a. Direct Laser Writing of Many Voxels Simultaneously

Applications of direct laser writing that enable simultaneous printing of many voxels, allowing the writing process to result in useful fabrication times. Novel approaches should target >100,000 voxels/second and demonstrate a roadmap to writing speeds at least two orders of magnitude greater than current state-of-the-art direct laser writing. Working distances greater than a centimeter and materials properties appropriate for end-use applications are also essential. Paths to employ affordable, continuous wave lasers with lower (<1 mW per voxel) writing powers are also necessary to achieve wide applicability in nanoscience and industry.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

References:

1. Saha, S.K., Wang, D., Nguyen, V.H., Chang, Y., Oakdale, J.S., and Chen, S.C. (2019). *Scalable Submicrometer Additive Manufacturing*, Science, Vol. 366(6461), p. 105-109. https://science.sciencemag.org/content/366/6461/105
2. Geng, Q., Wang, D., Chen, P., and Chen, S.C. (2019). *Ultrafast Multi-focus 3-D Nano-fabrication Based on Two-photon Polymerization*, Nature Communications, Vol. 10(1), p. 1-7. https://www.nature.com/articles/s41467-019-10249-2
3. LaFratta, C.N., and Li, L. (2020*). Making Two-photon Polymerization Faster*. In Three-Dimensional Microfabrication Using Two-Photon Polymerization, p. 385-408. William Andrew Publishing. https://www.sciencedirect.com/science/article/pii/B9780128178270000096?via%3Dihub
4. Rocheva, V.V., Koroleva, A.V., Savelyev, A.G., Khaydukov, K.V., Generalova, A.N., Nechaev, A.V., et al. (2018). *High-resolution 3D Photopolymerization Assisted by Upconversion Nanoparticles for Rapid Prototyping Applications*, Scientific Reports, Vol. 8(1), p. 1-10. https://www.nature.com/articles/s41598-018-21793-0

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19. NOVEL HIGH-FLUX, HIGH-SELECTIVITY MEMBRANES FOR ENVIRONMENTAL MEDIATION

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Grant applications are sought in the following subtopics:

a. Novel Membranes that Combine High Flux with High Selectivity for Low-Cost Carbon Capture

Separation membranes represent a promising approach to carbon capture from fossil fuel-based power plants and air due to their potential for greater energy efficiency, processability, and lower maintenance costs compared with contemporary reversible absorption techniques.[1-4] However, no commercial membrane for separating carbon dioxide (CO_2) from power plant flue gas or air yet exists. An efficient membrane should have both high permeance and high selectivity for CO_2. Permeance is the flux of CO_2 gas through the membranes, typically reported in gas permeation units [1 GPU = 10^{-6} cm^3 (standard temperature and pressure) $cm^{-2}s^{-1}(cm\ Hg)^{-1}$]. Selectivity is the capacity to separate two or more gases, typically reported as a dimensionless ratio of flux. Most existing membranes, including polymeric membranes, exhibit a sharp trade-off between flux and selectivity, and thus are impractical for CO_2 capture applications. Furthermore, most contemporary membranes, including polymeric membranes, show a flux that is strongly dependent on partial pressure of CO_2. That dependence is problematic because it raises the cost of capture from dilute mixtures of CO_2 where partial pressures are low, such as in air and power plant flue gases.

Grant applications are sought for 1) novel membranes that demonstrate both high flux (over 1200 GPU) and high selectivity (over 100) for CO_2 in dilute mixtures, and simultaneously 2) a mechanism that inherently allows rapid transport of CO_2 even for dilute mixtures, surpassing limitations of contemporary membranes and creating the conditions for efficient CO_2 capture. Applications that involve polymeric membranes will be considered non-responsive to this subtopic.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

b. Novel Hybrid Porous Materials for the Selective Capture of Contaminants and/or Valuable Metal Ions from Water

Since the recent industrial revolution there has been an increasing number of contaminants and valuable commodities that are discharged into industrial downstream operations and ultimately end up in the environment. Commercial remediation methods for these species such as chemical precipitation, sorbents, and membranes have many disadvantages that include high economic and energy cost, low removal efficiency, difficult regeneration and/or fouling, and the production of high quantities of chemical sludge [1]. The major drawback with current state-of-the-art adsorbents such as activated carbon is fouling due to inadequate selectivity [2]. Although these types of porous materials are extremely stable, they tend to foul quickly, compromising extraction rate, capacity, and overall energy efficiency [3]. As such, new hybrid porous materials that can selectively capture such species via energy-efficient processes and green principles are highly desirable. In order to steer the development of better-performing materials to address significant environmental and economic issues, applications addressing the following subtopics are sought.

Such materials should be constructed for sustainable environmental remediation, such as the rapid and selective extraction of toxic contaminants or valuable metal ions from water. The targeted toxic contaminants can be but are not limited to heavy metal ions such as lead, mercury, cadmium, arsenic, and chromium, or volatile organic compounds. These toxic species at trace amounts are problematic contaminants in water-purification applications. Another subarea is directed towards selective capture of valuable metal ions. The extraction of these commodities is a sustainability effort in the modern electronics industry. Other vital targets can also be valuable resources in the energy sector, such as uranium and lithium ions that are needed for energy production and storage. Exemplary hybrid porous materials may be composed of two or more of the following classes of materials: metal organic frameworks (MOFs), silica, activated carbons, polymers, nanoparticles, zeolites, covalent organic frameworks, and other competitive adsorbents. Such materials should target single metal ion selectivity and excel in the metrics mentioned above. Applications should focus on the capture of the aforementioned toxic contaminants from water for municipal use and/or the efficient purification of the targeted valuable commodities post-capture.

Grant applications are sought for hybrid porous materials for use in continuous flow devices for industrial operations. Novel techniques and formulations to optimally structure porous materials are sought to be implemented into filter devices to assess extraction performance.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

c. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: George Maracas, george.maracas@science.doe.gov

References: Subtopic a:

1. Aaron, D. & Tsouris, C. (2011). *Separation of CO_2 from Flue Gas: A Review*. *Sep. Sci. Technol.* 40, 321– 48 (2005). https://www.tandfonline.com/doi/abs/10.1081/SS-200042244
2. Rao, A. B. & Rubin, E. S. (2002). *A Technical, Economic, and Environmental Assessment of Amine-Based CO_2 Capture Technology for Power Plant Greenhouse Gas Control*. Environ. Sci. Tech. 36, 4467– 75 (Sept. 2002). https://pubs.acs.org/doi/abs/10.1021/es0158861
3. Khalilpour, R. et al. (2015). *Membrane-Based Carbon Capture From Flue Gas: A Review*, J. Clean. Prod. 103, 286–300 (Sept. 2015). https://www.sciencedirect.com/science/article/abs/pii/S0959652614010920
4. Kentish, S., Scholes, C. & Stevens, G. (2008). *Carbon Dioxide Separation through Polymeric Membrane Systems for Flue Gas Applications*. Recent Pat. Chem. Eng. 1, 52–66 (Jan. 2008). https://www.researchgate.net/publication/228676182_Carbon_Dioxide_Separation_through_Polymeric_Membrane_Systems_for_Flue_Gas_Applications

References: Subtopic b:

1. Shannon, M. A.; Bohn, P. W.; Elimelech, M.; Georgiadis, J. G.; Marinas, B. J.; Mayes, A. M. (2008). *Science and Technology For Water Purification In The Coming Decades*, Nature 2008, 452 (7185), 301-310. https://www.nature.com/articles/nature06599
2. Terdkiatburana, T.; Wang, S.; Tadé, M. O. (2007). *Competition and Complexation of Heavy Metal Ions and Humic Acid on Zeolitic MCM-22 and Activated Carbon.* Chemical Engineering Journal 2008, 139 (3), 437-444. https://www.sciencedirect.com/science/article/abs/pii/S1385894707005645
3. Tang, W.-W.; Zeng, G.-M.; Gong, J.-L.; Liang, J.; Xu, P.; Zhang, C.; Huang, B.-B. (2014). *Impact of Humic/Fulvic Acid On The Removal of Heavy Metals from Aqueous Solutions Using Nanomaterials: A*

Review, Science of the Total Environment 2014, 468–469, 1014-1027. https://www.sciencedirect.com/science/article/pii/S0048969713010826
4. Hong, Y, Thirion, D, et al. (2020). *Precious metal recovery from electronic waste by a porous porphyrin polymer*, PNAS (June 2020). https://doi-org.proxy.scejournals.org/10.1073/pnas.2000606117

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For more information see:
https://science.osti.gov/bes/suf/User-Facilities/Nanoscale-Science-Research-Centers
NSRC Portal: https://nsrcportal.sandia.gov/

20. INSTRUMENTATION AND TOOLS FOR MATERIALS RESEARCH USING NEUTRON SCATTERING

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

As a unique and increasingly utilized research tool, neutron scattering makes invaluable contributions to the physical, chemical, and nanostructured materials sciences. The Department of Energy supports neutron scattering and spectroscopy facilities at neutron sources where users conduct state-of-the-art materials research. Their experiments are enabled by the convergence of a range of instrumentation technologies. The Department of Energy is committed to enhancing the operation and instrumentation of its present and future neutron scattering facilities [1,2] so that their full potential is realized.

This topic seeks to develop advanced instrumentation that will enhance materials research employing neutron scattering. Grant applications should define the instrumentation need and outline the research that will enable innovation beyond the current state-of-the-art. Applicants are strongly encouraged to demonstrate applicability and proper context through a discussion with a user facility staff scientist or through a collaboration with a successful user of neutron sources. To this end, the STTR program would be an appropriate vehicle for proposal submission. Applicants are encouraged to demonstrate applicability by providing a letter of support from the user facility staff scientist or a successful user. Priority will be given to those grant applications that include such collaborations or letters of support.

A successful user is defined as someone at a research institution who has recently performed neutron scattering experiments and published results in peer reviewed archival journals. Such researchers are the early adopters of new instrumentation and are often involved in conceptualizing, fabricating, and testing new devices. A starting point for developing collaborations with either a staff scientist or an external user would be to examine the strategic plans and annual activity reports from neutron scattering facilities listed on the neutron facility web sites at: http://neutrons.ornl.gov and http://www.ncnr.nist.gov/.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought in the following subtopics:

a. Advanced Sample Environments

Develop instrumentation and techniques for advanced sample environments [3,4] for neutron scattering studies. Sample environments should provide a novel means of achieving controlled chemical and gaseous environment and extreme conditions of temperature, pressure, electric and magnetic fields, and mechanical loading including shear and strain or combinations thereof for *in situ* materials studies. Sample environments may enable conditions appropriate for *in situ* materials synthesis and support innovative approaches to incorporate diagnostic and characterization tools that complement neutron scattering data.

- Development of faster cooling furnace and cryostat: DOE's high flux sources enable faster data collection, but the existing furnaces and cryostats used for heating and cooling the samples significantly limit the efficient utilization of the valuable neutron beam time for experiments. An advancement in the technology and design of neutron scattering compatible cryostats and furnaces (with or without sample changer options) that can speed up the cooling and heating is needed to substantially decrease the down time for various types of high-throughput experiments.

- Development of steady state high field magnets: The steady-state high-field magnet systems currently available at US neutron scattering facilities are limited to a maximum field of 16 tesla, which prohibits the structure and dynamics studies of ultra-high magnetic field states of both quantum matter and in-situ materials processed at high magnetic fields [5-7]. To address this gap, development is needed for high field magnets, based on technologies employing composite conductors made of high temperature superconductor materials, suitable for neutron scattering applications.

- Development of neutron transparent sample environments for in-situ studies: Neutron scattering measurements to measure changes in samples in-situ and in-operando are of increasing importance to the neutron scattering user community. As such, sample environments that allow neutron scattering measurements on samples maintained at conditions relevant to the sample's synthesis, processing, or property are of interest. Such environments would require the use of neutron transparent windows with geometry and scattering characteristics compatible with instruments of the type on which they will be utilized and the possibility of control and reporting and recording of the key environmental parameters in coordination with the neutron scattering measurements. Examples of such environments include environments that allow simultaneous characterization of the same sample by neutron scattering techniques in coordination with optical techniques such as Raman spectroscopy [8], FTIR spectroscopy [9], or light scattering [10] during the processing or evolution of the sample.

- Advancements in automation in experimental setups and instruments: For neutron science, this is specifically interesting with respect to advancing self-centering furnaces, cryostats, magnets, and electrical voltage and current setups. This would include inserts, motorized mechanisms, and imaging to find and scan the beam center, self-align samples, and build a memory and database of such for each instrument to facilitate installation and use of interchangeable sample environments (SE).

Advanced SE needs to include artificial intelligence and machine learning (AI/ML) components to adjust according to conditions of instruments and to facilitate imaging at the beamline for sample position and sample movements. Example projects could include imaging samples with respect to movement in the neutron beam through a neutron IR camera, X-ray and gamma ray imaging with AI/ML sample-centering capability, tracking sample changes, and ultrasound imaging of samples within sample environments.

Questions – Contact: P. Thiyagarajan (Thiyaga), P.Thiyagarajan@science.doe.gov

b. Advanced Detectors

Several areas of neutron detector development are of interest to meet the existing and anticipated needs for detectors at neutron sources.

- High Spatial Resolution Detectors for Single Crystal Diffractometers: Novel detector technologies having resolutions from 300µm to 600µm FWHM with superior gamma rejection of < 1e-06 are needed to enable efficient measurement of small single crystals for diffraction and diffuse scattering measurements. Also, of interest are technologies that have curved detector surfaces allowing near 4π solid angle coverage with minimum dead area and reduced parallax. It is expected that these detectors have efficiencies >=60% for 1Å neutrons with a 10% dead time at 100K counts/sec.

- Large Area Time of Flight Detectors for Imaging Science: High rate > 20MHz time of flight (TOF) detectors are needed for novel science applications in neutron imaging. The goal is to replace frame-based systems for use at spallation neutron sources where simultaneous collection of position and wavelength allows for material identification and image enhancement. Large area detectors (10cmx10cm) with FWHM resolutions of 100µm or better are of highest interest. It is expected that these detectors have efficiencies >=40% for 2Å neutrons.

- High Data Rate Detectors for Neutron Reflectometers: The availability of detectors having resolutions of 1-2mm FWHM and very high rate capability (20 MHz) remains a challenge for neutron reflectometers where a large active area (15cmx15cm) and excellent gamma rejection < 2e-6 are required. Current detector technologies will likely fall short of the count rate requirements expected at new neutron sources by two orders of magnitude. It is expected that these detectors have efficiencies >=60% for 2Å neutrons.

Questions – Contact: P. Thiyagarajan (Thiyaga), P.Thiyagarajan@science.doe.gov

c. Advanced Choppers

Short-pulse neutron sources provide the brightest neutron beams and future sources will push this even further, particularly at longer wavelengths. Current Fermi choppers allow the use of only single-wavelength neutrons for measurements at pulsed neutron sources. Novel developments are needed in the design of Fermi choppers by incorporating neutron-reflecting mirrors. Such a device, known as Magic Chopper [11], will enable the use of a wide range of wavelengths available at pulsed neutron sources and maximize the scientific output.

Questions – Contact: P. Thiyagarajan (Thiyaga), P.Thiyagarajan@science.doe.gov

d. Novel Beam Conditioning Optics

The ability to produce neutrons is source limited. Therefore, development of improved optical components to control angular divergence and energy dispersion to maximize the usable flux on the sample while minimizing neutron and gamma background on the detectors is needed. Examples of such beam conditioning optics include but are not limited to advanced multilayer supermirrors for neutron beam transport [12], refractive and reflective focusing optics [13-16], and rotating absorbing-channel velocity selectors for wavelength and wavelength-dispersion control [17].

- Low-background apertures and collimators: Neutron scattering facilities are performing measurements using smaller samples and increasingly tight resolution, and many neutron scattering experiments are background-limited. Optics introduced into neutron scattering instruments to control beam size and divergence inescapably also introduce background into the data by scattering, reflection, and refraction, and are at risk of causing uncertainties in the resolution due to incomplete neutron absorption and wavelength distortion caused by incoherent scattering from hydrogenous binders. There is a need for precision apertures with minimal edge scattering and internal surface reflection, especially multiple confocal pinhole apertures [18], and for collimators with minimal surface reflection and scattering and minimal incoherent scattering.

- Spin manipulation optics: One of the key strengths of neutron scattering for condensed matter research is its ability to directly measure magnetic structure and dynamics through the interaction between the neutron spin and the nuclear spin of atoms. Experiments on magnetism are limited by the ability to manipulate, transport, and select the spin state of the neutron as it passes through the sample. Examples of areas where valuable advances can be made include spin-selective focusing devices capable of operation at time-of-flight sources, large-area superconducting foils for spin rotation[19], and improved actively-controlled and monitored He3 spin filters[20] with large areas and acceptance angles.

Questions – Contact: P. Thiyagarajan (Thiyaga), P.Thiyagarajan@science.doe.gov

e. Advanced Software Tools for Working with Multiple Related Data Sets and Automated Scattering Feature Recognition

In many experiments (single crystal diffraction, residual stress/ engineering diffraction, inelastic neutron scattering, tomography, etc.) the datasets comprise many runs at different orientations, times, and/or sample environment conditions. It is important to be able to look at the global picture through simultaneous visualization and analysis of the data. This can give important information on diffuse scattering, tracking phase transitions, and even diagnose experimental problems (non-centered rotations). Enabling the inspection of the data as a whole, especially with the possibility of automated detection of features and/or problems would greatly facilitate the experiment management and accelerate the analysis [21, 22, 23].

Questions – Contact: P. Thiyagarajan (Thiyaga), P.Thiyagarajan@science.doe.gov

f. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic descriptions above.

Questions – Contact: P. Thiyagarajan (Thiyaga), P.Thiyagarajan@science.doe.gov

References:

1. U.S. Department of Energy. (2020). *Neutron Scattering Facilities*, Office of Science. https://science.osti.gov/bes/suf/User-Facilities/Neutron-Scattering-Facilities

2. National Nanotechnology Initiative. (2005). *X-rays and Neutrons: Essential Tools for Nanoscience Research Workshop Report*. Report of the National Nanotechnology Initiative Workshop, p. 122. http://www.nano.gov/node/68.
3. Bailey, I.F. (2003). *A Review of Sample Environments in Neutron Scattering*, Zeitschrift für Kristallographie, Vol. 218, Issue 2, p. 84–95. https://www.degruyter.com/view/j/zkri.2003.218.issue-2/zkri.218.2.84.20671/zkri.218.2.84.20671.xml
4. Rix, J.E., Weber, J. K. R., Santodonato, L. J., Hill, B., et al. (2007). *Automated Sample Exchange and Tracking System for Neutron Research at Cryogenic Temperatures*, Review of Scientific Instruments, Vol. 78, Issue 1, p. 8. http://scitation.aip.org/content/aip/journal/rsi/78/1/10.1063/1.2426878
5. National Research Council. (2005). *Opportunities in High Magnetic Field Science*, The National Academies Press, Washington, D.C., ISBN: 978-0-309-09582-2. https://www.nap.edu/catalog/11211/opportunities-in-high-magnetic-field-science
6. Weijers, H.W., Markiewicz, W.D., Voran, A.J., Gundlach, S.R., et al. (2016). *Progress in the Development and Construction of a 32-T Superconducting Magnet*, IEEE Transactions on Applied Superconductivity Vol. 26, Issue 4, 4300807. https://ieeexplore.ieee.org/document/7383266
7. Smeibidl, P., Bird, M., Ehmler, H., Dixon, I., et al. (2016). *First Hybrid Magnet for Neutron Scattering at Helmholtz-Zentrum Berlin*, IEEE Transactions on Applied Superconductivity, Vol. 26, Issue 4, 4301606. https://ieeexplore.ieee.org/document/7399382
8. Adams, M.A., Parker, S.F., Fernandez-Alonso, F., Cutler, D.J., et al. (2009). *Simultaneous Neutron Scattering and Raman Scattering*, Applied Spectroscopy, Vol. 63, Issue 7, p. 727-732. https://www.ncbi.nlm.nih.gov/pubmed/19589208
9. Topham, P.D., Glidle, A., Toolan, D.T., Weir, M.P., et al. (2013). *The Relationship between Charge Density and Polyelectrolyte Brush Profile using Simultaneous Neutron Reflectivity and In Situ Attenuated Total Internal Reflection FTIR*, Langmuir, Vol. 29, Issue 20, p. 6068-6076. https://pubs.acs.org/doi/abs/10.1021/la4005592
10. Romer, S., Urban, C., Lobaskin, V., Scheffold, F., et al. (2003). *Simultaneous Light and Small-angle Neutron Scattering on Aggregating Concentrated Colloidal Suspensions*, Journal of Applied Crystallography, Vol. 36, Issue 1, p. 1-6. https://onlinelibrary.wiley.com/doi/abs/10.1107/S0021889802016291
11. Nakamura, M., Arai, M., Kajimoto, R., Yokoo, T., et al. (2008). *Conceptual Design of MAGIC Chopper Used for 4-SEASONS at JPARC*, Journal of Neutron Research, Vol. 16, Issue 3-4, p. 87-92. https://www.tandfonline.com/doi/abs/10.1080/10238160902819510
12. Hino, M., Hayashida, H., Kitaguchi, M., Kawabata, Y., et al. (2006). *Development of Large-m Polarizing Neutron Supermirror Fabricated by Using Ion Beam Sputtering Instrument at KURRI*, Physica B: Condensed Matter, Vol. 385, p. 1187-1189. https://www.sciencedirect.com/science/article/pii/S0921452606012968
13. Oku, T., Iwase, H., Shinohara, T., Yamada, S., et al. (2007). *A Focusing-geometry Small-angle Neutron Scattering Instrument with a Magnetic Neutron Lens*, Journal of Applied Crystallography, Vol. 40, Issue s1, p. s408-s413. https://journals.iucr.org/j/issues/2007/s1/00/aj6037/
14. Chen, H., Sharov, V.A., Mildner, D.F.R., Downing, R.G., et al. (1995). *Prompt Gamma Activation Analysis Enhanced by a Neutron Focusing Capillary Lens*, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, Vol. 95, Issue 1, p. 107-114. https://www.sciencedirect.com/science/article/pii/0168583X94003467
15. Oku, T., Morita, S., Moriyasu, S., Yamagata, Y., et al. (2001). *Development of a Fresnel Lens for Cold Neutrons based on Neutron Refractive Optics*, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Vol. 462, Issue 3, p. 435-441. https://www.sciencedirect.com/science/article/pii/S0168900200013140
16. Ice, G., Hubbard, C., Larson, B., Pang, J., et al. (2006). *High-performance Kirkpatrick-Baez Supermirrors for Neutron Milli-and Micro-beams*, Materials Science and Engineering: A, Vol. 437, Issue 1, p. 120-125. https://www.researchgate.net/publication/44061686_High-performance_Kirkpatrick-Baez_supermirrors_for_neutron_milli-_and_micro-beams

17. Peetermans, S., Grazzi, F., Salvemini, F., and Lehmann, E. (2013). *Spectral Characterization of a Velocity Selector Type Monochromator for Energy-selective Neutron Imaging, Physics Procedia*, Vol. 43, p. 121-127. https://www.sciencedirect.com/science/article/pii/S1875389213000291
18. Jaksch, S., Martin-Rodriguez, D., Ostermann, A., Jestin, J., Pinto, S.D., Bouwman, W.G., Uher, J., Engels, R. and Frielinghaus, H., (2014). *Concept for a time-of-flight Small Angle Neutron Scattering instrument at the European Spallation Source*. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 762, pp.22-30. https://arxiv.org/ftp/arxiv/papers/1403/1403.2534.pdf
19. Rekveldt, M.T., Bouwman, W.G. and Kraan, W.H. (2002). *Magnetized Foils as π Flippers in Neutron Spin-Echo Spectrometry*. Journal of applied physics, 92(6), pp.3354-3362. https://aip.scitation.org/doi/abs/10.1063/1.1499751
20. Chupp, T.E., Coulter, K.P., Kandes, M., Sharma, M., Smith, T.B., Jones, G., Chen, W.C., Gentile, T.R., Rich, D.R., Lauss, B. and Gericke, M.T. (2007). *A large area polarized 3He neutron spin filter*. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 574(3), pp.500-509. https://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-08-07265
21. Spinozzi, F., Ferrero, C., Ortore, M.G., De Maria Antolinos, A. and Mariani, P., 2014. *GENFIT: Software for the Analysis of Small-Angle X-ray and Neutron Scattering Data of Macromolecules in Solution*. Journal of applied crystallography, 47(3), pp.1132-1139. https://journals.iucr.org/j/issues/2014/03/00/to5062/to5062.pdf
22. Ewings, R.A., Buts, A., Le, M.D., van Duijn, J., Bustinduy, I. and Perring, T.G. (2016). *HORACE: Software for the Analysis of Data from Single Crystal Spectroscopy Experiments at Time-of-Flight Neutron Instruments.* Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 834, pp.132-142. https://www.sciencedirect.com/science/article/pii/S016890021630777X
23. McDonnell, M.T., Olds, D.P., Page, K.L., Neufeind, J.C., Tucker, M.G., Bilheux, J.C., Zhou, W. and Peterson, P.F. (2017). *ADDIE: ADvanced DIffraction Environment–A Software Environment for Analyzing Neutron Diffraction Data.* Foundations of Crystallography, 73, p.a377. https://www.researchgate.net/publication/321926871_ADDIE_ADvanced_DIffraction_Environment_-_a_software_environment_for_analyzing_neutron_diffraction_data

21. MEMBRANES FOR ELECTROCHEMICAL APPLICATIONS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Electrochemical membranes encompass a wide range of ceramic, polymeric, and composite materials that enable ion transport between electrodes in many electrochemical applications while acting as electrical insulators to direct electrical current through the external circuit. Accordingly, the Department of Energy supports the development of high-risk, innovative electrochemical membranes which possess greater thermal and chemical stability, greater reliability, improved fouling and corrosion resistance, and higher selectivity leading to better performance in a broad range of emerging applications involving electrochemical conversion and storage of energy. Electrochemical membranes with higher ion selectivity, increased stability, and better uniformity are critical for many electrochemical applications where the lack of a suitable membrane has hampered efforts to evaluate the system-level performance of the electrochemical device being developed.

Membranes that act as ionically-conductive, electrically-insulating separators are found in virtually every electrochemical device for energy conversion and storage, including Li-ion rechargeable batteries, proton-exchange membrane fuel cells, redox flow batteries, solar fuel generators, and electrolyzers. Membranes for electrochemical applications are increasingly viewed as complex, multifunctional materials that define the limits of device operation and often the overall lifetime of the device. Understanding the synthesis of electrochemical membranes, their stability and compatibility with other material in the system, and their detailed mechanism for ion transport will enable new materials with superior, longer-life performance for a wide range of electrochemical applications involving energy conversion and storage. An opportunity exists to develop novel, multifunctional membranes with superior ionic conductivity and stability that enable new chemistries, new device architectures, higher energy densities, and/or wider operational windows for an electrochemical application and have demonstrated lifetimes sufficient to encourage subsequent commercialization. Accordingly, grant applications that propose optimization of membrane materials for established or near-commercial electrochemical energy storage applications such as Li-ion intercalation batteries, Li-S conversion cells, proton-exchange membrane fuel cells, or aqueous all-vanadium redox flow batteries do not fall within this topic and will not be considered. Electrochemical applications focused on material synthesis (e.g., electrodeposition) primarily to achieve material separation, concentration, or purification will also not be considered within this topic.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought in the following subtopics:

a. Ion-Selective Membranes for use with Non-Traditional Chemistries, Electrolytes, and Architectures in Advanced Electrical Energy Storage

Membranes providing physical separation between the electrodes of a lithium-ion rechargeable battery are usually highly optimized polymeric materials or composite materials that prevent physical contact between the electrodes, allow transport of the Li working ion between electrodes, and accommodate a liquid electrolyte in its porous structure.[1] Battery separators typically have the morphology of a microporous membrane or nonwoven film and are designed to provide sufficient ionic conductivity with a high lithium transference number and minimal contribution to cell impedance. While a variety of membranes have been commercialized for use as separators in Li-ion cells with traditional electrolytes[2] consisting of a lithium phosphate salt dissolved in glycol/carbonate organic solvent, accurate assessment of the potential for new battery chemistries, electrolytes, and/or architectures is often complicated when borrowing membrane separators developed for Li-ion intercalation batteries. For example, development of highly ion-selective membranes that resist swelling and fouling in organic solvents and are mechanically robust could greatly accelerate the development of non-aqueous flow batteries for grid storage applications.[3] Similarly, the need to design new electrolytes for magnesium (Mg) batteries[4] will require that membranes designed to selectively transport magnesium ions in novel electrolytes such as organoborates will be needed for further research and development of Mg-ion batteries. Novel electrolytes based on ionic liquids have been designed for Na-ion batteries,[5] and high-performance membranes designed to selectively transport Na ions in these kinds of electrolytes will help further development of Na-ion energy storage. In many cases, the new chemistry or cell architecture involves differences in operating voltage, working ions, interfacial environments, or charge transport requirements that necessitate new electrolyte-membrane combinations or the development of an appropriate solid-state electrolyte that also serves as the membrane. Thus, there exists a need for advanced ion-selective membranes to enable new energy storage chemistries and architectures, especially when the introduction of a non-traditional liquid electrolyte is required.

In general, ion-selective membranes developed through this subtopic should have properties and characteristics required for advancing electrochemical energy storage beyond Li-ion batteries for new battery chemistries, architectures, and/or operating conditions that often require non-traditional electrolytes, which may include the following:

- Membranes with high ion-selectivity derived by physical, chemical, or combined means to prevent unwanted crossover in non-aqueous redox flow battery architectures
- Membranes designed for use with novel liquid electrolytes including ionic liquids, deep eutectics, or highly concentrated salt-in-solvent (either aqueous or non-aqueous)
- Membranes with a ion transference number approaching unity for non-Li working ions and/or non-traditional anions (e.g., organoborates or aluminates)
- Membranes for use with highly conducting, novel electrolytes designed for energy storage under extreme environments (low or high temperature, ultrafast (>6C) charge/discharge rate, etc.)
- Membranes with resistance to fouling, swelling, and other degradation mechanisms in non-aqueous redox flow batteries
- Membranes that self-heal, self-repair, or otherwise mitigate unwanted degradation of performance while in operation
- Membranes designed to enable dense 3D- or otherwise nanostructured cell architectures where conformal solid-state membrane separators also function as a solid-state electrolyte

Proposals to develop solid-state electrolytes to serve as electrochemical membranes will be considered for advanced battery applications, specifically excluding Li-ion intercalation batteries using conventional-style planar electrodes and similar cell architectures involving plating/stripping of metal anodes.

The goal of any proposed work under this subtopic should be to demonstrate a battery membrane material with improved, selective ion transport (with or without a non-traditional electrolyte) sufficient to support further development of a novel battery chemistry, cell architecture, or operating condition. For greater impact, demonstration of improved performance should be coupled with a basic scientific understanding of the mechanism(s) for selective ion transport in and/or stability of the advanced membrane. Advances in multimodal characterizations and in modeling and simulation may be appropriate where necessary to extend this fundamental understanding across length and time scales. Process-structure-property relationships should be developed where possible to guide future development activities for new promising families of membrane materials. Demonstrations of the relevance of the underlying advancement should be conducted at the full cell level with quantification of relevant electrochemical and mechanical parameters including lifetime at expected operational conditions.

Questions – Contact: Craig Henderson, Craig.Henderson@science.doe.gov

b. Polymeric Membranes for Solar Fuels Generators

The development of scalable systems that drive the conversion of water and carbon dioxide to storable chemical fuels using sunlight would be substantially beneficial for energy production and storage. The assembly of complete photoelectrochemical solar fuels generators is currently limited by the availability of several key components, including membrane separators that exhibit the transport and stability properties required for this application. The membrane separators must function in an appropriate electrolyte to efficiently and selectively transport desired ions while rejecting the flow of gases and other chemical species involved in the anodic and cathodic half reactions. For example, solar-to-hydrogen generators that operate in an acidic aqueous electrolyte require a robust proton exchange membrane with high proton conductivity and extremely low permeability for hydrogen and oxygen gases. Commercially available ion-conducting polymer membranes that have been optimized for related applications, such as fuel cells or electrolyzers, have been adequate for some initial solar fuels prototypes. However, further progress is hindered by a lack of membranes with properties that are optimized for specific solar fuels generator conditions. For some potentially promising conditions, the properties of all available membranes are completely inadequate.

Solar fuels generators target the production of either hydrogen through proton reduction, or carbon-based fuels that result from carbon dioxide reduction. The source of electrons and protons for either fuel products is water oxidation. The flux of photons from the sun typically limits the overall device operating currents to a range of tens of mA/cm^2, which is much lower than other related membrane applications. On the other hand, a particularly critical requirement for solar fuels applications concerns preventing crossover of gases and other chemical species in operating conditions. Mechanical and chemical stability are also critical issues, including considerations relevant to long-term function with diurnal cycling, seasonal temperature variations, and exposure to a solar spectrum that includes ultraviolet light.

Novel polymeric membranes suitable for the following solar fuels operating conditions are solicited through this subtopic:

- Proton exchange membranes for solar-to-hydrogen generators must operate in acidic (pH 1) aqueous electrolytes. In comparison with commercially available products, the membrane must exhibit good proton conductivity and far superior behavior preventing crossover of hydrogen and oxygen gases in a device-relevant geometry and conditions. It must be mechanically robust and chemically stable. This target condition is considered to be a lower priority than others due to the availability of minimally viable alternatives.

- Anion exchange membranes for solar-to-hydrogen generators must operate in alkaline (pH 14) aqueous electrolytes. In comparison with commercially available products, the membrane must exhibit good hydroxide conductivity and superior behavior preventing crossover of hydrogen and oxygen gases in a device-relevant geometry and conditions. A primary target is achieving good chemical stability in the strongly alkaline environment.

- Proton or anion exchange membranes for solar fuels generators that target carbon-based fuels through carbon dioxide reduction. Operating conditions are expected to involve aqueous electrolytes at more moderate pH conditions or potentially non-aqueous electrolytes. In addition to blocking transport of oxygen and carbon dioxide gases, the membrane must prevent crossover of carbon dioxide reduction products. Electrochemical carbon dioxide reduction produces a multiplicity of chemical species, including gases (e.g. carbon monoxide, methane, and ethylene), alcohols (e.g. methanol and ethanol) and charged organic species (e.g. formate and acetate). Even if the permeability of individual species is sufficiently reduced, limiting transport of multicomponent mixtures presents additional challenges. Although moderate pH conditions are less challenging, chemical stability can still be limited by plasticization in the presence of carbon dioxide. In comparison with commercially available products, the targeted membranes must exhibit good ion conductivity and stability while greatly reducing the crossover of multicomponent gas and carbon dioxide product mixtures.

Questions – Contact: Chris Fecko, Christopher.Fecko@science.doe.gov

c. Other

In addition to the specific subtopics listed above, the Department invites grant applications that focus on ion-selective membranes for electrochemical applications involving energy conversion and storage consistent with the general topic description and which act as ionically-conductive, electrically-insulating separators.

Questions – Contact: Craig Henderson, Craig.Henderson@science.doe.gov, or Chris Fecko, Christopher.Fecko@science.doe.gov

References: Subtopic a:

1. Lee, H., Yanilmaz, M., Toprakci, O., Fu, K., A., and Zhang, X. (2014). *A Review and Recent Developments in Membrane Separators for Rechargeable Lithium-ion Batteries,* Energy & Environmental Science, Vol. 7, p. 113. http://pubs.rsc.org/-/content/getauthorversionpdf/C4EE01432D
2. Jow, T. R., Xu, K., Borodin, O., and Ue, M. (2014). *Electrolytes for Lithium and Lithium-Ion Batteries*, Series: Modern Aspects of Electrochemistry, Vol. 58, Springer Science+Business Media, New York, USA, 2014, 476 pages, ISBN: 978-1-4939-0301-6. https://b-ok.cc/book/2348186/8cdeb4
3. Escalante-García, I, Wainright, J.S., Thompson, L.T., Savinell, R.F. (2014). *Performance of a Non-Aqueous Vanadium Acetylacetonate Prototype Redox Flow Battery: Examination of Separators and Capacity Decay*, J. Electrochem. Soc. 2015 volume 162, issue 3, A363-A372 DOI: 10.1149/2.0471503jes. https://iopscience.iop.org/article/10.1149/2.0471503jes/pdf
4. Muldoon, J., Bucur, C.B., Gregory, T. (2017). *Fervent Hype behind Magnesium Batteries: An Open Call to Synthetic Chemists—Electrolytes and Cathodes Needed*, Angew. Chem. Int. Ed. 2017, 56, 12064. DOI: 10.1002/anie.201700673. https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.201700673
5. Forsyth, M., Yoon, H., Chen, F., Zhu, H., MacFarlane, D.R., Armand, M., and Howlett, P.C. (2016). *Novel Na+ Ion Diffusion Mechanism in Mixed Organic–Inorganic Ionic Liquid Electrolyte Leading to High Na+ Transference Number and Stable, High Rate Electrochemical Cycling of Sodium Cells*, The Journal of Physical Chemistry C 2016 120 (8), 4276-4286 DOI: 10.1021/acs.jpcc.5b11746. https://pubs.acs.org/doi/10.1021/acs.jpcc.5b11746

References: Subtopic b:

1. Xiang, C., Weber, A.Z., Ardo, S., Berger, A., Chen,Y., Coridan, R., Fountaine, K.T., Haussener, S., Hu, S., Liu, R., Lewis, N.S., Modestino, M.A., Shaner, M.M., Singh, M.R., Stevens, J.C., Sun, K. and Walczak, K. (2016). *Modeling, Simulation, and Implementation of Solar-Driven Water-Splitting Devices*, Angewandte Chemie International Edition, Vol. 55, Issue 42, p. 12974-12988. https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.201510463
2. Berger, A., Segalman, R.A., and Newman, J. (2014). *Material Requirements for Membrane Separators in a Water-Splitting Photoelectrochemical Cell*, Energy & Environmental Science, Vol. 7, Issue 4, p. 1468-1476. http://pubs.rsc.org/en/content/articlelanding/2014/ee/c3ee43807d/
3. Beckingham, B.S., Lynd, N.A., Miller, D.J. (2018). *Monitoring Multicomponent Transport using In Situ ATR FTIR Spectroscopy*, Journal of Membrane Science, Vol. 550, p. 348-356. https://www.sciencedirect.com/science/article/pii/S0376738817317386

22. DEVELOPMENT OF LIGHT SOURCE X-RAY DETECTOR AND ELECTRON SPECTROMETER SYSTEMS FOR ADVANCED MATERIALS RESEARCH TECHNIQUES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Materials researchers using synchrotron and x-ray free electron laser (XFEL) light sources at national laboratories have a need for advanced spectrometers and detectors for x-ray scattering experiments [1]. The light source staff and user community engage in detector research to push the state of the art of x-ray scattering and imaging techniques. They often advance a detector technology to a level approaching a prototype stage and use it for a particular experiment. They have thus created some type of working detector or detector components as part of an imaging, diffraction, or spectrometer system. In other instances, a detector has been developed to a working level and there are enhancements that can be made to the established base platform to improve its functionality. However, the scientists and laboratories are not equipped to fully develop the detector into a final product, nor to transfer their technology readily into a stand-alone system for use by other researchers at another beamline or facility.

This topic seeks to move specific technology developed in conjunction with established light source facilities and move the technology into a commercialized product. A successful Phase I proposal and project will involve incorporating the specific technology listed in one of the sub-topics, in a collaboration with an experienced materials science light source user capable of utilizing the high-rate detector capability in new or improved x-ray techniques applied to materials research experiments. The experiments must be capable of obtaining competitive beam time at a light source user facility.

A feasibility study of the technology and the necessary development path should be part of the Phase I project. The study should determine the range of x-ray light source experiments that will be enabled or improved by the new spectrometer or detector system and quantify the number of users and experiments that will benefit from the improved system.

As part of the development strategy, the Phase I work should determine and quantify the level of effort involved in critical development tasks which must be made in order to make the detector commercially viable. (An outline of anticipated tasks should be part of the Phase I proposal and firmly established by the Phase I project.)

The Phase I project should perform systems research that will effectively determine and plan a path forward to completion of a user-friendly, fully functional new or improved spectrometer or detector system. The project should identify the development bottlenecks and describe separate development sub-projects, with delineated tasks, to resolve each commercialization barrier. The project should perform a risk analysis and market assessment that will enable funding agencies and investors to have confidence in the R&D path that will lead to a successful detector product.

Phase II will involve continued systems and sub-systems development to bring a spectrometer and detector system to a completed demonstration stage ready for investment in the manufacturing process. Production research will be completed in Phase II that resolves manufacturing feasibility issues and provides the necessary software control and systems integration.

Development aspects that do not involve proprietary information from Phase I (or from previous SBIR Phase II instances), may be openly competed in subsequent Phase I/II subset projects to be folded into successful prime Phase II projects. Possible Phase III funding would provide for actual working systems delivered to research groups who would be early adopters of the new technology and demonstrate the new capabilities in scientific research projects at x-ray light source facilities.

Systems are sought which enable or improve (especially in their time-resolved versions) the following state-of-the-art materials research x-ray scattering techniques: coherent x-ray diffraction imaging, x-ray photon correlation spectroscopy, resonant x-ray scattering (with chemical, orbital, or magnetic sensitivity), resonant inelastic x-ray scattering, pair distribution function analysis, surface truncation rod analysis, coherent grazing incidence or standing wave surface scattering, and time-resolved ARPES.

Grant applications are sought in the following subtopics:

a. MM-PAD Detector and Spectrometer Systems for X-ray Scattering

As an example of the research scenario described above, the Gruner group at Cornell [2] has developed what they call the MM-PAD detector system to support x-ray experiments at light source facilities. The original research phase was developed with DOE-BES research support. The base system technology for MM-PAD detectors has wide-ranging capability, including adaptability to other x-ray sources and to electron diffraction and imaging systems. The base system has been commercialized into a version one system by Sydor Technologies through a previous SBIR award. The original SBIR topic anticipated the need for follow-on development as identified through the original SBIR effort. This particular sub-topic is an instance of advancing the Version One MM-PAD technology into a more advanced version. The Cornell research group associated with the CHESS light source is willing to collaborate with qualified and experienced small business entities. This sub-topic is an opportunity to compete for SBIR support for the next version of MM-PAD detectors.

This sub-topic seeks to identify and perform the necessary research and development to move MM-PAD detector technology into a higher frame rate capability (>10 kHz) than is readily available throughout the light source community. The combined Phase I and II project should focus on the development of the MM-PAD technology into a user-friendly and fully implemented product that can be purchased by researchers and light source facilities. Special emphasis should be given to imaging techniques that require high dynamic range and high frame rate capabilities, such as coherent diffraction x-ray imaging.

Questions – Contact: Lane Wilson, Lane.Wilson@science.doe.gov

b. Time-of-Flight Electron Energy Analyzer for Multi-modal Spectroscopy

Another instance of the DOE-BES-funded detector development scenario described in the main heading of this topic involves a collaboration between the Lawrence Berkeley National Laboratory Materials Science Division and the Advanced Light Source. They have developed a multimodal spectroscopy spin-, time-, and momentum/angle-resolved photoemission spectrometer [3,4] which demonstrated unprecedented energy resolution and capabilities [5,6] not possible with any commercial instrument. (Another example of a leading TOF analyzer includes a momentum microscope which has been used at FLASH FEL, where it achieved a total resolution of 130 meV for time-resolved ARPES [7].)

For x-ray-stimulated electron spectroscopy, Time-of-Fight (TOF)-based detection schemes have specific advantages:

- TOF analyzers add an additional dimension channel by effectively utilizing the unique timing structures of XFEL, SR, and VUV Lasers.
- Availability of high-timing-resolution detectors and knowledge of utilizing aberration correction allows developing TOF electron energy analyzers where the experiment's energy resolution is limited by the physics of the materials being studied (wave function transform-limited).
- SASE XFEL operations add time and spatial jitter to the ultra-fast pulsed beam profile. TOF systems allow shot-by-shot readout and improved resolution in the face of jitter. This includes noise reduction through live time gating and pulse counting.

This sub-topic seeks proposals to improve and commercialize the referenced LBNL TOF technology into a stand-alone user-friendly system for use by other materials science researchers at XFEL or synchrotron facilities.

The resulting instrument should be suitable for the following types of measurements with the stated capabilities:

1. Angle-resolved photoemission spectroscopy (ARPES) with high momentum (0.005 $Å^{-1}$) and high energy resolution mode (1meV).
2. Shot-by-shot readout capability for use at XFELs operating up to 1 MHz.
3. Spin detection of all three spin polarization components (both in plane and out of the plane of the sample) with energy resolution down to 10 meV in spin ARPES mode.
4. Spatial resolution capability for ARPES down to 10 nm by utilizing imaging and aberration correction similar to what is used by atomic resolution TEM.
5. Suitable for carrying out ultrafast ARPES (100 fs).
6. Allow multimodal spectroscopy using lock-in techniques.

Questions – Contact: Lane Wilson, Lane.Wilson@science.doe.gov

c. Other

Developments advancing the Cornell MM-PAD detector and LBNL TOF spectrometer systems consistent with the topic description, and which enable synchrotron and XFEL scattering and spectroscopy materials research experiments not included in subtopics a and b, but with technical specifications and capabilities beyond those described in those sub-topics.

Questions – Contact: Lane Wilson, Lane.Wilson@science.doe.gov

References:

1. U.S. Department of Energy. (2012). *Report of the Basic Energy Sciences Workshop on Neutron and X-ray Detectors*, Office of Science, p. 87. http://science.osti.gov/~/media/bes/pdf/reports/files/NXD_rpt_print.pdf
2. Hugh T. Philippa, Mark W. Tatea, Katherine S. Shanksa, Prafull Purohita, Sol M. Gruner. (2020). *High Dynamic Range CdTe Mixed-Mode Pixel Array Detector (MM-PAD) for Kilohertz Imaging of Hard X-rays*. Cornell University. https://arxiv.org/pdf/2004.03421.pdf
3. Jozwiak, C., et al. “A High-Efficiency Spin-Resolved Photoemission Spectrometer Combining Time-of-Flight Spectroscopy with Exchange-Scattering Polarimetry”, Review of Scientific Instruments. 81, 053904 (2010). https://aip.scitation.org/doi/10.1063/1.3427223
4. Gotlieb, K., et al. (2013). *Rapid High-Resolution Spin- and Angle-Resolved Photoemission Spectroscopy with Pulsed Laser Source and Time-of Flight Spectrometer*, Review Scientific Instruments 84, 093904 (2013). https://aip.scitation.org/doi/10.1063/1.4821247
5. Jozwiak, C., et al. (2013). *Photoelectron Spin Flipping and Texture Manipulation in a Topological Insulator*, Nature Phys. 7, 13140 (2013). https://www.nature.com/articles/nphys2572
6. Jozwiak, C., et al. (2016). Spin Polarized Surface Resonance Accompanying Topological Surface State Formation. Nature Comm. 7, 13140 (2016). https://www.nature.com/articles/ncomms13143
7. Kutnyakhov, D., et al. (2020). *Time- and Momentum-Resolved Photoemission Studies Using Time-of-Flight Momentum Microscopy at a Free-Electron Laser*, Review Scientific Instruments 91, 013109 (2020). https://aip.scitation.org/doi/10.1063/1.5118777

23. HIGH PERFORMANCE MATERIALS FOR NUCLEAR APPLICATION

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

To achieve energy security and clean energy objectives, the United States must develop and deploy clean, affordable, domestic energy sources as quickly as possible. Nuclear power will continue to be a key component of a portfolio of technologies that meets our energy goals. Nuclear Energy R&D activities are organized along four main R&D objectives that address challenges to expanding the use of nuclear power: (1) develop technologies and other solutions that can improve the reliability, sustain the safety, and extend the life of current reactors; (2) develop improvements in the affordability of new reactors to enable nuclear energy to help meet the Administration's energy security and clean energy goals; (3) develop sustainable nuclear fuel cycles; and (4) understanding and minimization of risks of nuclear proliferation and terrorism.

To support these objectives, the Department of Energy is seeking to advance engineering materials for service in nuclear reactors.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought in the following subtopics:

a. Bimetallic Structures for Liquid-Cooled, High Temperature Reactor Systems

Advanced high temperature nuclear reactor systems may utilize liquid coolants to optimize heat transfer, neutronics, safety, and compactness of the nuclear supply system. Examples of such systems in which corrosion is a particular challenge are liquid-salt cooled reactors (both those in which the fuel is fixed and those where it is dissolved in the coolant) and lead- (or lead-bismuth) cooled reactors. In each of these reactors, the structural components of the primary systems in contact with the reactor coolant must be adequately compatible with the materials of the reactor components. While materials permitted for construction of high-temperature components of nuclear reactors are specified in Section III Division 5 of the ASME Boiler and Pressure Vessel Code, they may not provide adequate corrosion resistance with respect to the liquid coolants described for long corrosion lifetimes.

One alternative is to develop bimetallic structures consisting of a corrosion-resistant surface layer (e.g. weld overlay cladding, roll bonding, etc.) and a structural substrate approved for use in ASME Code Sec III Div 5. Grant applications are sought to develop such a system with emphasis on fabrication methods (including for complex 3-D structures) and projected metallurgical stability over an extended component lifetime (> 20 years). Corrosion, aging, diffusion-related changes in composition, and thermo-mechanical loading should be considered. Note: Thin coatings will not be considered due to high likelihood of peeling, spalling, scratching, debonding, etc., over long component lifetimes.

Questions – Contact: Sue Lesica, sue.lesica@nuclear.energy.gov

b. Material Development and Compatibility for Molten Salt Thermodynamic Reference Electrodes

Molten salts, including fluoride, chloride, and other high-temperature variants, find application in advanced nuclear technologies such as molten salt reactors and fuel processing equipment. These salts offer a number of advantages as fuel salts, coolants, and electrolytes; however, the aggressive nature of these fluids dictates that the salt redox state must be monitored to control the salt chemistry and to avoid corrosion of structural materials. A thermodynamic reference electrode, or an electrode that has a known, stable potential, can facilitate knowledge of the redox state. Corrosion and instability of containment cells, ionic membranes, and/or frits of a thermodynamic reference electrode due to chemical incompatibility, stress due to thermal cycling, and exposure to high temperature often limits the operational lifetime of these devices. Grant applications are sought to develop robust thermodynamic reference electrodes capable of extended use in nuclear-relevant molten salts. The developed technology must present high accuracy, stability, and lifetime (e.g., 6 months). The structural integrity of the containment cells and membranes/frits are of utmost importance in order to permit the deployment of the technologies in systems that may include flowing conditions. Demonstration of the compatibility and stable construction of the reference electrode through long duration tests including chemically corrosive conditions and temperature cycling is essential. New ion-conducting materials, containment cell construction, and reference chemistries (including salts, liquid metals, and other chemistries) will be considered.

Questions – Contact: Christina Leggett, Christina.Leggett@nuclear.energy.gov

c. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Sue Lesica, sue.lesica@nuclear.energy.gov

References:

1. U.S. Department of Energy. (2010). *Nuclear Energy Research and Development Roadmap*, Report to Congress, p. 60. http://energy.gov/sites/prod/files/NuclearEnergy_Roadmap_Final.pdf
2. U.S. Department of Energy. (2020). *Fuel Cycle Technologies*, Office of Nuclear Energy, Science and Technology. http://www.energy.gov/ne/nuclear-reactor-technologies/fuel-cycle-technologies
3. U.S. Department of Energy. (2020). *Nuclear Reactor Technologies*, Office of Nuclear Energy, Science and Technology. http://www.energy.gov/ne/nuclear-reactor-technologies
4. Greene, S.R., Gehin, J. C., Holcomb, D. E., Carbajo, J. J., et al. (2010). *Pre-Conceptual Design of a Fluoride-Salt-Cooled Small Modular Advanced High Temperature Reactor (SmAHTR)*, Oak Ridge National Laboratory, Oak Ridge, TN., ORNL/TM-2010/199, p. 125. http://info.ornl.gov/sites/publications/files/Pub26178.pdf
5. U.S. Department of Energy. (2020). *Light Water Reactor Sustainability (LWRS) Program,* Office of Nuclear Energy, Science and Technology. http://www.energy.gov/ne/nuclear-reactor-technologies/light-water-reactor-sustainability-lwrs-program

24. ADVANCED SUBSURFACE ENERGY TECHNOLOGIES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Subsurface sources constitute the Nation's primary source of energy (providing more than 80 percent of total U.S. energy needs today), and they are also critical to the Nation's secure energy future. Next-generation advances in subsurface technologies will enable access to more than 100 gigawatt-electric (GWe) of clean, renewable geothermal energy, as well as safer development of domestic natural gas supplies. The subsurface provides hundreds of years of safe storage capacity for carbon dioxide (CO_2) and opportunities for environmentally responsible management/disposal of hazardous materials and other energy waste streams. The subsurface can also serve as a reservoir for energy storage for power produced from intermittent generation sources, such as wind and solar. Increasing domestic hydrocarbon resource recovery enhances national security and fuels economic growth. Thus, understanding and effectively harnessing subsurface resources while mitigating impacts of their development and use are critical pieces of the Nation's energy strategy moving forward.

The Department of Energy's (DOE) Office of Basic Energy Sciences (BES) teams with the Geothermal Technologies Office (GTO) and Office of Fossil Energy (FE) in order to advance the state of the art for continued development of subsurface energy sources in a safe and sustainable matter through the focus areas and subtopics listed below.

Focus Area 1: Improvement of Subsurface Signals via Advanced Computational Methods

The goal of the first topic is to advance the state of the art in subsurface signals indicative of how stress, geologic features, fluids, and natural resources are distributed within the subsurface. Of particular interest is the development of advanced computational methods to describe and predict parameters including but not limited to temperature, fluid flow, mechanical stress, and chemical interactions within heterogeneous, time-dependent geologic systems. Computational methods may include software or algorithm development, data science/data-driven analysis, machine learning methods, quantum information science and quantum sensing, etc.

Responsive applications to this topic could include (but are not limited to) advances in:

- Imaging subsurface stress, incorporating rheological properties of rocks and effects of mechanical discontinuities to improve our understanding of the initial and evolving state of stress;
- Measuring geochemical characteristics and processes to include imaging subsurface fluid flow;
- Modeling how mechanical and geochemical perturbations to subsurface rock systems are coupled through fluid and mineral interactions; and
- Understanding how heterogeneous time-dependent geologic systems can improve models of hydraulic fracturing and its environmental impacts.

Grant applications are sought in the following subtopics:

a. Advanced Computing: Geothermal

Applications of interest under this subtopic should focus on the challenges related to improving subsurface signals specific to geothermal energy development in conditions with elevated temperatures (> 200°C) and crystalline lithology. Specifically of interest are advanced computational methods that improve the understanding of how fractures within geothermal reservoirs evolve over time, both naturally and under the influence of operations such as well stimulation, maintenance, or flexible operating conditions. This can include improving analysis and visualization techniques for application to magnetotelluric (MT), gravity, magnetic, or other subsurface geophysical data. Proposed projects could propose analysis of new data sets, existing data sets within the Geothermal Data Repository (GDR) at https://gdr.openei.org/, or other existing data sets. DOE is seeking as much emphasis on open-source data and/or methods as possible.

Questions – Contact: William Vandermeer, william.vandermeer@ee.doe.gov

Focus Area 2: Improving Ultimate Recovery from Unconventional (Tight) Oil and Gas Reservoirs

The Oil and Gas Program's Unconventional Oil and Natural Gas (UOG) R&D Technology Area supports research to advance the economic viability and environmentally prudent development of domestic UOG resources. These efforts include (1) improving understanding of the processes involved in UOG resource development; (2) advancing technologies and engineering practices to ensure these resources are developed efficiently; and (3) increasing the supply of U.S. oil and natural gas resources to enhance national energy security.

This Area of Interest seeks applications which propose research to develop tools, methods, and/or technologies that 1) improve the ultimate recovery of UOG resources and 2) improve the understanding and economic viability of emerging UOG plays. Applications under this Area of Interest are encouraged to consider data needs with respect to big data and machine learning concepts. As such, technologies developed under this Area of Interest may address how the proposed technology fills critical data gaps needed for advanced data analytics.

b. Tight Reservoir Recovery: Oil and Gas

Grant applications are sought in the following subtopics:

- Innovative and breakthrough technologies for improved subsurface characterization, visualization, and diagnostics. This may include approaches and/or technologies to inform hydraulic fracture stimulation treatment effectiveness, including characterization of fracture development and propagation, fluid and proppant emplacement, reservoir response, and stimulated rock volume. These approaches could include fracture diagnostic tools (for direct measurement of fracture dimensions, orientation and proppant distribution) as well as improved methods for subsurface imaging of stimulated reservoir volume throughout the lifecycle of a well.
- Cost-effective tools for real-time monitoring of well performance data not routinely collected (e.g., downhole pressure, geochemistry, etc.) that would fill critical data gaps in big data analytics and machine learning applications in order to inform decision making and improve the ultimate recovery of UOG.
- New resource development approaches that can enable or accelerate dramatic improvements in drainage volume, per-well resource recovery efficiency, and ultimate field resource recovery. These approaches may include the development of new tools or methods for identifying the optimal placement of fracturing stages, improved technologies for the optimization of stimulation treatment design, and improved methods for effective refracturing.

Questions – Contact: William Fincham william.fincham@netl.doe.gov

Focus Area 3: Sensors to Provide New Measurements in Carbon Storage Complexes to Improve Plume and Leak Detection and to Document Plume Containment

Accurate monitoring at a carbon storage site is necessary to track the movement of CO_2 and document permanence for geologic storage. Therefore, advanced monitoring technologies, as well as supporting protocols, are needed to decrease the cost and uncertainty in measurements and to satisfy requirements for tracking the fate of subsurface CO_2. These can help to confirm that CO_2 stays in the target reservoir, to assist in optimizing storage operations, as well as to find leaks and assist with remediation.

An initial focus of Carbon Storage R&D activities has been to adapt technologies and methods to the specific requirements of CO_2 injection, storage, and long-term monitoring. Some technologies, such as well logging and reflection seismic imaging, have reached a highly sophisticated level as a result of decades of use and development in the petroleum industry. These subsurface monitoring technologies are being used to track CO_2 migration and pressure changes in the reservoir. Improved techniques are being developed to augment seismic methods for improved spatial and temporal mapping of the CO_2 plume. Other technologies are currently in the development phase (e.g., downhole pH sensing, strain sensing) to directly observe parameters associated with CO_2 injection and CO_2 plume location.

Grant applications are sought in the following subtopics:

c. Plume Detection: Carbon Storage

Grant applications are sought to develop new or adapt existing sensors for subsurface parameters that have not previously been measured but could be used to decrease uncertainty in plume location, identify leaks, or document containment of CO_2 in the reservoir. Capabilities to detect and measure new parameters/properties of the subsurface that would help improve the ability to track and detect plume location, pressure front, and leakage conditions are sought. The goal is to be able to combine these sensor capabilities with those currently available or under development to improve confidence that the geophysical and geochemical conditions are understood and to document those things required by Underground Injection Control regulations and Class VI well permits.

Questions – Contact: Kyle Smith, kyle.smith@netl.doe.gov

Focus Area 4: Other Topics Related to Advanced Computing, Wellbore Integrity, Tight Reservoir Recovery, or Plume Detection

d. Other

In addition to the specific subtopics listed above, the Department solicits applications in other areas that fall within the specific scope of the topic description above, but is either outside of the scope of any of the subtopics or span multiple subtopic scopes. This subtopic also encompasses innovations in computational methods that support advances in fundamental geosciences or foundational aspects of wellbore integrity.

Questions – Contact: James Rustad, James.Rustad@science.doe.gov

References:

1. U.S. Department of Energy Office of Science. (2015). *Controlling Subsurface Fractures and Fluid Flow: A Basic Research Agenda*, DOE Roundtable Report, p. 24. https://www.energy.gov/sites/prod/files/2016/01/f28/BES%20Report%20Controlling%20Subsurface%20Fractures%20and%20Fluid%20Flow.pdf

References: Subtopic c:

1. U.S. Department of Energy. (2020). *Unconventional Resources,* National Energy Technology Laboratory. https://netl.doe.gov/unconventional

References: Subtopic d:

1. U.S. Department of Energy. (2020). *Storage Complex Efficiency and Security,* National Energy Technology Laboratory. https://www.netl.doe.gov/coal/carbon-storage/advanced-storage-r-d/storage-complex-efficiency-and-security

25. ADVANCED FOSSIL ENERGY TECHNOLOGY RESEARCH

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

For the foreseeable future, the energy needed to sustain economic growth will continue to come largely from hydrocarbon fuels. Advanced Fossil Energy technologies must allow the Nation to use its secure indigenous fossil energy resources more wisely, cleanly, and efficiently. This topic addresses grant applications for the development of innovative, cost-effective technologies for improving the efficiency and environmental performance of advanced industrial and utility fossil energy power generation and natural gas recovery systems.

The only areas considered in this opportunity announcement include research and technology issues and opportunities in advanced technology development of oxygen separation from air for small, modular systems, supercritical fluid extraction using CO_2, coal-derived graphene, and ultrafast laser processing of sapphire optical fiber. In addition, refer to the FE related collaborative topic: Improvement of Subsurface Signals via Advanced Computational Methods and Assessment of Legacy Wellbore Integrity. This topic serves as a bridge between basic science and the fabrication and testing of new technologies. Small scale applications, such as residential, commercial and transportation will not be considered. Applications determined to be outside the mission or not mutually beneficial to the Fossil Energy and Basic Energy Sciences programs will not be considered.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought in the following subtopics:

a. Technology Development of High Purity Oxygen Separation from Air

The Gasification Systems Program, conducted under the U.S. Department of Energy's Office of Fossil Energy (FE), is developing innovative, flexible, and small-scale, modular systems for converting diverse types of U.S. domestic coal into clean syngas to enable the production of affordable, reliable, and low-cost electricity, hydrogen, high-value chemicals, and liquid fuels, and a market-flexible slate of by-products with greatly reduced greenhouse gas emissions [1,2]. The small-scale modular systems offer distinct advantages against big commercial scales, expediting technology development, cutting capital investment and operating costs, improving availability, and offering flexibility in meeting location-specific needs.

Since gasification is the partial oxidation of combustible materials and operates in an oxygen-lean environment, oxygen can be provided by either air or high-purity oxygen produced by an oxygen separation unit from air. Air-blown gasifiers avoid the large capital cost of an oxygen separation from air but produce a much lower calorific value syngas than oxygen-blown gasifiers due to nitrogen in air. Air-blown gasifiers also have a lot bigger systems than oxygen-blown gasifiers due to high volume of nitrogen in air. Because of the dilution effect of the nitrogen, the partial pressure of CO_2 in air-blown gasifier syngas will be one-third of that from an oxygen-blown gasifier. In addition, air-blown gasifiers have a negative impact on CO_2 capture. This increases the cost and decreases the effectiveness of the CO_2 removal equipment. Current commercially available cryogenic distillation-based oxygen separation from air is costly and energy-intensive. This system cannot be scaled down cost-effectively because of huge balance of plant costs. An innovative technology development of oxygen separation from air for small-scale, modular gasification systems is encouraged to increase deployment opportunities.

Grant applications are sought for research and development to have high-purity oxygen (above 95%) from air that can show significant capital cost reduction compared with a commercial/conventional cryogenic distillation-based oxygen separation from air, in application of smaller, modular systems. Areas of interest are limited to any technology whose operation temperature should be lower than 300 °C (572 °F). However, electrochemical membrane and magnetic technologies will not be accepted.

The applicant must provide how their proposed technology would reduce capital cost and improve performance to obtain at least 95% oxygen purity from air. Phase I effort should demonstrate the feasibility of the concept in a lab-scale testing. Phase II effort should demonstrate the oxygen generation of a pilot scale.

Questions – Contact: Jai-woh Kim, jai-woh.kim@hq.doe.gov

References:

1. U.S. Department of Energy. (2020). Gasification Systems, Office of Fossil Energy. https://www.energy.gov/fe/science-innovation/clean-coal-research/gasification
2. U.S. Department of Energy. (2020). Gasification – Yesterday, Today, and Tomorrow, National Energy Technology Laboratory. https://netl.doe.gov/coal/gasification/background

26. ADVANCED FOSSIL ENERGY CROSSCUTTING RESEARCH

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The ***Crosscutting Research Portfolio of programs*** is unique in its ability to see and foster applications of a given enabling technology across multiple fossil energy systems and operational platforms and to efficiently leverage resources to accomplish the strategic goals, objectives, and performance measures common to several fossil research areas. Often, processes and materials that advance one technology platform may well have application in another with little to no modification.

Crosscutting Research leverages the latest technology trends such as artificial intelligence, advanced manufacturing, and high-performance computing. These advanced capabilities accelerate progress toward addressing the challenges facing today's fossil power plants and realize the next generation of fossil energy technology platforms. The technologies developed improve power plant efficiency and reduce operating and maintenance costs while maintaining reliable and resilient energy infrastructure.

The programs also accelerate the development of science and engineering-based solutions across a range of technology maturities from concept to market through the creation of strategic partnerships with stakeholders who share our interest in maximizing the value of our nation's fossil resources. In this context, the SBIR program is a key component to developing and commercializing technology to realize program goals and public benefit.

Grant applications are sought in the following subtopics:

a. Low-Cost Energy Storage Materials and Technologies for Fossil-Integrated Systems

As part of FE's new Advanced Energy Storage Program, The National Energy Technology Laboratory (NETL) invests in energy storage technologies ranging from innovative concepts with game-changing potential to components and integrated systems. The Program emphasizes the integration of storage with fossil assets such as natural gas combined cycles, coal plants, and others with a focus on ultimately commercializing and widely deploying technology to benefit the nation.

Benefits for co-location include improved asset utilization, grid reliability, and enhanced environmental performance. For fossil generating units, energy storage increases power plant lifetimes by reducing component stress and promotes efficient plant operations by decreasing the need to load follow. Current energy storage technologies exist but miss the mark. For integration with fossil generation, long-duration energy storage technologies (greater than 4 hours) provide the needed capacity to enable slower ramping and reduced turndowns as well as a host of other benefits for efficient operations. Longer duration is best, but cost is also a key metric to keep in mind for generating units with limited enhancement budgets. Integration between energy storage and fossil generation provides the dynamic feedback loop necessary to charge or discharge power based on the needs of the grid through control systems.

Proposals are sought to develop or enhance long-duration energy storage technologies from materials or processes which are low-cost. Materials or systems with a well-established domestic supply chain are particularly of interest. Technologies sought include, but are not limited to, thermal, chemical, thermo-chemical, and phase change materials; and systems built around these materials. Goals include low overall capital cost, long duration (in excess of 4 hours), and ease of integration with fossil assets. Successful projects will address key barriers to energy storage integration with fossil assets. By Phase II, the projects must have demonstrated the novel technology as a packaged energy storage system; assessed performance, cost, and benefits; and designed plans for integration with at least one fossil asset class. An industrial end-user partner is highly recommended.

Questions – Contact: Jason Hissam, jason.hissam@netl.doe.gov

b. Supply Chain Enhancements for Fossil Energy Alloy Production

Supply chain innovation is critical to the development of next-generation fossil energy (FE) power generation technologies, and in improving the performance and reliability of existing FE power plants.

Improved methods to manufacture alloys used for large steam cycle components in pulverized coal and natural gas combined-cycle power plants are sought. Gas turbine applications are not of interest.

Nickel superalloys offer improved cycle performance with enhanced flexibility; however, costs remain a barrier to widespread implementation. For these superalloys, the goal of this topic is improved material yield, improved material quality, and/or decreased component cost.

For existing plants, ferritic and austenitic stainless steels are of central interest. They suffer under cyclic loading conditions, particularly at joints and dissimilar metal welds. Failure mechanisms include thermal fatigue, corrosion fatigue, creep, corrosion, oxidation, and erosion – with relative predominance dependent on a host of material- and system-specific factors. For existing plants, the goal of this topic is to develop a material, model, or repair technology that increases plant life and reliability and decreases Operations and Maintenance (O&M) costs.

Applications should address key barriers to producing a robust domestic supply chain. This work should take the form of supply chain assessment, market analysis, industrial manufacturing trials, end-user value proposition demonstration, and technoeconomic analysis. Industrial supply chain partners are required. Applicants must specify the manufacturing process or component of interest, relevant specification for material performance (microstructure, mechanical properties, etc.), proposed manufacturing approach, and summary of critical fabrication issues. Suggested topics include but are not limited to the following:

1. **Ingot Cost Reduction**: Reduce the cost of producing basic ingots from their alloying elements without loss of product quality (chemical purity, microstructure, and physical properties (mechanical strength)).
2. **Surface Technologies**: Materials and processes for enhancing the resistance of base alloy materials to environmental constituents.
3. **High-Throughput, Large-scale Advanced Manufacturing**: Feedstock materials and process improvements suitable for fabricating large components with high throughput rates, consistent with the needs of fossil power plant applications.

Questions – Contact: Richard Dunst, richard.dunst@netl.doe.gov

c. Dewatering Coal and Other Porous Materials using Novel Techniques

Moisture in coal has a very large negative impact on boiler efficiency and the power plant heat rate. For instance, on a 600MW coal-fired unit that uses lignite, a fuel that comes with high moisture content, the reduction in moisture from 38% to 29% improves the Higher Heating Value (HHV) of the coal by 14% while improving coal flow rates, reducing flue gas flow rate and lowering operating and maintenance costs while allowing the plant to operate more efficiently[1].

The Department of Energy Fossil Energy Office is seeking novel proposals that help dewater such coals that come with high moisture, using benign solvents that are easily recoverable, environmentally friendly, and can be recyclable. Energy efficiencies would also be realized if the use of such benign solvents can convert part of the bound water to free water and also if the degree of free water removal could be increased. The conversion of bound to free water has been demonstrated. For example, freeze-thawing various sludges increases the free water content, which leads to increased cake solids.[2-4] Surfactants can also aid in the bound-to-free water conversion of wastewater sludge.[5]

Such crosscutting applications are given as examples where novel techniques, other than thermal and mechanical dewatering, could yield economic and environmentally friendly techniques to dewater porous materials such as coal.

Technologies that increase the energy efficiency of dewatering porous matrices are of interest. These include new methods for higher bound water conversion, improved techniques for mechanical water expression, and combinations thereof. The overall goal is to develop sustainable energy-efficient dewatering technologies.

The Phase I proposal would then consist of trying out various solvents and/or surfactants (positive, negative, neutral, etc.) and then removing the water in an efficient way. A pilot would be built in Phase II.

The Phase project should result in the following information being included in the Phase I final report

a. Feasibility study of various types of coal processing with the optimum conditions for operation
b. Quantification of value addition using the novel technique vs. the traditional thermal-mechanical route
c. Show a viable path to building and demonstrating a pilot if the project moves to Phase II

Questions – Contact: Bhima Sastri, bhima.sastri@hq.doe.gov

References: Subtopic a:

1. U.S. Department of Energy. (2020). *Energy Storage For Fossil Fuel Energy Systems*, 2020. https://netl.doe.gov/coal/crosscutting/energy-storage

2. U.S. Department of Energy. (2020). *Crosscutting Research Program*, Energy Storage Overview hosted by the United States Energy Association Webinar, 2020 https://netl.doe.gov/crosscutting/resources
3. U.S. Department of Energy. (2020). *2nd Thermal-Mechanical-Chemical Energy Storage Workshop Agenda*, hosted by the Elliot Group, 2019. https://www.netl.doe.gov/coal/crosscutting/energy-storage/2020-TMCES-Workshop
4. U.S. Department of Energy. (2020). *DOE Energy Storage Global Database*, 2020. https://www.sandia.gov/ess-ssl/global-energy-storage-database/

References: Subtopic b:

1. National Energy Technology Laboratory. (2018). *DOE Crosscutting Workshop on Developing a Domestic Supply Chain for High Temperature Steam Cycles*, 2018 https://edx.netl.doe.gov/dataset/doe-crosscutting-workshop-on-developing-a-domestic-supply-chain-for-high-temperature-steam-cycles
2. deBarbadillo J., et al. (2016). *Alloy 740H – Development of Fittings Capability for AUSC Applications*, Presented at the 8th International Conference on Advances in Materials Technology for Power Plants, Albufeira, Portugal, October 2016. https://s3.amazonaws.com/v3-app_crowdc/assets/d/da/da77d8e83c0796b6/File_4_FINAL_-_deBarbadillo_-_Alloy_740H_%E2%80%93_Development_of_Fittings_Capability_for_AUSC_Applications.original.1473277539.pdf
3. White, B. (2019). *Crosscutting Research Program Overview*, Proceedings from 2019 Annual Project Review Meeting. https://www.netl.doe.gov/sites/default/files/2019-05/2019_Annual_Reports/1%20NETL%20DOE%20Crosscutting_Annual%20Review%20Meeting_2019_Final%20Draft.pdf
4. Smith, D. (2017). *Boiler Maintenance and Upgrades – Attacking Tube Failures*, Power Engineering. Issue 2 and Volume 108. https://www.power-eng.com/2004/02/01/boiler-maintenance-and-upgrades-mdash-attacking-tube-failures/
5. Pfeuffer, S. (2009). *Update: Benchmarking Boiler Tube Failures*, Power. https://www.powermag.com/update-benchmarking-boiler-tube-failures/

References: Subtopic c:

1. World Coal. (2014). *Drying Lignite – How and Why?.* https://www.worldcoal.com/power/01102014/iea-ccc-report-on-drying-lignite-1381/
2. Hu, Y., and Wang, Y. (2017). *Study on the Dewatering Process for Water Treatment Residuals: Applicability of Freezing–Thawing, Compression, and Electro-Osmotic Treatment*, Drying Technol., 35, 1450-1459, 2017. https://www.tandfonline.com/doi/full/10.1080/07373937.2016.1253021
3. Parker, P. J., Collins, A. G., and Dempsey, J. P. (1998). *Alum Residual Floc Interactions with an Advancing Ice/Water Interface*, J. Environ, Eng. 124(3): 249-253, 1998. https://ascelibrary.org/doi/10.1061/%28ASCE%290733-9372%281998%29124%3A3%28249%29
4. Jean, D. S., Lee, D. J., and Chang, C. Y. (2001). *Direct Sludge Freezing Using Dry Ice*, Adv. Environ. Res., 5, 145-150, 2001. https://www.sciencedirect.com/science/article/abs/pii/S1093019100000526
5. Wu, C. C., Huang, C., and Lee, D. J. (1997). *Effects of Polymer Dosage on Alum Sludge Dewatering Characteristics and Physical Properties*, Colloids and Surfaces A, 122, 89-96, 1997. https://www.sciencedirect.com/science/article/abs/pii/S092777579700006X

27. RARE EARTH ELEMENTS

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

America's critical materials and manufacturing supply chains for production of commodity and national defense products no longer reside on our domestic shores, but are controlled predominantly by off-shore markets. Recent efforts at DOE-NETL under the *Feasibility of Recovering Rare Earth Elements (REE)* program have successfully demonstrated the very first step for the utilization of coal and coal-based resources to produce critical elements needed for our commodity and defense industries. This achievement was marked by demonstrating the technical feasibility and processing capability to extract and separate REEs at low 300ppm concentrations contained in our coal-based resources, and to recover these materials as mixed rare earth oxides or salts (REOs/RESs) at levels of 96-98% purity (960,000-980,000ppm) in three, first-of-a-kind, domestic, small pilot-scale facilities.

As individual high-purity rare earth oxides, phosphates, or fluorides, these materials are often used as automotive pollution-abatement catalysts (oxides), fluorescent lamps (phosphates), and electrowinning electrolytes (fluorides). Approximately 40% of mined rare earth production is reduced to metals and alloys, including most of neodymium (Nd), samarium (Sm), and dysprosium (Dy), for applications such as neodymium metal for Nd-Fe-B permanent magnets, samarium metal for Sm-Co permanent magnets, and lanthanum (La), cerium (Ce), praseodymium (Pr), and neodymium (Nd) for rechargeable battery electrodes.

Grant applications are sought in the following subtopics:

a. Advanced Technology Development for Production of Rare Earth Metals

The objective of this Phase I subtopic is to continue to expand technology development beyond production of salable REOs and/or RESs from coal-based resources, ultimately producing individually separated rare earth metals (REMs) for use in intermediate and/or end product commercial and/or defense equipment through development of advanced processing metalization concepts.

The Phase I efforts shall include:

- Development of advanced, novel, rare earth oxide/salt-to-rare earth metal (REO/RES-REM) reduction techniques.
- Production and analytic characterization of small quantities of individually separated, high-purity REMs resulting from advanced, novel, REO-REM reduction processes.
- Preliminary techno-economic assessment (TEA).
- Preliminary design for process scale-up.

Questions – Contact: Mark Render, mark.render@netl.doe.gov

b. Transformational Technology Development for the Separation and Recovery of Rare Earth Elements (REE) and Critical Minerals (CM) from Coal-Based Resources

The objective of this Phase I subtopic is the development of advanced, economic, transformational separation and recovery processes for the generation of mixed and/or individually separated, high-purity REEs and CMs from coal and coal-based resources.

The Phase I efforts shall include:

- Identify and select coal-based resource(s) (e.g., coal, coal refuse, power generation ash, clay/shale over/under-burden materials, acid mine drainage fluids and/or sludges, etc.). Acquire field sample materials.
- Identify rare earth element(s) (e.g., Sc, Nd, Pr, etc.) and critical mineral(s) (e.g., Li, Co, Mn, Al, etc.), and their respective phase(s) (e.g., elemental, oxide, salt, etc.) that will be recovered through advanced transformational processing.

- Demonstrate proof-of-concept lab/small bench-scale processing capability to produce the above identified REEs and CMs.
- Address economic feasibility for production of REEs and CMs from coal-based resources.
- Address co-product production to support process economic viability.

Questions – Contact: Mark Render, mark.render@netl.doe.gov

References: Subtopic a:

1. U.S. Department of Energy. (2020). *Feasibility of Recovering Rare Earth Elements,* National Energy Technology Laboratory._ https://netl.doe.gov/coal/rare-earth-elements
2. Alvin, M. A. (2019). *Meeting USA's Critical Minerals Need*, Global Critical Minerals and Mining 2019 Summit, Perth, Australia, November 21, 2019. http://claridenglobal.com/conference/criticalminerals-miningsummit-au/
3. Alvin, M. A. (2020). *US-DOE Approach to Increasing Strategies for Critical Minerals Sourcing*, Argus US Specialty Metals. https://www.argusmedia.com/en/conferences-events-listing/us-specialty-metals

References: Subtopic b:

1. U.S. Department of Energy. (2020). *Feasibility of Recovering Rare Earth Elements,* National Energy Technology Laboratory. https://netl.doe.gov/coal/rare-earth-elements
2. Alvin, M. A. (2019). *Meeting USA's Critical Minerals Need*, Global Critical Minerals and Mining 2019 Summit, Perth, Australia, November 21, 2019. http://claridenglobal.com/conference/criticalminerals-miningsummit-au/
3. Alvin, M. A. (2020). *US-DOE Approach to Increasing Strategies for Critical Minerals Sourcing*, Argus US Specialty Metals. https://www.argusmedia.com/en/conferences-events-listing/us-specialty-metals

28. TECHNOLOGY TRANSFER OPPORTUNITIES: BASIC ENERGY SCIENCES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Applicants to TECHNOLOGY TRANSFER OPPORTUNITIES (TTO) should review the section describing these opportunities on page 8 of this document prior to submitting applications.

Grant applications are sought in the following subtopics:

a. Technology Transfer Opportunity: Torsionally Flexible Bellows

Argonne's researchers developed a bellows that allows for rotational motion while still maintaining vacuum integrity. The designed bellows consists of thin-walled material that flexes within its elastic limit when twisted, thanks to the ability to flex through thin convolutions angled at 45 degrees from the horizontal that run the length of the bellows. These thin convolutions act as flexures and become smaller or larger when the bellows is rotated in a counterclockwise or clockwise direction respectively, requiring only a minimal amount of torque to rotate. The ability to rotate about the central axis while maintaining vacuum integrity will allow the coupling of misaligned vacuum components as well as the ability to rotate in-vacuum components from their respective vacuum chambers.

ANL is looking for the industrial partner to provide this low-cost and added rotational flexibility to users requiring UHV conditions. The invention can benefit "clean" production environments including semiconductor manufacturing, synchrotrons or other research systems, precision optics, or other general vacuum or pressurized systems.

Licensing Information:
Argonne National Laboratory
Contact: Eric Tyo, (etyo@anl.gov, (630) 252-4924)
ANL Technology ID: ANL-IN-18-027
Patent Status: US Patent Pending 16/286,193

Technology Available for Licensing Link: https://www.anl.gov/tcp/torsionally-flexible-attachment-system-and-method-anlin18027

Questions – Contact: Eliane Lessner, eliane.lessner@science.doe.gov

b. Technology Transfer Opportunity: Bio-based Base-oils from Fatty Acids and Biomass

University of Delaware researchers have developed a method for the synthesis of bio-based lubricant base-oils from renewable feedstock. This method creates high-carbon, branched alkanes from fatty acids and furans, which are biomass platform chemicals. The renewable lubricant product is composed of a unique composition of matter that can be tuned to suit lower-temperature applications. It has a structure similar to synthetic poly-alpha-olefins. The resulting bio-lubricant base oil is produced in high yield and selectivity via an energy-efficient pathway. The technology enables production of high-carbon-number bioproducts for lubricant and cosmetic applications from low-carbon-number biorefinery feedstock. Benefits include biodegradability, low toxicity, appropriate viscosity, and high yield/selectivity. The University of Delaware is looking for an industrial partner to help develop this exciting new technology.

Licensing Information:
University of Delaware
Contact: Will Johnson, (techtransfer@udel.edu)
Univ. of Delaware ID: UD19-11
Patent Status: Patent application 62/772,672; PCT/US2019/063325

Website: http://innovation.oeip.udel.edu/technologies/ud19-11_bio-based-base-oils-from-fatty-acids-and-biomass

Questions – Contact: Andrew Schwartz, andrew.schwartz@science.doe.gov

PROGRAM AREA OVERVIEW: OFFICE OF BIOLOGICAL AND ENVIRONMENTAL RESEARCH

The mission of the Biological and Environmental Research (BER) program 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. The program seeks to understand the biological, biogeochemical, and physical principles needed to fundamentally understand and be able to predict processes occurring at the molecular and genomics-controlled smallest scales to environmental and ecological processes at the scale of planet Earth. Starting with the genetic information encoded in organisms' genomes, BER research seeks to discover the principles that guide the translation of the genetic code into the functional proteins and metabolic and regulatory networks underlying the systems biology of plants and microbes as they respond to and modify their environments. Gaining a predictive understanding of biological processes will enable design and reengineering of microbes and plants for improved energy resilience and sustainability, including improved biofuels and bioproducts, improved carbon storage capabilities, and controlled biological transformation of materials such as nutrients and contaminants in the environment. BER research also advances the fundamental understanding of dynamic, physical, and biogeochemical processes required to systematically develop process and Earth system models that integrate across the atmosphere, land surfaces, oceans, sea ice, coasts, terrestrial ecosystems, watersheds and subsurface required for predictive tools and approaches responsive to future energy and resource needs.

BER has interests in the following areas:

(1) Biological Systems Science subprogram carries out basic research to underpin development of sustainable bioenergy production and to gain a predictive understanding of carbon, nutrient, and metal transformation in the environment in support of DOE's energy and environmental missions. Genomic Science research is multifaceted in scope and includes a complementary set of activities in basic biological research focused on DOE's efforts in bioenergy development. The portfolio includes the DOE Bioenergy Research Centers (BRCs), team-oriented research within the DOE National Laboratories and focused efforts in plant feedstocks genomics, biosystems design, sustainability research, environmental microbiology, computational bioscience, and microbiome research. These activities are supported by a bioimaging technology development program and user facilities and capabilities such as the Joint Genome Institute (JGI), a primary source for genome sequencing and interpretation, the DOE Systems Biology Knowledgebase (KBase) for advanced computational analyses of "omic" data and, instrumentation at the DOE synchrotron light and neutron sources for structural biology. The research is geared towards providing a scientific basis for producing cost effective advanced biofuels and chemicals from sustainable biomass resources.

(2) Earth and Environmental Systems Sciences Division (EESSD) activities include fundamental science and research capabilities that enable major scientific developments in Earth system-relevant atmospheric and ecosystem process and modeling research in support of DOE's mission goals for transformative science for energy and national security. This includes research on components such as clouds, aerosols, terrestrial ecology, watersheds, terrestrial-aquatic interfaces, as well as modeling of component interdependencies under a variety of forcing conditions, interdependence of climate and ecosystem variabilities, vulnerability and resilience of the full suite of energy and related infrastructures to extreme events, and uncertainty quantification. It also supports terrestrial ecosystem and subsurface biogeochemical research that advances fundamental understanding of coupled physical, chemical, and biological processes controlling energy byproducts in the environment. The subprogram supports three primary research activities, two national scientific user facilities, and a data activity. The two national scientific user facilities are the Atmospheric Radiation Measurement Research Facility (ARM) and the Environmental Molecular Sciences Laboratory (EMSL). ARM provides unique, multi-instrumented capabilities for continuous, long-term observations and

model-simulated high resolution information that researchers need to develop and test understanding of the central role of clouds and aerosols on a variety of spatial scales, extending from local to global. EMSL provides a wide range of premier experimental and computational resources for studying the physical, biogeochemical, chemical, and biological processes that underlie DOE's energy and environmental mission. The data activity encompasses observations collected by dedicated field experiments, routine and long term observations accumulated by user facilities, and model generated information derived from Earth models of variable complexity and sophistication.

For additional information regarding the Office of Biological and Environmental Research priorities, click here.

29. TECHNOLOGIES FOR HYDROBIOGEOCHEMICAL MEASUREMENTS IN COASTAL SYSTEMS

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The mission of the Biological and Environmental Research (BER) program 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, independence, and prosperity. The mission of the Earth and Environmental Systems Sciences Division (EESSD) within BER is to enhance the seasonal to multi-decadal predictability of the Earth system using long term field experiments, DOE user facilities, modeling and simulation, uncertainty characterization, best-in-class computing, process research, and data analytics and management (Reference 1). EESSD scientific grand challenges include the integrated water cycle, biogeochemistry, high latitudes, drivers and responses in the Earth system, and data-model integration (Reference 1).

Within EESSD, the Environmental System Science (ESS) activity supports experimental and process modeling research to improve understanding of the coupled physical, chemical and biological interactions that control the structure and functioning of watershed systems, terrestrial ecosystems, and coastal interfaces. These systems extend across a vast range of spatial and temporal scales from bedrock to the top of the vegetative canopy, Arctic to tropical vegetation, surface water to groundwater, and freshwater to saline coastal interfaces. Key challenges for the ESS scientific community include dealing with the extremely heterogeneous and complex data that are generated from observations and field experiments within these watersheds, terrestrial ecosystems, and coastal interfaces, integrating these data; and facilitating their use to test and further advance predictive models of the functioning and dynamics of these systems.

This topic is specifically focused on addressing measurement and data challenges within the complex environment of coastal systems, defined as the broad zones where the land margin meets the fresh and/or salt-water environment. For field observations and experiments, coastal systems as a component of terrestrial-aquatic interfaces (TAIs) represent a major knowledge gap in understanding and scaling. This is because coastal systems are home to extremely rich and complex processes that interact at the transition between fully terrestrial and fully aquatic environments (Reference 2). Measurements that can adequately capture and quantify these hydro-biogeochemical processes are subject to a number of challenges.

Coastal systems are characterized by steep environmental and process gradients at plot and landscape scales and are subject to wide ranges of forcing and environmental conditions that hydro-biogeochemical sensors must both withstand and measure. Gradients at a plot or reach scale are often embedded with complex fine-scale structural patterns and environmental and hydrologic forcing that vary in space and time, complicating scaling from small-scale process understanding to system-level predictions. Multi-cyclical (e.g. daily, seasonal, interannual) variability and intermittent and chronic shifts in environmental drivers layer additional dimensions of complexity on the multi-scale patterns. Collectively, these complexities require recurrent observations across these dynamic spatial and temporal conditions to properly represent ecosystem function and response, particularly spatially transient and temporally episodic “hot spots” and “hot moments” of biogeochemical activity resulting from the ephemeral confluence of dynamic factors. Many current technologies are extractive or require disturbance or synoptic sampling, which complicates fully capturing and characterizing these dynamic processes. Grant applications submitted to this topic must emphasize development of technologies that will help address these measurement challenges in coastal systems.

Applications should (1) demonstrate performance characteristics of proposed measurement systems, and (2) show a capability for deployment at field scales ranging from experimental plot size (meters to a hectare) to nominal dimensions of ecosystems and watersheds (hectares to kilometers). Phase I projects must perform feasibility and/or field tests of proposed measurement systems to assure a high degree of reliability and robustness. Grant applications based on satellite remote sensing platforms are beyond the scope of this topic, and will be declined. Grant applications are sought in the following two subtopics:

a. Integrated Surface/Near-surface Sensors and Arrays for Real-Time, *In situ* Measurements of Hydro-Biogeochemical Processes in Coastal Terrestrial-Aquatic Interfaces

Sensitive, accurate, and real-time characterization and monitoring of hydro-biogeochemical processes are needed for coastal outlets and interfaces, e.g. freshwater to freshwater (stream to lake) and freshwater to saline/tidal interfaces (river to ocean), estuarine systems, and transitional terrestrial ecosystems at the interface with aquatic systems (marshes, swamps, riparian zones, and shorelines). Rugged, portable, and sensitive *in situ* devices capable of continuous or repetitive high-precision measurements are needed for low-cost field deployment in remote locations that often have little to no power available, may be under heavy vegetation cover with thick organic soil layers, and subject to daily-to-seasonal surface water inundation, high humidity, and a halophytic environment. Specific areas of interest include:

- Measurement systems for emissions of trace greenhouse gas (e.g., CH_4, N_2O) or other gas (hydrogen, oxygen) at the water- or soil-atmosphere boundary capable of capturing both sustained emissions as well as spatially variable, temporally discrete episodic emission events (hot spots/hot moments);
- Sensing arrays, networks and instrument clusters for vertical profiles (water surface into the sediments) and lateral transport of chemical parameters in both fresh and brackish waters. Example parameters include Total Suspended Solids (TSS); dissolved and/or particulate organic carbon; salinity; redox potential; major/minor cations and other trace metals; and compounds that are signatures of microbial/fungal/algal activity;
- Sensors for minimally invasive estimation/quantification of depth-resolved soil porosity (amount of gas/water-filled space), particularly for high-organic matter soils in varied freshwater and brackish wetland environments, to enable repetitive *in situ* measurement of soil physical structure (with application for assessment of fluid or gas conductivity and soil subsidence/accretion). Sensors should be self-powered, suitable for use in submerged/saturated soils, and capable of extended (e.g., 3-12 months) *in situ* deployment and data retrieval with minimal disturbance to the surrounding soils or have non-invasive surface-based capability to enable repeated measurements of the same location, with an integrated measurement depth interval of no more than 10cm. Of particular interest are integrated sensors providing simultaneously measured or derived key soil environment parameters (e.g., temperature, moisture content, redox potential, dissolved oxygen, conductivity).

Questions – Contact: Jennifer Arrigo, jennifer.arrigo@science.doe.gov or Brian Benscoter, brian.benscoter@science.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department invites grant applications in areas that more generally fall within the scope of the topic description above.

Questions – Contact: Jennifer Arrigo, jennifer.arrigo@science.doe.gov

Grant applications involving these topics must provide convincing documentation (experimental data, calculations, and simulation as appropriate) to show that the sensing method is both highly sensitive (i.e., low detection limit), precise, and highly selective to the target analyte, parameter or biological component (i.e., with minimal or no confounding of results due to other physical/chemical/biological interferences typically found in natural systems/in the field). Of particular interest are individual or networked systems that are autonomous or can be left unattended, and that have independent/low power requirements and a centralized data storage/download location. Approaches that leave significant doubt regarding sensor functionality or characteristics for real-time and/or multi-component sampling under realistic field conditions will not be considered. Technologies whose application is exclusive to open waters of marine (e.g., ocean) or freshwater systems (e.g., lakes) rather than terrestrial or across terrestrial-aquatic interfaces will not be considered.

Applications submitted to these topics must describe why and how the proposed in situ fieldable technologies will substantially improve the state-of-the-art, include bench and/or field tests to demonstrate the technology, and clearly state the projected dates for likely operational deployment. New or advanced technologies, which can be demonstrated to operate under field conditions and can be deployed in 2-3 years, will receive selection priority. Demonstration and/or deployment plans (e.g. taking samples, deploying/testing sensors) that would require access to DOE sites or laboratories must include a letter of support for such access from the relevant field site manager or equivalent. Grant applications that propose incremental improvements to existing technologies are not of interest and will be declined. Coordination and/or collaboration with government laboratories or universities, either during or after the SBIR/STTR project, is encouraged insofar that this may accelerate the development and field evaluation of the measurement or monitoring technology.

References:

1. U.S. Department of Energy. (2018). *Earth and Environmental Systems Sciences Division, Strategic Plan,* DOE/SC-019. https://science.osti.gov/-/media/ber/pdf/workshop-reports/2018_CESD_Strategic_Plan.pdf
2. U.S. Department of Energy. (2017). *Research Priorities to Incorporate Terrestrial-Aquatic Interfaces in Earth System Models: Workshop Report,* DOE/SC-0187. https://tes.science.energy.gov/files/TAI_Workshop2016.pdf

30. ATMOSPHERIC MEASUREMENT TECHNOLOGY

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The mission of the Biological and Environmental Research (BER) program 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, independence, and prosperity. The mission of the Earth and Environmental Systems Sciences Division (EESSD) within BER is to enhance the seasonal to multi-decadal predictability of the Earth system using long term field experiments, DOE user facilities, modeling and simulation, uncertainty characterization, best-in-class computing, process research, and data analytics and management (Reference 1). EESSD scientific grand challenges include the integrated water cycle, biogeochemistry, high latitudes, drivers and responses in the earth system, and data-model integration (Reference 1).

Addressing these scientific grand challenges requires a combination of theoretical, experimental, and modeling research across a variety of relevant scientific disciplines. For the atmospheric sciences discipline, data from field campaigns and long-term observations are needed to quantify local atmospheric processes including aerosol formation; chemical composition and optical properties of aerosols; initiation and microphysical properties of cloud droplets, ice crystals, and precipitation; details of atmospheric state structure including turbulence, temperature, trace gas, and water vapor profiles; and feedbacks involving the terrestrial-aerosol-cloud-precipitation system. These data are necessary both for fundamental process understanding and for evaluation of numerical models that are used to assess the predicted impacts on global and regional systems (References 2-5).

This topic is specifically focused on developing technologies for robust and well-characterized airborne measurements of atmospheric aerosol, cloud, turbulence, precipitation, temperature, trace gas, or water vapor properties that are relevant to Earth system understanding and that are suitable for deployment on airborne research platforms including manned aircraft, unmanned aerial systems (UAS), or tethered balloon systems (TBS) such as those operated by the Atmospheric Radiation Measurement (ARM) user facility (www.arm.gov and Reference 6). ARM has recently acquired a new piloted aircraft that will be modified for atmospheric research (the Bombardier Challenger 850 regional jet) and continues to develop measurement capabilities for its midsize unmanned aerial system (the ArcticShark UAS) and its tethered balloon systems (TBS).

While instrumentation currently exists for airborne measurements of many atmospheric properties, the scientific questions of interest to the community require technological innovations and improvements to develop instrumentation and measurement techniques that have faster sampling, higher accuracy and precision, larger sampling ranges, and/or lower weight and power requirements. Additionally there is interest in development of measurement techniques for atmospheric parameters that cannot currently be measured on airborne platforms or for which robust, miniaturized instruments suitable for deployment on small aerial platforms do not currently exist. To identify scientific questions and opportunities, specific observational needs, and research challenges associated with aerial measurements, DOE held a workshop on aerial measurement needs in 2015 (Reference 7) and the ARM facility held a workshop in early 2020 (Reference 11).

Grant applications submitted to this topic must propose development of measurement technologies **suitable for deployment on airborne research platforms** (manned aircraft, unmanned aerial systems, or tethered balloon systems). Therefore applications must consider and discuss factors such as the weight and power requirements, resistance to vibration, and/or other factors critical to successful operation of the proposed technology on an airborne research platform.

Applications should demonstrate performance characteristics of proposed measurement systems and must propose Phase I bench tests of critical technologies ("critical technologies" refers to components, materials, equipment, or processes that overcome significant limitations to current capabilities). In addition, grant applications must (1) specifically describe how the proposed work is a technical advance over existing commercial instrumentation and how it will either improve the robustness, automation, precision, accuracy, calibration, resolution, sampling rate, or weight/power requirements compared to existing instrumentation or provide measurements of parameters not currently available with existing commercial instrumentation, (2) describe the purpose and benefits of any proposed teaming arrangements with government laboratories or universities, and (3) support claims of commercial potential for proposed technologies (e.g., endorsements from relevant industrial sectors, market analysis, or identification of potential spin-offs or interested users for the proposed technology). Grant applications for development of new instrument components or instrument systems that propose only computer modeling without physical testing will be considered non-responsive.

Grant applications must provide convincing documentation (experimental data, calculations, and/or simulations as appropriate) to show that the proposed sensing method is appropriate to make the desired measurements.

Approaches that leave significant doubt regarding sensor functionality in realistic field conditions or that do not specifically discuss application to airborne platforms will not be considered. Applications focused primarily on technologies for air quality measurements will not be considered.

a. Fast Response Aircraft Temperature and/or Water Vapor Measurements

Specification of the atmospheric state, especially high resolution spatial information about water vapor mixing ratio and temperature, is important for understanding many aerosol, cloud, and radiative processes. Of particular importance is using these two measurements in combination to compute supersaturation, which cannot be measured directly and is fundamental to cloud droplet growth. Cloud physics studies require accuracy in supersaturation with respect to ice to be within a few percent for cold clouds, whereas warm clouds need accuracy of 0.1% in supersaturation with respect to liquid (Reference 7). Temperature and water vapor properties may vary on quite small spatial scales due to turbulent fluctuations in the atmosphere. Therefore it is important to have fast response sensors for measuring these quantities on airborne platforms in order to get the desired spatial resolution. In addition, these measurements need to be made accurately within clouds and to cover the full range of atmospheric conditions. Capabilities of some existing sensors are discussed in References 8, 9.

This sub-topic seeks grant applications for fast temperature and/or water vapor/humidity measurements suitable for airborne platforms and capable of operation within cloud and across a range of atmospheric conditions. Applications may propose measurement technologies for manned aircraft or miniaturized versions for unmanned aerial systems/tethered balloons. Applications must discuss precision and accuracy of the proposed measurements and required calibration procedures. Accuracy specification may include anchoring/calibration of the fast response instrument to a slower, more accurate, measurement instrument typically flown on the same platform. Applications should also discuss the “time response” of the proposed technology, i.e., the time required by the sensor to get within 10% of the real value after a step function change of the measured parameter. Applications must clearly indicate suitability of the proposed techniques for airborne applications and must clearly indicate how their proposed technology is a significant advance over existing commercial instrumentation available for the given airborne platform type (manned aircraft, UAS, or TBS).

Desired specifications:

- Temperature measurement: > 100 Hz, 5 ms time response
- Humidity/water vapor measurement: > 50 Hz, 20 ms time response

Questions – Contact: Sally McFarlane, Sally.McFarlane@science.doe.gov

b. Airborne Instruments for Water Cloud Measurements

Improving representation of cloud microphysical processes in numerical weather and Earth system models requires detailed information on cloud properties such as cloud droplet size distributions and cloud water mass, along with detailed measurements of atmospheric state discussed above. While many aircraft instruments exist for measurements of liquid water content (LWC) or droplet size distribution (DSD), there are still uncertainties regarding sampling characteristics of the droplet size distribution and uncertainties in measurements in cases of high droplet concentrations, large droplets, or high LWC (Reference 7, 10). Additionally there are often inconsistencies in measurements of water mass derived from cloud droplet size distributions compared to those derived from sensors that solely measure LWC (Reference 10).

This sub-topic seeks grant applications for an airborne instrument to measure an ensemble of drops in a water cloud and accurately determine simultaneously both the liquid water content (LWC) and drop size distribution (DSD) for clouds with drop diameters ranging from about 2 to 65 µm and LWC up to 4 g m-3. Applications must discuss precision and accuracy of the proposed measurements and required calibration procedures. Applications must clearly indicate suitability of the proposed techniques for airborne applications and must clearly indicate how their proposed technology is a significant advance over existing commercial instrumentation available for the given airborne platform type (manned aircraft, UAS, or TBS).

Desired specifications:

- Droplet size resolution of 1 µm or better
- Sampling frequency of at least 1 Hz; with 10 Hz preferred
- Able to measure droplet size range from 2 to 65 µm
- LWC accuracy of 10% or better across full range

Questions – Contact: Sally McFarlane, Sally.McFarlane@science.doe.gov

c. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Sally McFarlane, Sally.McFarlane@science.doe.gov

References:

1. U.S. Department of Energy. (2018). *Earth and Environmental Systems Sciences Division, Strategic Plan,* DOE/SC-0192. https://science.osti.gov/-/media/ber/pdf/workshop-reports/2018_CESD_Strategic_Plan.pdf
2. Stith, J. L., and Coauthors. (2019). *100 years of progress in atmospheric observing systems. A Century of Progress in Atmospheric and Related Sciences: Celebrating the American Meteorological Society Centennial,* Meteor.Monogr., No. 59, Amer.Meteor. Soc. https://doi.org/10.1175/AMSMONOGRAPHS-D-18-0006.1
3. Kreidenweis, S., Petters, M., and Lohmann, U. (2019). *100 years of progress in cloud physics, aerosols, and aerosol chemistry. A Century of Progress in Atmospheric and Related Sciences: Celebrating the American Meteorological Society Centennial,* Meteor. Monogr., No. 59, Amer. Meteor. Soc. https://doi.org/10.1175/AMSMONOGRAPHS-D-18-0024.1
4. Wood R., Jensen, M. P., Wang, J., Bretherton, C. S., Burrows, S. M., Del Genio, A. D., Fridlind, A. M., Ghan, S. J., Ghate, V.P., Kollias, P., Krueger, S. K., MGraw, R. L., Miller, M. A., Painemal, D., Russell, L. M., Yuter, S.E., and Zuidema, P. (2016). *Planning the Next Decade of Coordinated Research to Better Understand and Simulate Marine Low Clouds.* Bulletin of the American Meteorological Society, 97(9). https://journals.ametsoc.org/bams/article/97/9/1699/69544/Planning-the-Next-Decade-of-Coordinated-Research
5. Shrivastava M, Cappa, C. D., Fan, J., Goldstein, A., Guenther, A., Jimenez, J., Kuang, C., Laskin, A., Martin, S. Ng, N., Petaja, T., Pierce, J., Rasch, P., Roldin, P., Seinfeld, J., Shilling, J., Smith, J., Thornton, J., Volkamer, R., Wang, J., Worsnop, D., Zaveri, R., Zelenyuk, A., and Zhang, Q. (2017). *Recent advances in understanding secondary organic aerosol: Implications for global climate forcing.* Reviews of Geophysics, 55(2). https://agupubs.onlinelibrary.wiley.com/doi/full/10.1002/2016RG000540
6. Schmid, B., Tomlinson, J. M., Hubbe, J. M., Comstock, J.M., Mei, F., Chand, D., Pekour, M. S., Kluzek, C. D., Andrews, E., Biraud, S. C., and McFarquhar, G.M. (2014). *The DOE ARM Aerial Facility. Bull. Amer. Meteor.* Soc., 95, 723–742. https://doi.org/10.1175/BAMS-D-13-00040.1

7. de Boer G., Dafflon, B., Guenther, A., Moore, D., Schmid, B., Serbin, S., and Vogelmann, A. (2015). *Climate and Environmental Sciences Division,* Aerial Observation Needs Workshop May 13-14, 2015 Report. DOE/SC-0179. https://science.osti.gov/-/media/ber/pdf/workshop-reports/CESD_AerialObsNeeds_Workshop_2015web.pdf?la=en&hash=BDF3483C2D32A9E57669EA52E9349AE01A03FF07
8. Zondlo, M. A., Paige, M. E., Massick, S. M., and Silver, J. A. (2010). *Vertical cavity laser hygrometer for the National Science Foundation Gulfstream-V aircraft.* Journal of Geophysical Research 115(D20): D20309. https://doi.org/10.1029/2010JD014445
9. Goldberger L. (2019). *Chilled Mirror Hygrometer Aboard Aircraft (CMH-AIR) Instrument Handbook.* Ed. by Robert Stafford, ARM user facility. DOE/SC-ARM-TR-235.
10. Faber, S., French, J. R., and Jackson, R. (2018). *Laboratory and in-flight evaluation of measurement uncertainties from a commercial Cloud Droplet Probe (CDP).* https://ra9r13nh313ew0s1pxuptw7p-wpengine.netdna-ssl.com/wp-content/uploads/2020/01/CDP-18-01-faberEtAl2018amtBeamMapping.pdf
11. Mei, F., D. Dexheimer, J. Fast, M. Diao, B. Geerts, A. Bucholtz, L. Riihimaki, C. Flynn, T. Thornberry, T. Campos, S. Springston, C. Kuang, J. Tomlinson, and B. Schmid (2020). ARM Aerial Instrument Workshop Report. DOE/SC-ARM-20-010. https://www.arm.gov/publications/programdocs/doe-sc-arm-20-010.pdf

31. ENABLING TOOLS FOR STRUCTURAL BIOLOGY OF MICROBIAL AND PLANT SYSTEMS RELEVANT TO BIOENERGY

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Biological Systems Science Division (BSSD) supports research to understand, predict, and design biological processes that underpin innovations for bioenergy and bioproduct production and to enhance the understanding of natural environmental processes relevant to DOE. Structural characterization of biological systems and their components provide critical insights that illuminate these processes. Powerful experimental approaches to structural characterization include scattering and imaging techniques at the DOE synchrotron and neutron user facilities (which are funded by Basic Energy Sciences; see https://www.energy.gov/science/bes/basic-energy-sciences) as well as cryo-electron microscopy (cryoEM) for molecular or tomographic characterization of biological samples. BER supports access, training and user support for experimental capabilities described at www.BERStructuralBioPortal.org to enable experiments for studying and understanding structural and functional processes of importance to the BER Genomic Science program (GSP; see https://genomicscience.energy.gov/index.shtml). These BER-supported capabilities are freely available to all researchers through peer-reviewed facility proposal processes. This SBIR-STTR topic encourages the development of tools necessary for doing experiments at the beamlines or that can facilitate cryoEM investigations.

a. Tools or Instruments for Structural Characterization of Biological Systems Ranging from Atomic to Multi-cellular Scales

This subtopic solicits the development of robust tools that are needed to improve structural biology capabilities for researchers studying microbial or plant systems relevant to DOE mission interests. For this solicitation, structural biology targets range from the atomic to multi-cellular scale. For this solicitation, technology areas for structural characterization include x-ray or neutron-based techniques and cryo-EM for determining the 3D structures of macromolecules, macromolecular complexes, cells, cellular components or tissues. Examples of concepts responsive to this announcement include but are not restricted to tools or instruments for beam focus or alignment, sample preparation, handling, positioning or detection for any of the above mentioned technology areas. The purpose is to encourage development

and commercialization of tools that ease use, improve results or overcome obstacles associated with existing technologies.
Algorithm development, software or informatics solutions are not included under this subtopic, but could be submitted under the SBIR/STTR Topic 1a, Application Area 1 “Advanced Data Analytic Technologies for Systems Biology and Bioenergy”.

Questions – Contact: Amy Swain, Amy.Swain@science.doe.gov

b. Other
In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Amy Swain, Amy.Swain@science.doe.gov

References:

1. U.S Department of Energy, Office of Biological and Environmental Research. (2019). *BER Structural Biology Resources at Synchrotron and Neutron Facilities.* http://www.BERStructuralbioportal.org
2. U.S Department of Energy, Office of Biological and Environmental Research. (2017). *Technologies for Characterizing Molecular and Cellular Systems Relevant to Bioenergy and Environment Workshop,* September 21-23, 2016, DOE/SC-0189. https://genomicscience.energy.gov/technologies/Technologies_highres.pdf
3. U.S. Department of Energy, Office of Biological and Environmental Research. (2015). *Biological Systems Science Division,* Strategic Plan*,* p. 18. https://genomicscience.energy.gov/pubs/BSSDStrategicPlan.pdf

32. BIOIMAGING TECHNOLOGIES FOR BIOLOGICAL SYSTEMS

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The mesoscale to molecules Bioimaging Technology development effort in BER is targeted at creating novel multifunctional technologies to image, measure, and model key metabolic processes within and among microbial cells and multicellular plant tissues. BER’s current focus on developing a scientific basis for plant biomass-based biofuel production requires detailed understanding of cellular metabolism to incorporate, modify, or design beneficial properties into bioenergy-relevant plants and microbes. Likewise, the ability to track materials and chemical exchanges within and among cells and their environment is crucial to understanding the activity of microbial communities in environmental settings. New imaging and measurement technologies that can characterize multiple metabolic transformations will provide the integrative systems-level data needed to gain a more predictive understanding of complex biological processes relevant to BER. Grant applications are sought in the following subtopics:

a. New Instrumentation and Bioimaging Devices for Non-destructive, Functional Metabolic Imaging of Plant and Microbial Systems
Applications are invited to develop new imaging instrumentation and imaging devices for in situ, non-destructive, functional imaging and quantitative measurement of key metabolic processes in living organisms such as within and among microbial cells and microbial communities in terrestrial environments, and/or multicellular plant tissues. The instrumentation and devices to be developed for imaging biological systems will have high likelihood to enable an understanding of the spatial/temporal relationships, physical connections, and chemical exchanges that facilitate the flow of information and materials across membranes and between intracellular partitions. The primary interest for this solicitation

is for new innovative, bioimaging devices with small footprints, which are fully capable of operation independently of heavy equipment and large instruments (e.g. neutron and light sources, cryoelectron microscopes, high resolution mass spectrometers), and can be easily deployed in public and private sector to make them accessible to the larger scientific community.

For the purpose of this announcement, the following clarification is provided: The "bioimaging technology" of interest is defined as an imager or an imaging device deployable for non-destructive metabolic imaging of living biological systems. However, the tools, techniques and methodologies to construct and develop the technical components of such systems including objects or platforms as models for imaging are excluded from this solicitation.

Questions – Contact: Prem Srivastava, Prem.Srivastava@science.doe.gov

b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Prem Srivastava, Prem.Srivastava@science.doe.gov

References:

1. U. S. Department of Energy. (2019). *Bioimaging Science Program, Principal Investigator Meeting Proceedings,* Office of Science, p. 36. https://doegenomestolife.org/characterization/2019_Bioimaging_Program_PI_Meeting.pdf
2. U. S. Department of Energy. (2017). *Funding Opportunity Number: DE-FOA-0001868 Announcement, Office of Science, Biological and Environmental Research, Bioimaging Research and Approaches for Bioenergy, p. 66.* https://science.osti.gov/-/media/grants/pdf/foas/2018/SC_FOA_0001868.pdf

33. TECHNOLOGIES TO ENABLE THE SYNTHESIS OF LARGE DNA FRAGMENTS FOR SYNTHETIC BIOLOGY

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Synthetic genomic science is an emerging research frontier that offers substantial promise for fundamental discoveries and practical applications in many of the research areas related to BER's vision. The ability to design, build, and test large genomic fragments or whole chromosomes (Cello et al. 2002; Smith et al. 2003; Huchinson et al. 2015; Richardson et al. 2017) offers the potential to purposefully engineer entire genetic regulatory networks, genomes, or organisms. Major breakthroughs in DNA sequencing technologies over the past two decades constitute some of the most enabling and transformative technological advances in biology and have resulted in a precipitous decline of DNA sequencing cost. While technologies for DNA synthesis are widely used, their capacity and throughput has not kept pace, leading to a "DNA read-write bandwidth gap" that represents an important obstacle to biological research and developing a future bioeconomy. Novel, high-throughput DNA synthesis technologies, or related, enabling technologies, are therefore needed to fundamentally enhance our ability to design, edit, and construct artificial genomes (Wang et al. 2018).

a. Technologies for the Synthesis of Large DNA Fragments

This topic addresses the DNA read-write bandwidth gap in synthetic biology. The purposeful production of genomic-scale DNA fragments is a profoundly enabling technology. Current DNA synthesis technology is, however, directly tied to the cost of oligonucleotide production, which has not decreased appreciably in a decade (Hughes and Ellington, 2019). Advanced synthesis technologies would enhance capabilities in a wide range of fundamental biological research disciplines, including biochemistry, whole pathway and bio-systems design, metabolic engineering, microbiome engineering, ecology, and developmental as well as structural biology. This topic therefore encourages applications that aim at developing innovative, next-generation DNA synthesis technologies that are more efficient and cost-effective than existing approaches. Of interest to the program are technologies that have the potential for high-fidelity, high-throughput production of very large DNA fragments (10^4-10^6 base pairs). Applications should be focused on approaches that are both flexible and scalable. Also, technologies that broadly enable large DNA fragment synthesis and handling are of interest. This could include commercialization of tools that are not directly used for oligonucleotides production, yet are broadly enabling capabilities for DNA synthesis. Examples may include approaches to create large numbers of specific, high-fidelity oligos of known sequence and at low cost, or technologies to handle large numbers of large DNA fragments. A clear case should be made how the technology is directly enhancing DNA synthesis efficiency. Proposals that incrementally improve existing commercial technologies, or those that would have only narrow applications, are not encouraged.

Questions – Contact: Boris Wawrik, boris.wawrik@science.doe.gov

b. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Boris Wawrik, boris.wawrik@science.doe.gov

References:

1. Cello J., Paul, A.V., and Wimmer, E. (2002). *Chemical Synthesis of Poliovirus cDNA: Generation of Infectious Virus in the Absence of Natural Template, Science,* Vol. 297, Issue 5583, p. 1016-1018. https://www.ncbi.nlm.nih.gov/pubmed/12114528
2. Hutchison, C. A. III, Chuang, R. Y., Noskov, V. N., Assad-Garcia, N., et al. (2016). *Design and Synthesis of a Minimal Bacterial Genome*, Science, Vol. 351, Issue 6280, aad6253, p. 13. https://www.ncbi.nlm.nih.gov/pubmed/27013737
3. Hughes, R.A. and Ellington, A.D. (2017). *Synthetic DNA Synthesis and Assembly: Putting the Synthetic in Synthetic Biology*, Cold Spring Harb Perspect Biology, Vol. 9, Issue 1. pii: a023812, p. 18. https://www.ncbi.nlm.nih.gov/pubmed/28049645
4. Richardson, S. M., Mitchell, L. A., Stracquadanio, G., Yang, K., et al. (2017). *Design of a Synthetic Yeast Genome*, Science, Vol. 355, Issue 6329, p. 1040-1044. https://science.sciencemag.org/content/355/6329/1040
5. Smith, H. O., Hutchison C. A., Pfannkuch C., and Venter, J. C. (2003). *Generating a Synthetic Genome by Whole Genome Assembly: phiX174 Bacteriophage from Synthetic Oligonucleotides*, Proc Natl Acad Sci U S A, Vol. 100, Issue 26, p. 15440-15445. https://www.ncbi.nlm.nih.gov/pubmed/14657399
6. Wang, L., Jiang, S., Chen, C., He, W., et al. (2018). *Synthetic Genomics: From DNA Synthesis to Genome Design*, Angewandte Chemie (Int Ed. in English), Vol. 57, Issue 7, p. 1748-1756. https://www.ncbi.nlm.nih.gov/pubmed/29078032

34. BIOLOGICAL APPROACHES AND TECHNOLOGIES FOR BIOENERGY: ENZYMATIC AND MICROBIAL TECHNOLOGIES FOR BIOENERBGY AND BIOPRODUCTS PRODUCTION FROM LIGNOCELLULOSIC FEEDSTOCKS

Maximum Phase I Award Amount: $250,000	Maximum Phase II Award Amount: $1,600,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

BER's major efforts in bioenergy research seek to couple a basic understanding of plant and microbial biology to sustainably produce fuels, chemicals, and other bioproducts from plant biomass. Dedicated crops grown on marginal lands and converted to renewable sources of fuels, chemicals and other bioproducts have the potential to significantly offset the reliance on fossil resources for production of these critical materials. This is of importance to DOE, as fossil resources are ultimately finite and subject to economic and geopolitical uncertainty. Renewable sources for the fuels and products that support our modern society are thus a long-term strategic need for the Nation and a burgeoning bioeconomy. These topics target key areas to broaden development of enzymes capable of deconstructing lignocellulose, synthetic biology approaches to convert lignocellulosic components to bioproducts, and microbial amendments that could help facilitate the growth of bioenergy crops. Specific details are provided below:

a. Lignocellulose Deconstructing Enzymes

The objective of this topic area is to support the development of enzymes for the deconstruction of lignocellulose with particular interest in lignin deconstructing enzymes. Deconstruction of lignocellulose continues to be an expensive process that can also result in toxic compounds being produced. Cost of enzymes contribute significantly to the overall cost of biofuel and bioproduct production when enzymes are utilized.

Enzymatic deconstruction of lignocellulose may contribute to a controlled, predictable, and reproduceable conversion of cellulose, hemicellulose and lignin polymer into bioproduct or useful intermediates. In particular, enzymatic depolymerization is expected to reduce production of toxic compounds during deconstruction and will facilitate the creation of value from lignin.

This topic may support the discovery of new lignocellulose deconstructing enzymes, optimization of known enzymes, and research toward production scale-up and commercialization. The resulting enzyme products are expected to reduce the cost of deconstruction and reduce the production of toxic compounds.

Questions – Contact: Kent Peters, Kent.Peters@science.doe.gov

b. Synthetic Biology Approaches for the Microbial Conversion of Lignocellulose to Bioproducts

The objective of this topic area is to support approaches that leverage microbial metabolic capabilities and engineering in bacteria, fungi, archaea, and/or mixed communities for the conversion of lignocellulosic biomass. Specifically, enhanced degradation of lignocellulosic bioenergy feedstocks to simple sugars and further conversion to a flexible range of higher value products is desired. Projects should focus on the development and eventual commercialization of metabolically engineered microbes designed to simultaneously or sequentially utilize both C5 and C6 sugars to produce bioproducts. Relevant targets should replace petroleum-derived non-pharmaceutical chemicals and/or chemicals that are non-domestically sourced to broadly support a growing US bioeconomy. Projects focused on the initial stage of microbial isolation with the intent of looking for specific biochemical characteristics are not requested for this topic. Projects focused on the following areas are also NOT encouraged for this topic: starch-derived fuels and products; natural gas-, petroleum-, or coal-derived biofuels and bioproducts; bioethanol or other short chain alcohols, biohydrogen, and biogas production; pharmaceuticals; nutraceuticals; cosmetics;

food products; municipal solid waste; microbial fuel cells; wastewater treatment; biomimetic hydrogen production; and microbial bioremediation.

Questions – Contact: Dawn Adin, Dawn.Adin@science.doe.gov

c. Microbial Amendments for Enhanced Bioenergy Crop Production

The objective of this topic area is to support research using microbes to increase biomass in large-scale bioenergy crop production. Projects should focus on manipulating microbes or microbial communities that result in increases in biomass in bioenergy crops under non-stress and/or abiotic stress growth conditions. Microbial effects on plant characteristics may include, but are not limited to: plant architecture and development, plant resilience and adaptation to abiotic stress such as nutrient availability, water availability, or tolerance to temperature variations. Although an understanding of the molecular mechanisms underlying the increase in biomass would be ideal, experimentation to determine these mechanisms is not required for this topic area.

Questions – Contact: Shing Kwok, Shing.Kwok@science.doe.gov

d. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Kent Peters, Kent.Peters@science.doe.gov

References: Subtopic a:

1. U. S. Department of Energy. (2020). *Bioenergy Research Centers: 2020 Program Update*, DOE/SC-0201. https://www.genomicscience.energy.gov/centers/BRC_Booklet_2020LR.pdf
2. U.S. Department of Energy. (2015). *Lignocellulosic Biomass for Biofuels and Bioproducts: Workshop Report*, DOE/SC-0170. https://www.genomicscience.energy.gov/biofuels/lignocellulose/BioenergyReport-February-20-2015LR.pdf
3. U.S. Department of Energy. (2015). *Basic Research Opportunities in Genomics Science to Advance the Production of Biofuels and Bioproducts from Plant Biomass,* DOE/SC-0177. https://www.genomicscience.energy.gov/biofuels/BER-Bioenergy-WhitePaper-Final.pdf
4. U.S. Department of Energy. (2018). *Bioenergy Research Centers 10-Year Retrospective: Breakthroughs and Impacts 2007-2017 Report,* DOE/SC-0193, September 2018. https://www.genomicscience.energy.gov/centers/brcretrospective.pdf

References: Subtopic b:

1. U. S. Department of Energy. (2018). Funding Opportunity Number: DE-FOA-0001865 Announcement, Systems Biology of Bioenergy-Relevant Microbes to Enable Production of Next-Generation of Biofuels and Bioproducts. https://science.osti.gov/-/media/grants/pdf/foas/2018/SC_FOA_0001865.pdf
2. U.S. Department of Energy. (2015). Lignocellulosic Biomass for Biofuels and Bioproducts: Workshop Report, DOE/SC-0170. https://www.genomicscience.energy.gov/biofuels/lignocellulose/BioenergyReport-February-20-2015LR.pdf
3. U.S. Department of Energy. (2011). Biosystems Design Report from the July 2011 Workshop, DOE/SC-0141. https://www.genomicscience.energy.gov/biosystemsdesign/report/biosystemsdesignreport2012.pdf

References: Subtopic c:

1. U. S. Department of Energy. (2020). Funding Opportunity Number: DE-FOA-0002214 Announcement, Systems Biology Research to Advance Sustainable Bioenergy Crop Development. https://science.osti.gov/-/media/grants/pdf/foas/2020/SC_FOA_0002214.pdf
2. U.S. Department of Energy. (2018). Bioenergy Research Centers 10-Year Retrospective: Breakthroughs and Impacts 2007-2017 Report, DOE/SC-0193, September 2018. https://www.genomicscience.energy.gov/centers/brcretrospective.pdf
3. U. S. Department of Energy. (2017). Funding Opportunity Number: DE-FOA-0001650 Announcement, Biosystems Design to Enable Next-Generation of Biofuels and Bioproducts. https://science.osti.gov/-/media/grants/pdf/foas/2017/SC_FOA_0001650.pdf

PROGRAM AREA OVERVIEW: OFFICE OF NUCLEAR PHYSICS

Nuclear physics (NP) research seeks to understand the structure and interactions of atomic nuclei and the fundamental forces and particles of nature as manifested in nuclear matter. Nuclear processes are responsible for the nature and abundance of all matter, which in turn determines the essential physical characteristics of the universe. The primary mission of the Office of Nuclear Physics (NP) Program is to develop and support the scientists, techniques, and facilities that are needed for basic nuclear physics research. Attendant upon this core mission are responsibilities to enlarge and diversify the Nation's pool of technically trained talent and to facilitate transfer of technology and knowledge to support the Nation's economic base.

Nuclear physics research is carried out at national laboratories, international accelerator facilities, and universities. The Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF) allows detailed studies of how quarks and gluons bind together to make protons and neutrons. The Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory (BNL) is forming new states of matter which have not existed since the first moments after the birth of the Universe. The Argonne Tandem Linac Accelerator System (ATLAS) at Argonne National Laboratory (ANL) which provides stable and radioactive beams directed toward understanding the properties of nuclei at their limits of stability. NP is constructing the Facility for Rare Isotope Beams (FRIB) at Michigan State University, which is nearing completion. NP is supporting the community that is developing technologies necessary for construction of the electron ion collider (EIC) at BNL.

The NP program supports an in-house program of basic research focused on heavy elements at the 88-Inch Cyclotron of the Lawrence Berkeley National Laboratory (LBNL); the operations of accelerators for in-house research programs at two universities (Texas A&M University and the Triangle Universities Nuclear Laboratory (TUNL) at Duke University), which provide unique instrumentation with a special emphasis on the training of students; and non-accelerator experiments, such as large stand-alone detectors and observatories for rare events. Of particular interest is R&D related to future experiments in fundamental symmetries such as neutrinoless double-beta decay experiments and measurement of the electric dipole moment of the neutron, where extremely low background and low count rate particle detections are essential. Another area of R&D is rare isotope beam capabilities, which could lead to a set of accelerator technologies and instrumentation developments targeted to explore the limits of nuclear existence. By producing and studying highly unstable nuclei that are now formed only in supernovae and neutron star mergers, scientists could better understand stellar evolution and the origin of the elements.

Our ability to continue making a scientific impact on the general community relies heavily on the availability of cutting edge technology and advances in detector instrumentation, electronics, software, and accelerators. The technical topics that follow describe research and development opportunities in the equipment, techniques, and facilities needed to conduct and advance nuclear physics research at existing and future facilities.

For additional information regarding the Office of Nuclear Physics priorities, click here.

35. NUCLEAR PHYSICS SOFTWARE AND DATA MANAGEMENT

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Large scale data storage and processing systems are needed to store, retrieve, distribute, and process data from nuclear physics experiments conducted at large facilities, such as Brookhaven National Laboratory's (BNL) Relativistic Heavy Ion Collider (RHIC) and the Thomas Jefferson National Accelerator Facility (TJNAF). In addition, data acquisition for the Facility for Rare Isotope Beams (FRIB) that is nearing completion will require considerable speed and flexibility in collecting data from its detectors. An electron ion collider (EIC), undergoing design and eventual construction at BNL, is anticipated to produce data at rates that will also challenge current computing and storage resources. Experiments at such facilities are extremely complex, involving thousands of detector elements that produce raw experimental data at rates in excess of several GB/sec, resulting in the annual production of raw data sets of size 5 to 10 Petabytes (PB). A single experiment can produce reduced data sets of many 100s of Terabytes (TB) which are then distributed to institutions worldwide for analysis, and with the increasing data generation rates at RHIC and TJNAF, multi-PB reduced datasets will soon be common. Increased adoption and implementation of streaming readout protocols will only accelerate the data acquisition rates. Research on the management of such large data sets, and on high speed, distributed data acquisition will be required to support these large scale nuclear physics experiments.

All grant applications must explicitly show relevance to the DOE Nuclear Physics (NP) program. Grant applications must be informed by the state of the art in nuclear physics applications, commercially available products, and emerging technologies. A proposal based on merely incremental improvements or little innovation will be considered non-responsive unless context is supplied that convincingly shows its potential for significant impact or value to the DOE nuclear physics program.

Applications which are largely duplicative of previously funded research by the Office of Nuclear Physics will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from the Office of Nuclear Physics. Those awards can be found at https://science.osti.gov/sbir/Awards (Release 1, DOE Funding Program: Nuclear Physics).

The subtopics below refer to innovations that will advance our nation's capability to perform nuclear physics research, and more specifically to improve DOE NP Facilities and the wider NP community experimental programs. Although applicants may wish to gather information from and collaborate with experts at DOE National Laboratories to establish feasibility for their innovations, DOE expects all applicants to address commercialization opportunities for their product or service in adjacent markets such as medicine, homeland security, the environment and industry. Grant applications that propose using the resources of a third party (such as a DOE laboratory) must include in the application, a letter of certification from an authorized official of that organization.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought only in the following subtopics:

a. Tools for Large Scale Distributed Data Storage

A trend in nuclear physics is to maximize the use of distributed storage and computing resources by constructing end-to-end data handling and distribution systems, with the aim of achieving fast data processing and/or increased data accessibility across many disparate computing facilities. Such facilities include local computing resources, university based clusters, major DOE funded computing resources, and commercial cloud offerings.

Grant applications are sought for (1) hardware and/or software techniques to improve the effectiveness and reduce the costs of storing, retrieving, and moving such large volumes of data (> 1 PB/day), possibly including but not limited to automated data replication, data transfers from multiple sources, or network bandwidth scheduling to achieve the lowest wait-time or fastest data processing at low cost; (2) effective new approaches to data mining or data analysis through data discovery or restructuring (examples of such approaches might include fast information retrieval through advanced metadata searches or in-situ data reduction, and repacking for remote analysis and data access); (3) new tools for co-scheduling compute, network and storage resources for distributed data-intensive high performance computing tasks, such as user analyses in which repeated passes over large datasets are needed.

Open source software solutions are strongly encouraged. Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and declined without review.

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b. Applications of AI/ML to Nuclear Physics Data Science

As discussed above, analysis of experimental data from accelerator-based detector systems is a central task in the NP community. In the case of medium scale experiments, data sets will be collected with each event having a large number of independent parameters or attributes. The manipulation of these complex datasets into summaries suitable for the extraction of physics parameters and model comparison is a difficult and time-consuming task. Currently, both the accelerator facilities and university-based groups carrying out analysis maintain local computing clusters running domain specific software, often written by the experimentalists themselves. Recently, the data science community has developed tools and techniques to apply machine learning (ML) and artificial intelligence (AI) for handling such tasks at scale in an efficient and more generic manner. These tools are generally open-source and can be effectively deployed on platforms ranging from distributed computing resources provided by commercial web services to leadership computing facilities. Furthermore, these tools hide many of the implementation details required to run efficiently on distributed systems allowing the experimenter to focus on the physics analysis task at hand while fully utilizing a modern computing infrastructure

Application of these new ML and AI technologies to the analysis of nuclear physics data requires the development of domain specific tools. Sources of such data are described in Topic 39 (Nuclear Instrumentation, Detection Systems and Techniques).

Applicants are expected to address a specific application domain in experimental nuclear physics data analysis. Proposals should address performance and plan to demonstrate feasibility to non-experts in computer systems with working prototypes and comprehensive tutorials and/or documentation.

Open source software solutions are strongly encouraged. Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and declined without review.

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c. Heterogeneous Concurrent Computing

Computationally demanding theory calculations as well as detector simulations and data analysis tasks can be significantly accelerated through the use of general purpose Graphics Processing Units (GPUs). The ability to exploit these graphics accelerators has been significantly constrained by the effort required to port the software to the GPU environment. Much more capable cross compilation or source-to-source translation tools are needed that are able to convert conventional as well as very complicated templatized C++ code into high performance implementations for heterogeneous architectures.

Utilizing High Performance Computing (HPC) and Leadership Computing Facilities (LCFs) is of growing relevance and importance to experimental NP as well. Most HPC and LCF facilities are evolving toward hybrid CPU and GPU architectures oriented toward machine learning. Existing analysis codes do not sufficiently reveal the concurrency necessary to exploit the high performance of the architectures in these systems. NP analysis problems do have the potential data concurrency needed to perform well on multi- and many-core architectures but currently struggle to achieve high efficiency in both thread-scaling and in vector utilization. NP experimental groups are increasingly invited and encouraged to use such facilities, and DOE is assessing the needs of computationally demanding experimental activities such as data analysis, detector simulation, and error estimation in projecting their future computing requirements. Proposals are sought to develop tools and technologies that can facilitate efficient use of large-scale CPU-GPU hybrid systems for the applications and data-intensive workflows characteristic of experimental NP. Ideally, tools should be designed, and interfaces constructed in such a way to abstract low-level computational performance details away from users who are not computer scientists. At a higher level, new analysis algorithms would be designed for the user and not necessarily focused on technical efficiencies. An example would be an online web portal which could simulate a basic x86 processor, compile custom code and run it with an *in situ* analyzer running in the background to detect and recommend different HPC tools and techniques automatically.

Open source software solutions are strongly encouraged. Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and declined without review.

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d. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the general description at the beginning of this topic.

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References:

1. Paschalis, S., Lee, I.Y., Macchiavelli, A.O., Campbell, C.M., et. al. (2013). *The Performance of the Gamma-Ray Energy Tracking In-beam Nuclear Array GRETINA,* Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Vol. 709, p. 44–55. https://www.sciencedirect.com/science/article/pii/S0168900213000508
2. Aschenauer, E., Kiselev, A., Petti, R., Ullrich, T., et al. (2019). *Electron-Ion Collider Detector Requirements and R&D Handbook*, Electron-Ion Collider User Group, p. 56. http://www.eicug.org/web/sites/default/files/EIC_HANDBOOK_v1.1.pdf
3. National Computational Infrastructure for Lattice Quantum Chromodynamic. (2020). *USQCD: US Lattice Quantum Chromodynamics*. www.usqcd.org/
4. Fowler, R. J. (2012). *The Secret Life of Quarks, Final Report For The University of North Carolina at Chapel Hill*, U.S. Department of Energy, doi: 10.2172/1062585. https://www.osti.gov/servlets/purl/1062585
5. The Globus Alliance. (2020). *Homepage*, University of Chicago and Argonne National Laboratory. https://www.globus.org/
6. University of Wisconsin. (2020). *HTCondor: High Throughput Computing*, University of Wisconsin. www.cs.wisc.edu/condor/
7. CERN. (2020). *CERN VM Software Appliance*. http://cernvm.cern.ch/portal/
8. The Virtual Data Toolkit (VDT). (2020). V*DT Software Distribution*, Open Science Grid (OSG). http://vdt.cs.wisc.edu/index.html/
9. CERN. (2020). *Welcome to the Worldwide LHC Computing Grid*, Worldwide Large Hadron Collider (LHC), Computing Grid (WLCG). http://wlcg.web.cern.ch/
10. European Grid Infrastructure (EGI). (2020). *European Grid Infrastructure (EGI).* http://www.egi.eu/
11. Baru, C. (2015). *SDSC's Storage Resource Broker Links, NPACI Data-Intensive Infrastructure*, San Diego Supercomputer Center (SDSC). https://www.sdsc.edu/pub/envision/v14.1/srb.html
12. Wikipedia. (2020). *Event-Driven Architectures (EDA),* Wikipedia. http://en.wikipedia.org/wiki/Event_driven_architecture
13. National Institute of Standards and Technology. (2014). *NIEEE 1588TM Standard for A Precision Clock Synchronization Protocol for Networked Measurement and Control Systems*, National Institute of Standards and Technology. https://www.nist.gov/el/intelligent-systems-division-73500/ieee-1588
14. SLAC/CERN. (2020). *Welcome to the XRootD Webpage*, XRootD. http://xrootd.slac.stanford.edu/
15. CERN. (2018). *PROOF (Parallel ROOT Facilities),* ROOT Data Analysis Framework. http://root.cern.ch/drupal/content/proof
16. Open Hardware Repository. (2020). *The White Rabbit Project Webpage*, Open Hardware Repository. https://www.ohwr.org/projects/white-rabbit
17. Martoiu, S., Muller, H., Tarazona, A., and Toledo, J. (2012). *Development of the Scalable Readout System (SRS) for Micro-pattern Gas Detectors and Other Applications*, Journal of Instrumentation, Vol. 8, p. 12. https://iopscience.iop.org/article/10.1088/1748-0221/8/03/C03015/pdf
18. Muller, H., (2017). *Scalable Readout System: from APV to VMM frontends*, p. 37. https://indico.cern.ch/event/676702/contributions/2818988/attachments/1575628/2488041/From_APV_to_VMM_frontends.pdf
19. Hasell, D. and Bernauer, J. (2017). *Summary of the Streaming Readout Workshop*, p. 4. https://eic.jlab.org/wiki/images/c/c4/SR_Summary.pdf
20. Purschke, M. L., et al. (2019). *Streaming Readout V, Developing a Common, Community-Wide Standard for Streaming Readout*, RIKEN BNL Research Center Workshop Hosted at Brookhaven National Laboratory, November 13-15, 2019. https://www.bnl.gov/srv2019/
21. Bedaque, P., et al. (2020). *Report from the A.I. For Nuclear Physics Workshop*, Cornell University. https://arxiv.org/abs/2006.05422

36. NUCLEAR PHYSICS ELECTRONICS DESIGN AND FABRICATION

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The DOE Office of Nuclear Physics (NP) seeks new developments in detector instrumentation electronics with significantly improved energy, position, timing resolution, sensitivity, rate capability, stability, dynamic range, and background suppression. Of particular interest are innovative readout electronics for use with the nuclear physics (NP) detectors described in Topic 39 (Nuclear Instrumentation, Detection Systems and Techniques). An important criterion is the cost per channel of electronic devices and modules.

Nuclear physics detectors range in complexity, from those that fill a modest-sized laboratory to those that fill a multistory building. While most detectors may operate at or near room temperature, those used in rare decay experiments like neutrinoless double beta decay operate at cryogenic temperatures, below 20 mK for some experiments. This underscores that in general, nuclear physics electronics operate in extreme environments, whether it be where there is high radiation, or extreme cryogenic temperatures.

All grant applications must explicitly show relevance to the DOE Nuclear Physics program. Grant applications must be informed by the state of the art in nuclear physics applications, commercially available products and emerging technologies. A proposal based on incremental improvements or little innovation will be considered non-responsive unless context is supplied that convincingly shows its potential for significant impact or value to the DOE nuclear physics program.

Applications which are largely duplicative of previously funded research by the Office of Nuclear Physics will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from the Office of Nuclear Physics to avoid duplication. Those awards can be found at https://science.osti.gov/sbir/awards/ (Release 1, DOE Funding Program: Nuclear Physics).

The subtopics below refer to innovations that will advance our nation's capability to perform nuclear physics research, and more specifically to improve scientific productivity at DOE Nuclear Physics Facilities and the wider NP community experimental programs. Applicants may wish to gather information from and collaborate with experts at DOE National Laboratories to establish feasibility for their innovations. DOE expects all applicants to address commercialization opportunities for their product or service in adjacent markets such as medicine, homeland security, the environment and industry. Grant applications that propose using the resources of a third party (such as a DOE laboratory) must include in the application, a letter of certification from an authorized official of that organization.

Grant applications are sought only in the following subtopics:

a. Advances in Digital Processing Electronics

Digital signal processing electronics are needed to replace analog signal processing, following low noise amplification and anti-aliasing filtering, in nuclear physics applications. Grant applications are sought to develop high speed digital processing electronics that, relative to current state of the art, improve the effective number of bits to 16 at sampling rates of > 4GHz and a bandwidth > 2 GHz, with minimal integral non-linearity. Such devices should have 64 channels with fast timing (< 10 ps) and be rad-hard (tolerate 10 Mrad with 10^{15} n/cm^2). Emphasis should be on low power dissipation and cost.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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b. Front-End Application-Specific Integrated Circuits

Grant applications are sought to develop front-end application-specific integrated circuits (ASICs) for amplifying and processing data from highly-segmented solid-state and gas detectors in pixels, strips or drift configurations, including silicon photomultipliers (SiPM), multi-channel plate photomultipliers (MCP-PMTs), large area picosecond photodetectors (LAPPD) and germanium detectors.

Microelectronics of specific interest include:

1. Very low power and very low noise charge amplifiers and filters, very high rate photon-counting circuits, high-precision charge and timing measurement circuits, low-power and small-area ADCs and TDCs, efficient sparsifying and multiplexing circuits.
2. Two-dimensional high-channel-count circuits for small pixels combined with high-density, high-yield, and low-capacitance interconnection techniques.
3. Microelectronics for extreme environments such as high-radiation (both neutron and ionizing) and low temperature, depending on the application. Specifications for the former are: high channel count (64 channels) ASIC with fast timing (< 10 ps), high radiation hardness (10 mrad with 10^{15} n/cm^2), fast waveform sampling (> 4GHz) and bandwidth (> 2GHz).
4. Very-large-scale systems-on-chip or experiments-on-chip characterized by high functionality, high programmability, DSP capabilities, high data rate interface.

Relative to the state of the art these circuits should be low-cost, user friendly, and capable of communicating with commercial auxiliary electronics.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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c. Next Generation Pixel Sensors

Active pixel sensors (APS) in CMOS (complementary metal-oxide semiconductor) technology have largely replaced charge coupled devices (CCDs) as imaging devices and cameras for visible light. Nuclear physics experiments at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory and at the Large Hadron Collider (LHC) at CERN have developed and used APS devices as direct conversion minimum ionizing particle detectors. As an example, the innermost tracking detector of the STAR experiment at RHIC contained 356 million (21x21x50 µm) APS elements. Future proposed high luminosity colliders such as the Electron Ion Collider (EIC) plan to operate at luminosities in the range 10^{33}–10^{34} cm^{-2} s^{-1} and will require radiation hard tracking devices placed at radii below 10 cm from the beam axis. Therefore, cost effective alternatives to the present generation high density APS devices will be required. An ambitious goal is to develop extremely thin ~0.1% radiation length detector modules capable of high rate readout. In low energy nuclear physics applications, the bulk silicon substrate is used as the active volume given it is highly-resistive and depleted. A major advance in CMOS would be to introduce an electric field into the passive substrate region and to deplete it. This would result in a much shorter collection time and negligible charge dispersion allowing sensitivity to non-minimum ionizing particles, such as MeV-range gamma rays. Grant applications are also sought for the next generation of active pixel sensors. Options may include integrated CMOS detectors which combine initial signal processing and data sparsification on a high-resistivity silicon, superconducting large area pixel detectors, and novel 2.5D- and 3D-pixel materials and geometric structures.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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d. Manufacturing and Advanced Interconnection Techniques

Many next-generation detectors will have highly segmented electrode geometries covering areas up to several square meters. Conventional packaging and assembly technology cannot be used with these large areas. Grant applications are sought to develop (1) advanced microchip module interconnect technologies that address the issues of high-density area-array connections – including modularity, reliability, repair/rework, and electrical parasitics; (2) technology for aggregating and transporting the signals (analog and digital, optically and/or wirelessly) generated by the front-end electronics, and for distributing and conditioning power and common signals (clock, reset, etc.); and (3) low-cost and low-mass methods for grounding and shielding.

Lastly, highly-segmented detectors with pixels smaller than 100 microns present a significant challenge for integration with frontend electronics. New monolithic techniques based on vertical integration and through-silicon vias have demonstrated advantages. Grant applications are sought to demonstrate reliable, readily-manufacturable technologies to interconnect silicon pixel detectors with CMOS front-end integrated circuits. Of great interest are high-density front-end CMOS circuits directly bonded to a high resistivity silicon detector layer. The high resistivity detector layer would be fully depleted to enable fast charge collection with very low diffusion. The thickness of this layer would be optimized for the photon energy of interest or to obtain sufficient signal from a minimum number of ionizing particles.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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e. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the general description at the beginning of this topic.

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References:

1. Adare, A., et al. (2015). *An Upgrade Proposal from the PHENIX Collaboration*, p.243. sPHENIX. https://arxiv.org/abs/1501.06197
2. Adare, A., Aidala, C., Ajitanand, N.N., Akiba, Y., et al. (2014). *Concept for an Electron Ion Collider (EIC) Detector Built Around the BaBar Solenoid*, The PHENIX Collaboration, p. 59. https://arxiv.org/abs/1402.1209v1
3. Abelev, B., Adam, J., Adamova, D., Aggarwal, M.M., et. al. The ALICE Collaboration. (2014). *Technical Design Report for the Upgrade of the ALICE Inner Tracking System*, Journal of Physics G: Nuclear and Particle Physics, Vol. 41, Issue 8, p. 181. http://iopscience.iop.org/article/10.1088/0954-3899/41/8/087002/meta
4. The SoLID Collaboration. (2014). *SoLID (Solenoidal Large Intensity Device) Preliminary Conceptual Design Report*, p. 225. http://hallaweb.jlab.org/12GeV/SoLID/files/solid_precdr.pdf
5. EIC. (2020). *Generic Detector R&D for an Electron Ion Collider*, Wikipedia. https://wiki.bnl.gov/conferences/index.php/EIC_R%25D
6. Aune, S., Delagnes, E., Garcon, M., Mandjavidze, I., et. al. (2012). *Design and Assembly of Fast and Lightweight Barrel and Forward Tracking Prototype Systems for an EIC*, p. 11. https://wiki.bnl.gov/conferences/images/6/6f/RD_2011-2_F.Sabatie.pdf
7. Adrian, P.H., Field, C., Graf, N., Graham, M., et. al. (2012). *Status of the Heavy Photon Search Experiment at Jefferson Laboratory*, p. 89. https://www.jlab.org/exp_prog/proposals/12/C12-11-006.pdf
8. Niinikoski, T.O., Abreu, M., Anbinderis, P., Anbinderis, T., et al. (2004). *Low-temperature Tracking Detectors*, Nuclear Instruments and Methods in Physics Research, Section A--Accelerators, Spectrometers, Detectors and Associated Equipment, Vol. 520, Issues 1-3, p. 87-92. https://www.sciencedirect.com/science/article/pii/S0168900203031310
9. Paschalis, S., Lee, I.Y., Machiavelli, A.O., Campbell, C.M., et al. (2013). *The Performance of the Gamma-Ray Energy Tracking In-beam Nuclear Array GRETINA*, Nuclear Instruments and Methods Physics Research A, Vol. 709, p. 44-55. http://adsabs.harvard.edu/abs/2013NIMPA.709...44P
10. Ionascut-Nedelcescu, A., Carlone, C., Houdayer, A., Raymond, S., et al. (2002). *Radiation Hardness of Gallium Nitride*, IEEE Transactions on Nuclear Science, Vol. 49, Issue 6, Part 1, p. 2733-2738, ISSN: 0018-9499. http://ieeexplore.ieee.org/abstract/document/1134213/
11. Schwank, J.R., Dodd, P.E., Shaneyfelt, M.R., Vizkelethy, G., et al. (2002). *Charge Collection in SOI (Silicon-on-Insulator) Capacitors and Circuits and Its Effect on SEU (Single-Event Upset) Hardness*, IEEE Transactions on Nuclear Science, Vol. 49, Issue 6, Part 1, p. 2937-2947, ISSN: 0018-9499. http://ieeexplore.ieee.org/xpl/abstractKeywords.jsp?arnumber=1134244
12. IEEE. (2014). *IEEE Nuclear Science Symposium and Medical Imaging Conference*, Seattle, WA, Complete Technical Program, November 8-15. https://ieeexplore.ieee.org/xpl/mostRecentIssue.jsp?punumber=7422433
13. Polushkin. V. (2004). *Nuclear Electronics: Superconducting Detectors and Processing Techniques*, J. Wiley, p. 402, ISBN: 0-470-857595. https://www.wiley.com/en-us/Nuclear+Electronics%3A+Superconducting+Detectors+and+Processing+Techniques-p-9780470857687

14. Argonne National Laboratory. (2014). *Front End Electronics (FE 2014),* 9th International Meeting on Front-End Electronics, May 19-23. http://indico.cern.ch/event/276611/
15. De Geronimo, G., D'Andragora, A., Li, S., Nambiar, N., et al. (2011). *Front-end ASIC for a Liquid Argon TPC*, IEEE Transactions on Nuclear Science, Vol. 58, Issue 3, p. 1376-1385. https://ieeexplore.ieee.org/document/5752881
16. Institut Pluridisciplinaire Hubert Curien (IPHC). (2020). *Physics with Integrated CMOS Sensors and Electron Machines (PICSEL),* Institut Pluridisciplinaire Hubert Curien (IPHC). http://www.iphc.cnrs.fr/-PICSEL-.html
17. L'Ecole Polytechnique. (2020). *Omega – Centre De Microelectronique*. http://omega.in2p3.fr/
18. PSEC. (2020). *Large-Area Picosecond Photo-Detectors Project*, PSEC. psec.uchicago.edu
19. Paul Scherrer Institut. (2020). *DRS Chip Home Page*, Paul Scherrer Institut (PSI). drs.web.psi.ch
20. Ritt, S. (2014). *A New Timing Calibration Method for Switched Capacitor Array Chips to Achieve Sub-picosecond Timing Resolutions*, Workshop on Picosecond Photon Sensors, Scherrer Institute, p.26. http://psec.uchicago.edu/library/chipdesign/ritt_timing_calibration_method.pdf
21. RD51 Collaboration. (2010). *Development of Micro-Pattern Gas Detectors Technologies,* CERN. https://ep-news.web.cern.ch/content/rd51-collaboration-development-micro-pattern-gas-detectors-technologies
22. Bedaque, P., et al. (2020). *Report from the A.I. For Nuclear Physics Workshop* (2020), https://arxiv.org/abs/2006.05422
23. Purschke, M. L., et al. (2019). *Streaming Readout V, Developing a Common, Community-Wide Standard for Streaming Readout*, RIKEN BNL Research Center Workshop Hosted at Brookhaven National Laboratory, November 13-15, 2019. https://www.bnl.gov/srv2019/

37. NUCLEAR PHYSICS ACCELERATOR TECHNOLOGY

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The Nuclear Physics (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 their associated systems. Research and development is desired that will advance fundamental accelerator technology and its applications to nuclear physics scientific research. Areas of interest include the enabling technologies of the Brookhaven National Laboratory's Relativistic Heavy Ion Collider (RHIC), linear accelerators such as the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF) and the Argonne Tandem Linac Accelerator System (ATLAS) at Argonne National Laboratory, development of devices and/or methods that would be useful in the generation of intense rare isotope beams at the Facility for Rare Isotope Beams (FRIB) linac nearing completion at Michigan State University, and technologies relevant to the development of the future Electron Ion Collider (EIC), A major focus in all of the above areas is superconducting radio frequency (SRF) accelerators, superconducting magnets, and related technologies. Relevance to nuclear physics must be explicitly described, as discussed in more detail below.

All grant applications must explicitly show relevance to the DOE NP Program. Grant applications must be informed by the state of the art in nuclear physics applications, commercially available products, and emerging technologies. A proposal based on merely incremental improvements or little innovation will be considered non-responsive unless context is supplied that convincingly shows its potential for significant impact or value to the DOE NP Program.

Applications which are largely duplicative of previously funded research by the Office of Nuclear Physics will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from the Office of Nuclear Physics to avoid duplication. Those awards can be found at https://science.osti.gov/sbir/awards/ (Release 1, DOE Funding Program: Nuclear Physics).

The subtopics below refer to innovations that will advance our nation's capability to perform nuclear physics research, and more specifically to improve DOE NP Scientific User Facilities and the wider NP community's experimental programs. Although applicants may wish to gather information from and collaborate with experts at DOE National Laboratories, for example, to establish feasibility for their innovations, DOE expects all applicants to address commercialization opportunities for their product or service in adjacent markets such as medicine, homeland security, the environment and industry. Grant applications that propose using the resources of a third party (such as a DOE laboratory) must include in the application, a letter of certification from an authorized official of that organization.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought only in the following subtopics:

a. Materials and Components for Radio Frequency Devices

Grant applications are sought to improve or advance superconducting and normal-conducting materials or components for RF devices used in particle accelerators. Areas of interest include;

1. peripheral components for both room temperature and superconducting structures, such as beam pipe absorbers, SRF HOM loads, possibly based on metamaterials, and capable of being cleaned, particulate-free bellows and gate valves and associated low-loss cryogenic beam line flange connections, with diameters ranging from 2" to 36";
2. cleaning techniques for removal of > 0.01 µm particulates in diameter from superconducting cavities which can replace or compliment high-pressure water rinsing e.g., methods for cleaning whole cryomodules, alternative techniques to dry ice and high pressure water cleaning;
3. novel techniques for producing the higher order mode (HOM) or fundamental power coupler (FPC) end groups of elliptical cavities at low cost, including e.g. additive manufacturing, hydroforming or impulse forming. End groups must sustain ~10% of the surface fields in the cells or ~10-20 mT without degrading the cavity Q0 below $1X10^{10}$; and
4. metal forming techniques, including the use of bimetallic materials, with the potential for significant cost reductions by simplifying cavity sub-assemblies e.g., dumbbells and end groups, as well as eliminating or reducing the number of electron beam welds.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov

b. Design and Operation of Radio Frequency Beam Acceleration Systems

Grant applications are sought for the design, fabrication, and operation of radio frequency accelerating structures and systems for electrons, protons, and light- and heavy ion particle accelerators. Areas of interest include;

1. innovative techniques for relative field control and synchronization of multiple crabbing structures (0.1° of phase and 0.01% amplitude RMS jitter) in the presence of 10-100 Hz microphonics-induced variations of the structures' resonant frequencies (0.1-1.5 GHz);
2. active methods for damping microphonic modes of cavities installed in cryomodules , such as mode-by-mode piezo feedback, fast active tuners or variable couplers, to reduce microphonic excursions in power-limited SRF cavities;
3. development of wide tuning (with respect to the center frequency of up to 10^{-4}) superconducting RF cavities for acceleration and/or storage of relativistic heavy ions;
4. devices and methods for accurate in-situ measurement of SRF cavity Qo's at very high values where an individual cavity's dynamic losses may be small compared to the static background;
5. development of an inexpensive low noise fast switching DC high voltage power supply suitable for driving a L-band CW magnetron with amplitude modulations up to 1 kHz; and
6. Development of a compact RF chopping system to reduce bunched ion beam frequency from about 100 MHz to about 20 MHz at roughly 500 keV/u. The system should be capable to operate near SRF cryomodule and dump up to 500 W heavy ion beam power.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov

c. Particle Beam Sources and Techniques

Grant applications are sought to develop

1. methods and/or devices for improving emission capabilities of photocathode sources (polarized and unpolarized) used by the NP community, such as improving charge lifetime, bunch charge, average current, emission current density, emittance, or energy spread (Note, Letters of Intent or applications proposing the use of diamond amplifiers and variants will be considered nonresponsive.);
2. novel technologies for ion sources capable of generating high-intensity, high-brightness, high charge state heavy ion beams, for example: ~12 pμA of uranium beam at charge states between q=32 and 46 with an rms emittance of 0.1π mm-mrad. If an oven is used to provide uranium beams with these properties, the high temperature oven must reliably reach 2300 °C within the high field of the ECR ion source injection region;
3. novel technologies for liquid helium (4 K and 1.9 K) high voltage breaks to supply helium to ECR ion sources on high voltage platforms. Such a break would be useful to overcome the cryogenic cooling limitations of high performance ECR ion sources on high voltage platforms that need to use cryo-coolers;
4. passivation techniques or other treatments to ECR components to reduce contamination from the alloys used in the source;
5. novel quench protection systems for Nb3Sn and HTS superconducting 4^{th} and 5^{th} Generation ECR ion source combined function magnets (sextupole and solenoids); and

6. efficient cw positron beam sources (polarized and unpolarized) motivated by the NP community, aimed at improving aspects of pair-production targets, operating at low energy (10-100 MeV), high power (50-100 kW), and at several 100 MHz.

Accelerator techniques for an energy recovery linac (ERL) based electron cooling facility for medium to high energy bunched proton or ion beams are of great interest for next generation colliders, like the Electron-Ion Collider (EIC). Grant applications are sought for

1. High voltage pulse generators matched to 50 or 75 Ω with >50 kV 10-200 ns flat-top pulse profiles, <10 ns rise and fall times and repetition rates >100 Hz for high-energy beam kickers, and
2. Novel methods for clearing electrons or ions trapped in intense hadron beams.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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d. Polarized Beam Sources and Polarimeters

With respect to polarized sources, grant applications are sought to develop

1. CW polarized electron sources and/or associated components delivering beams of ~1 mA for at least 24 hours, with longitudinal polarization greater than 90%; and a photocathode quantum efficiency > 5% at ~780 nm. At these beam currents, the cw polarized source should be capable of delivering high bunch charges > 100 pC/bunch for EIC based storage rings. (Note: applications proposing the use of diamond amplifiers and variants will be considered nonresponsive.);
2. advanced software and hardware to facilitate the manipulation and optimized control of the spin of polarized beams;
3. absolute polarimeters for spin polarized ^{3}He beams with energies up to 160 GeV/nucleon;
4. polarimeter concepts for bunch by bunch hadron polarimetry with a bunch spacing as short as 2 ns; and
5. advanced electron or positron beam polarimeters such as those that operate in the energy range of 10-100 MeV, with average currents exceeding 200 uA, and with accuracies that are <1%.

For applications involving software, open source solutions are strongly encouraged. Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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e. Rare Isotope Beam Production Technology

Grant applications are sought to develop

1. Radiation resistant stepper motor with integrated captive leadscrew with the following features: a) NEMA size 23 with max thrust force > 300 lbs; b) 0.9 degree resolution and micro stepping compatible; c) Radiation tolerance to 10^4 Gy (10^6 rad); and
2. Development of a non-destructive diagnostics system to measure intensities of fast (~100-200 MeV/u) rare isotope beams in the range from 10^4 to 10^{11} ions/sec.

(Additional needs for high-radiation applications can be found in subtopic e "Technology for High Radiation Environments" of Topic 39, Nuclear Physics Instrumentation, Detection Systems and Techniques.)

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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f. Accelerator Control and Diagnostics

As accelerator facilities advance in their capabilities, it is important that diagnostics and controls keep pace. Grant applications are sought to develop advanced beam diagnostics for concepts and devices that provide high speed measurements, real-time monitoring, and readout of particle beam intensity, position, emittance, polarization, luminosity, transverse profile, longitudinal phase space, time of arrival, and energy. More specifically:

For facilities that produce high average power beams, grant applications are sought for

1. measurement devices/systems for cw beam currents in the range 0.01 to 100 μA, with very high precision ($<10^{-4}$) and short integration times;
2. non-intercepting beam diagnostics for stored proton/ion beams, and/or for ampere class electron beams;
3. devices/systems that measure the emittance of intense (>100 kW) CW ion beams; and
4. particulate counters that can be integrated into ultra-high vacuum, cryogenic and radiation environments

For heavy ion linear accelerator beam facilities, grant applications are sought for

1. beam diagnostics for ion beams with intensities less than 10^7 nuclei/second over a broad energy range up to 400 MeV/u (an especially challenging region is for intensities of 10^2 to 10^5 with beam energy from 25 keV to 1 MeV/nucleon);
2. diagnostics for time-dependent, multicomponent, interleaved heavy ion beams. The diagnostic system must separate time-dependent constituents (total period for switching between beams >10 ms), where one species is weaker than the other, and is ~5% of a 30 - 100 ms cycle. The more intense beam would account for the remainder. Proposed solutions which work over a subset of the total energy range are acceptable;
3. on-line, minimally interceptive systems for measurement of beam contaminant species or components. (Energy range of primary ion species should be 500 keV/nucleon to 2 MeV/nucleon.); and
4. advanced diagnostic methods and devices for fast detection (e.g. < 10 us) of stray beam loss for low energy heavy ion beams (e.g. ions heavier than Argon at energies above 1 MeV/nucleon and below 100 MeV/nucleon) to facilitate accelerator machine protection.

For accelerator controls, grant applications are sought to develop:

1. a Webkit application framework to enable the development of data visualization and controls tools;
2. a runtime environment - an extendable framework to process and display real time data that supports control system protocols (e.g. EPICS v3, v4), web services, and integration patterns. The model would accept development of advanced control systems for tuning and stabilizing beam transport and higher-moment properties such as emittance, luminosity, etc., including real-time fast feedforward and

optimization methods through active manipulation of critical components' parameters using Machine Learning (ML) techniques or other Artificial Intelligence (AI) expert systems. Submissions with ML/AI applications should be explicit in what problem is being addressed and the methods that will be applied; and
3. software applications for collection, visualization, and analysis of post-mortem data from beam line data acquisition and storage devices.

Applications to this subtopic should indicate familiarity with complex accelerator systems and the interfaces between the beamline diagnostics and the control systems in use at large accelerator installations. That could also include accelerators like those at Texas A&M's Cyclotron Institute, TUNL at Duke University, and tandem accelerator facilities supported by the National Science Foundation at universities like Notre Dame and Ohio University.

For applications involving software, open source solutions are strongly encouraged. Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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g. Magnet Development for Future Electron-Ion Colliders (EIC)

A full utilization of the discovery potential of the EIC will require a full-acceptance system that can provide detection of reaction products scattered at small angles with respect to the incident beams over a wide momentum range. Grant applications are sought for hardware developments to reduce the costs of production of these interaction region magnets and to the supporting subsystems.

1. cost-effective materials and manufacturing techniques for interaction region magnets, including components for an integrated cold magnet assembly such as support systems, compact cold to warm transitions, and cold BPMs; and
2. high efficiency cooling methods and cryogenic systems; power supplies and the interaction magnets.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics accelerator facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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h. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov

References:

1. U.S. Department of Energy. (2015). *The 2015 Long Range Plan for Nuclear Science, Reaching for the Horizon*, Office of Science, p. 160. http://science.osti.gov/~/media/np/nsac/pdf/2015LRP/2015_LRPNS_091815.pdf

2. U. S. Department of Energy. (2020). *Argonne Tandem Linac Accelerator System (ATLAS),* U. S. Department of Energy. https://science.osti.gov/np/facilities/user-facilities/atlas/
3. U.S. Department of Energy. (2020). *Labs at-a-Glance: Thomas Jefferson National Accelerator Facility,* Future Science at Thomas Jefferson National Accelerator Laboratory, U.S. Department of Energy. http://science.osti.gov/laboratories/thomas-jefferson-national-accelerator-facility/
4. U.S. Department of Energy. (2020). *Relativistic Heavy Ion Collider (RHIC),* U.S. Department of Energy, Office of Science. https://science.osti.gov/np/facilities/user-facilities/rhic/
5. Michigan State University. (2020*). Facility for Rare Isotope Beams*, Michigan State University. http://frib.msu.edu/
6. Leitner, D., Abbot, S.R., Abell, D., Aberle, O.,et al. (2003). *Proceedings of 2003 Particle Accelerator Conference*, PAC 2003 Particle Accelerator Conference, Portland, OR, May 12-16, p. 3377. http://accelconf.web.cern.ch/accelconf/p03/INDEX.HTM
7. Angoletta, M.E. (2006). *Digital Low Level RF*, Proceedings of the European Particle Accelerator Conference, CERN, AB/RF, EPAC'06, Edinburgh, WEXPA03, p. 19. https://accelconf.web.cern.ch/accelconf/e06/TALKS/WEXPA03_TALK.PDF
8. Thomas Jefferson National Accelerator Laboratory. (2012). *7th SRF Materials Workshop*, Thomas Jefferson National Accelerator Laboratory, July 2012. https://www.jlab.org/indico/conferenceDisplay.py?confId=20
9. Freeman, H. (2000). *Heavy Ion Sources: The Star, or the Cinderella, of the Ion-Implantation Firmament?,* Review of Scientific Instruments, Vol. 71, Issue 2, p. 603-611, ISSN: 0034-6748. http://adsabs.harvard.edu/abs/2000RScI...71..603F
10. Trbojevic, D., Berg, J.S., Brooks, S., Hao, Y., et al. (2015). *ERL with Non-scaling Fixed Field Alternating Gradient Lattice for eRHIC*, Proceedings of the International Particle Accelerator Conference (IPAC'15), Richmond, VA, p. 6. https://www.bnl.gov/isd/documents/88876.pdf
11. Hayano, H. (2014). *TESLA Technology Collaboration Meeting*, KEK, Dec 2-5, 2014. https://indico.desy.de/indico/event/10663/
12. Schwarz, S., Bollen, G., Kester, O., Kittimanapun, K., et al. (2010). *EBIS/T Charge Breeding for Intense Rare Isotope Beams at MSU*, Journal of Instrumentation, Vol. 5, Issue 10, C10002, p. 10. https://iopscience.iop.org/article/10.1088/1748-0221/5/10/C10002/pdf
13. SRF2015 Whistler. (2015). *17th International Conference on RF Superconductivity*, Whistler Conference Center September 13-18, 2015. http://srf2015.triumf.ca
14. Perry, A., Mustapha, B., and Ostroumov, P.N. (2013). *Proposal for Simultaneous Acceleration of Stable and Unstable Ions in ATLAS*, Proceedings of PAC2013, p. 306-308. http://accelconf.web.cern.ch/accelconf/pac2013/papers/mopma06.pdf
15. Afanasev, A., et al. (2019). *Physics with Positron Beams at Jefferson Lab 12 GeV* (2019) https://arxiv.org/abs/1906.09419
16. Solopova, A.D., Carpenter, A., Powers, T., Roblin, Y., et al. (2019). *SRF Cavity Fault Classification Using Machine Learning at CEBAF*, Proc. IPAC'19, Melbourne, Australia, May 2019, p. 17. http://accelconf.web.cern.ch/AccelConf/ipac2019/talks/tuxxplm2_talk.pdf
17. Edelen, A.L., Biedron, S.G., Chase, B.E., Milton, S.V., et al. (2016). *Neural Networks for Modeling and Control of Particle Accelerators*, IEEE Transactions on Nuclear Science, Vol. 63, Issue 2, p. 878-897. https://fast.fnal.gov/papers/07454846.pdf
18. Bedaque, P., et al. (2020). *Report from the A.I. For Nuclear Physics Workshop* (2020), https://arxiv.org/abs/2006.05422
19. U.S. Department of Energy. (2017*). Report of the Community Review of Electron Ion Collider (EIC) Accelerator R&D for the Office of Nuclear Physics*, Office of Nuclear Physics, p. 62. https://science.osti.gov/~/media/np/pdf/Reports/Report_of_the_Community_Review_of_EIC_Accelerator_RD_for_the_Office_of_Nuclear_Physics_20170214.pdf
20. Wang, J. B., et al. (2019). *An Electron-Ion Collider Study*, Brookhaven National Laboratory. https://wiki.bnl.gov/eic/upload/EIC.Design.Study.pdf

38. NUCLEAR PHYSICS INSTRUMENTATION, DETECTION SYSTEMS AND TECHNIQUES

Maximum Phase I Award Amount: $200,000	Maximum Phase II Award Amount: $1,100,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The Office of Nuclear Physics (NP) is interested in supporting grants that will lead to advances in detection systems, instrumentation, and techniques for nuclear physics experiments. Opportunities exist for developing equipment beyond the present state-of-the-art needed at universities, national scientific user facilities, and facilities worldwide. Next-generation detectors are needed for the 12 GeV Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF), the future Facility for Rare Isotope Beams (FRIB) nearing completion at Michigan State University, the Relativistic Heavy Ion Collider (RHIC), the future Electron Ion Collider (EIC) at Brookhaven National Lab, and the Argonne Tandem Linac Accelerator System (ATLAS) at Argonne National Laboratory). Also of interest is technology related to future experiments in fundamental symmetries, such as neutrinoless double-beta decay (NLDBD). In the case of NLDBD experiments, extremely low background and low count rate particle detection are essential.

All grant applications must explicitly show relevance to the DOE NP Program. Grant applications must be informed by the state of the art in nuclear physics applications, commercially available products and emerging technologies. A proposal based on merely incremental improvements or little innovation will be considered non-responsive unless context is supplied that convincingly shows its potential for significant impact or value to the DOE NP Program.

Applications which are largely duplicative of previously funded research by the Office of Nuclear Physics will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from the Office of Nuclear Physics to avoid duplication. Those awards can be found at https://science.osti.gov/sbir/Awards (Release 1, DOE Funding Program: Nuclear Physics).

The subtopics below refer to innovations that will advance our nation's capability to perform NP research, and more specifically to improve scientific productivity at DOE NP Facilities and the wider NP community experimental programs. Applicants may wish to gather information from and collaborate with experts at DOE National Laboratories to establish feasibility for their innovations. DOE expects all applicants to address commercialization opportunities for their product or service in adjacent markets such as medicine, homeland security, the environment and industry. Grant applications that propose using the resources of a third party (such as a DOE laboratory) must include in the application, a letter of certification from an authorized official of that organization.

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC) resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at http://www.nersc.gov/users/accounts/allocations/request-form/.

Grant applications are sought in the following subtopics:

a. Advances in Detector and Spectrometer Technology

Nuclear physics research has a need for devices to detect, analyze, and track photons, charged particles, and neutral particles such as neutrons, neutrinos, and single atoms. Grant applications are sought to develop and advance the following types of detectors:

Particle identification and counting detectors such as:

- Low cost large area Multi-channel Plate (MCP) type detector with high spatial resolution (≤ mm2), high rate capability (≥200 kHz/cm^2), radiation tolerance (10 Mrad with 10^{15} n/cm^2), magnetic field tolerance(2-3 T) for imaging Cherenkov detectors, and timing resolution of < 10 ps for time-of-flight detectors. The accompanying readout system (i.e. electronics, application-specific integrated circuit, etc.) should be compatible with the above requirements; high speed data buffering compatible with trigger decisions up to 1 usec later and fast data ports to allow second level triggers; "dead time less data acquisition" when incorporated as a tracker for beam identification and beam particle phase space determination.
- Large area Multigap Resistive Plate Chamber (MRPC) detectors with very high rate capability, radiation and magnetic field tolerance and high timing resolution, with the same specs as above for time-of-flight detectors. The accompanying readout system (i.e., electronics, application-specific integrated circuit, etc.) should be compatible with the above requirements as well;
- Cherenkov detectors (Threshold, Ring-Imaging (RICH), Detection of Internally Reflected Cherenkov Light (DIRC)) with broad particle identification capabilities over a large momentum range and/or large area that can operate at a high rate in noisy (very high rate, low-energy background) environments and that are also magnetic field tolerant;
- Low cost large area electromagnetic calorimetry with high energy and spatial resolution, and capability to operate for extended periods in a high-radiation environment;
- Low cost large area hadronic calorimetry with high energy resolution (<50% sqrt(E)/E) capable of operating for extended periods in a high-radiation environment;

Enhancement of particle identification using machine learning techniques, such as:

- Particle Flow algorithms to enhance hadron calorimetry;
- Pattern recognition in Cerenkov, e.g., Ring-Imaging and DIRC detectors;
- Shower shape recognition to enhance electromagnetic calorimetry;
- Event identification for low background detectors, such as those used in neutrinoless double beta decay;
- Assisted beam tuning of separators and spectrometers for rare isotope beams;
- Pattern recognition and/or physics-informed machine learning approaches for gamma-ray tracking to improve source localization and energy reconstruction;
- Algorithms for event classification, track recognition and particle identification (implantation-decay experiments) in time projection chambers and active targets;
- Heavy-ion particle identification in magnetic spectrometers and separators based on measurements of energy loss, total energy, time of flight, and momentum; and
- Position determination and track reconstruction algorithms for state-of-the-art beam tracking detectors with optical readout arrays (i.e. Optical Parallel Plate Avalanche Counters – OPPAC).

For applications involving software, open source solutions are strongly encouraged. Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate for Instrumentation, Detection Systems and Technique: Elizabeth Bartosz, Elizabeth.Bartosz@science.doe.gov

b. Development of Novel Gas and Solid-State Detectors

Nuclear physics research has the need for devices to track charged and neutral particles such as neutrons and photons. Items of interests are detectors with very good energy resolution for low- and medium-energy applications, high precision tracking of different types of particles, with fast triggering capabilities, as well as detectors that provide high energy and position resolution at high count rates (e.g. > 1 Mcps).

Grant applications are sought to develop detector systems with focus on:

- Next generation, heavy ion focal plane detectors or detector systems for magnetic spectrometers and recoil separators with high time resolution (< 150ps FWHM), high energy loss resolution (<1%), and high total energy resolution (<1%), and high position resolution (<0.4 mm FWHM), including associated readout electronic and data acquisition systems;
- Novel detector concepts such as Micropattern Gas Detectors (GEMs, Micromegas, MicroRWELLs, etc) and Parallel Plate Avalanche Chambers, for charged particle tracking, capable of submillimeter position resolution (less than a few hundred micrometers), using novel readout plane geometries offering low channel counts, high counting rate capability (> 1 MHz and/or (>200 kHz/cm^2), uniform energy-losses independent of the position, high dynamic range and low thickness (< a few mg/cm2);
- New charged particle detectors for particle identification based energy loss measurement, with energy resolution (< 1 % at 1 MeV), uniform response to a wide variety of heavy-ions (from ^{1}H to ^{235}U), and with high rate capability (> 1 MHz);
- High-rate, high-radiation hard, precision tracking devices capable of detecting low-energy reaction products such as those from few-GeV Compton and Moller scattering;
- Large area monocrystalline diamond detectors of uniform thickness and strip or pixelated readout capable of submillimeter position resolution; and
- Cost effective readout for the above with high speed data buffering compatible with trigger decisions up to 1 μsec later and fast data ports to allow second level triggers. “Dead time-less data acquisition” when incorporated as a tracker for beam identification and beam particle phase space determination.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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c. Technology for Rare Decay and Rare Particle Detection

Grant applications are sought for detectors and techniques to measure very weak or rare event signals. Such detector technologies and analysis techniques are required in searches for rare events such as NLDBD and for new isotopes produced far from stability at rare isotope beam and high intensity stable beam facilities. Rare decay and rare event detectors require large quantities of ultra-clean materials for shielding and targets. Future detectors require unprecedented sensitivity and accuracy and could benefit from the use of quantum information sensors and adjacent supporting technologies. The adoption of these sensors in NP applications depends on the development of fabrication techniques at scale to increase availability at lower cost.

Grant applications are sought to develop:

- Detectors based on uniquely quantum properties such as superposition, entanglement, and squeezing;
- Detectors with very high resolution (tenths of micrometers spatial resolution and tenths of eV energy resolution). Bolometers, including the required thermistors, based on cryogenic semiconductor materials, transition edge sensors, Superconducting Tunnel Junction (STJ) radiation detectors, or other new materials are eligible, as well as;
- Ultra-low background techniques and materials for supporting structural and vacuum-compatible materials, hermetic containers, cabling, connecting and processing signals from high density arrays of detectors (such as radio-pure signal cabling, optical fibers, signal and high voltage interconnects, vacuum feedthroughs, front-end amplifier FET assemblies and front-end ASICs). The radiopurity goals are less than 0.1 mBq/kg [Th or U]. Values for surface alphas and ^{222}Rn are contained in references 10-12;
- Ultra-sensitive assay or mass-spectrometry methods for quantifying contaminants in ultra-clean materials;
- Cost-effective production of large quantities of ultra-pure liquid scintillators;
- Novel methods capable of discriminating between interactions of gamma rays and charged particles in rare event experiments; and
- Methods by which the background interactions in rare event searches, such as those induced by gamma rays or neutrons, can be tagged, reduced, or removed entirely;

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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d. High Performance Scintillators, Cherenkov Materials and Other Optical Components

Nuclear physics research has the need for high performance scintillator and Cherenkov materials for detecting and counting photons and charged particles over a wide range of energies (from a few keV to up to many GeV). These include crystalline, ceramic, glass, and liquid scintillators (both organic and cryogenic noble liquids) for measuring electromagnetic properties (e.g., for high resolution EM calorimetry) as well as for particle identification. The majority of these detectors e.g., calorimeters, require large area coverage and therefore cost-effective methods for producing the materials are required.

Grant applications are sought to develop:

- New high density, nonhygroscopic scintillating crystals with high light output and fast decay times;
- Scintillators materials that can be used for n/gamma discrimination over large areas using timing and pulse shape information or other method. Thermal neutron sensitivity is not required;
- Radiation resistant scintillating fiber assemblies for beam tracking of rare isotope beams at rates of up to 1MHz. The position resolution should be better than 1 mm; and
- Radiation resistant fast scintillators with timing resolution better than 100 ps.

Grant applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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e. Technology for High Radiation Environments

Next generation rare isotope beam facilities require new and improved techniques, instrumentation and strategies to deal with the anticipated high radiation environment in the production, stripping and transport of ion beams. These could also be useful for existing facilities. Therefore grant applications are sought to develop:

- Efficient tools to convert 3D-CAD geometries into geometry models that can to be used in common radiation transport codes like Mars, PHITS, MCNPx and others and advanced visualization and analysis tools of radiation transport calculation results and for these geometries

Open source solutions are strongly encouraged. Applications must clearly indicate how Phase I research and development will result in a working prototype or method that will be completed by the end of Phase II. The prototype or method must be suitable for testing in a nuclear physics application and/or at a nuclear physics facility. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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f. Other

In addition to the specific subtopics listed above, the Department invites grant applications in other areas that fall within the scope of the topic description above

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate for Instrumentation, Detection Systems and Technique: Elizabeth Bartosz, Elizabeth.Bartosz@science.doe.gov

References:

1. U.S. Department of Energy. (2020). *Facility for Rare Isotope Beams (FRIB),* Michigan State University, DOE Office of Science. http://frib.msu.edu/
2. Wei, J., Ao, H., Beher, S., Bultman, N., et al. (2019). *Advances of the FRIB Project*, International Journal of Modern Physics E, Vol. 28, Issue 3, 1930003. https://www.researchgate.net/publication/331838290_Advances_of_the_FRIB_project
3. The EDM Collaboration. (2007). *The Neutron Electric Dipole Moment Project (nEDM)*, Conceptual Design Report for the Measurement of Neutron Electric Dipole Moment, nEDM, Los Alamos National Laboratory, p. 105. http://p25ext.lanl.gov/edm/pdf.unprotected/CDR(no_cvr)_Final.pdf
4. Adare, A., Daugherity, M.S., Gainey, K., Isenhower, D., et.al., 2012, sPHENIX: An Upgrade Proposal from the PHENIX Collaboration, p. 200. https://wiki.bnl.gov/sPHENIX/index.php/SPHENIX

5. Adare, A., Aidala, C., Ajitanand, N.N., Akiba, Y., et al. (2014). *Concept for an Electron Ion Collider (EIC) Detector Built Around the BaBar Solenoid*, The PHENIX Collaboration, p. 59. https://inspirehep.net/literature/1280344#
6. Andersen, T. C., Blevis, I., Boger, J., Bonvin, E., et al. (2003). *Measurement of Radium Concentration in Water with Mn-coated Beads at the Sudbury Neutrino Observatory*, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Vol. 501, Issues 2-3, p. 399-417. https://www.sciencedirect.com/science/article/pii/S0168900203006168
7. Andersen, T. C., Black, R.A., Blevis, I., Boger, J.N., et al. (2003). *A Radium Assay Technique Using Hydrous Titanium Oxide Absorbant for the Sudbury Neutrino Observatory*, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Vol. 501, Issues 2-3, p. 386-398. https://www.researchgate.net/publication/222666014_A_radium_assay_technique_using_hydrous_titanium_oxide_adsorbent_for_the_Sudbury_Neutrino_Observatory
8. Batignani, G., Cervelli, F., Chiarelli, G., and Scribano, A. (2001). *8th Pisa Meeting on Advanced Detectors for Frontier Physics*, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Vol. 461, Issue 1-3, ISSN: 0168-9002. https://inspirehep.net/record/972299
9. Alduino, C., Alfonso, K., Artusa, D.R., Avignone, F.T., et al. (2016). *CUORE-0 Detector: Design, Construction and Operation*, Journal of Instrumentation, Vol. 11, P07009. https://iopscience.iop.org/article/10.1088/1748-0221/11/07/P07009
10. W. Rau and G. Heusser. (2000). *{222}Rn Emanation Measurements at Extremely Low Activities*, Applied Radiation and Isotopes 53 (2000) 371-375. https://www.sciencedirect.com/science/article/abs/pii/S096980430000155X#:~:text=%20222Rn%20emanation%20measurements%20at%20extremely%20low%20activities,of%20materials%20that%20are%20planned%20to...%20More%20
11. Heusser, G. (1995). *Low-Radioactivity Background Techniques*, Annu. Rev. Nucl. Part. Sci. 1995.45:543-590. https://www.deepdyve.com/lp/annual-reviews/low-radioactivity-background-techniques-E1yhJfauLr#:~:text=Low-Radioactivity%20Background%20Techniques%20The%20basic%20sources%20of%20background,with%20particular%20emphasis%20on%20the%20cosmic%20ray-induced%20component.
12. Radiopurity, *Public database of material radio-purity measurements*. https://www.radiopurity.org
13. Adare, A., Aidala, C., Ajitanand, N.N., Akiba, Y., et al. (2014). *Concept for an Electron Ion Collider (EIC) Detector Built Around the BaBar Solenoid*, The PHENIX Collaboration, p. 59. https://inspirehep.net/literature/1280344#
14. Abelev, B., Adam, J., Adamova, D., Aggarwal, M.M., et. al. The ALICE Collaboration. (2014). *Technical Design Report for the Upgrade of the ALICE Inner Tracking System*, Journal of Physics G: Nuclear and Particle Physics, Vol. 41, Issue 8, p. 181. http://iopscience.iop.org/article/10.1088/0954-3899/41/8/087002/meta
15. The SoLID Collaboration. (2014). *SoLID (Solenoidal Large Intensity Device) Preliminary Conceptual Design Report*, p. 225. http://hallaweb.jlab.org/12GeV/SoLID/files/solid_precdr.pdf
16. EIC, (2020). *Generic Detector R&D for an Electron Ion Collider,* Wikipedia. https://wiki.bnl.gov/conferences/index.php/EIC_R%25D
17. Aune, S., Delagnes, E., Garcon, M., Mandjavidze, I., et. al. (2012). *Design and Assembly of Fast and Lightweight Barrel and Forward Tracking Prototype Systems for an EIC*, p. 11. https://wiki.bnl.gov/conferences/images/6/6f/RD_2011-2_F.Sabatie.pdf
18. Adrian, P.H., Field, C., Graf, N., Graham, M., et. al. (2012). *Status of the Heavy Photon Search Experiment at Jefferson Laboratory*, p. 89. https://www.jlab.org/exp_prog/proposals/12/C12-11-006.pdf
19. Niinikoski, T.O., Abreu, M., Anbinderis, P., Anbinderis, T., et al. (2004). *Low-temperature Tracking Detectors*, Nuclear Instruments and Methods in Physics Research, Section A--Accelerators, Spectrometers,

Detectors and Associated Equipment, Vol. 520, Issues 1-3, p. 87-92. https://www.sciencedirect.com/science/article/pii/S0168900203031310

20. Lawrence Berkeley National Laboratory. (2019). *Scintillator Properties Database*, Lawrence Berkeley National Laboratory. http://scintillator.lbl.gov/
21. Nakamura, T. and Heilbronn, L. (2005). *Handbook of Secondary Particle Production and Transport by High-Energy Heavy Ions*, World Scientific Publishing Co. Pte. Ltd., Singapore, p. 236, ISBN: 978-981-256-558-7. http://www.worldscientific.com/worldscibooks/10.1142/5973
22. Sato, T., Niita, K., Matsuda, N., Hashimoto, S., et al. (2013). *Particle and Heavy Ion Transport Code System (PHITS),* Journal of Nuclear Science and Technology, Vol. 50, Issue 9, p. 913-923. http://www.tandfonline.com/doi/full/10.1080/00223131.2013.814553
23. Los Alamos National Laboratory, (2019). *Monte Carlo Methods, Codes, and Applications Group*, X Theoretical Design (XTD) Division, Los Alamos National Laboratory, MCNPX. http://mcnpx.lanl.gov/
24. CERN, INFN. (2010). *FLUKA*, Fluktuierende Kaskade. http://www.fluka.org/fluka.php
25. Cooper, R.J., Amman, M., and Vetter, K. (2018). *High Resolution Gamma-ray Spectroscopy at High Count Rates with a Prototype High Purity Germanium Detector*, Nuclear Instruments and Methods in Physics A, Vol. 886, p. 1-6. https://www.sciencedirect.com/science/article/pii/S0168900217314596
26. Cooper, R.J., Amman, M., Luke, P.N., and Vetter, K. (2015). *A Prototype High Purity Germanium Detector for High Resolution Gamma-ray Spectroscopy at High Count Rates*, Nuclear Instruments and Methods in Physics A, Vol. 795, p. 167-173. https://www.sciencedirect.com/science/article/pii/S0168900215007123
27. U.S. Department of Energy. (2019). *QUANTUM HORIZONS: QIS RESEARCH AND INNOVATION FOR NUCLEAR SCIENCE*, Office of Science, Nuclear Physics, p. 5-10. https://science.osti.gov/-/media/grants/pdf/foas/2019/SC_FOA_0002210.pdf
28. U.S. Department of Energy. (2018). *Opportunities for Nuclear Physics & Quantum Information Science*, Office of Science, p. 22. https://science.osti.gov/~/media/np/pdf/Reports/npqi_whitepaper_20Feb2019.pdf
29. Francesco Armando Di Bello, et al. (2020). *Towards a Computer Vision Particle Flow*. https://arxiv.org/abs/2003.08863
30. E. Cisbani, et al., (2019). *AI-Optimized Detector Design For The Future Electron-Ion Collider: The Dual-Radiator RICH Case*, Journal of Instrumentation, vol. 15, May 2020. https://arxiv.org/abs/1911.05797
31. Strong, G. C. (2020). *On The Impact of Selected Modern Deep-Learning Techniques To The Performance and Celerity of Classification Models in an Experimental High-Energy Physics Use Case*. https://arxiv.org/abs/2002.01427
32. Kim Albertsson et al., (2018) *Machine Learning in High Energy Physics Community White Paper*. https://arxiv.org/abs/1807.02876
33. Boehnlein, A. (2020). *Report from the A.I. For Nuclear Physics Workshop*. https://arxiv.org/abs/2006.05422