U.S. Department of Energy

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

Topics

FY 2022

Phase I

Release 1

Version 5, September 15, 2021

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 12, 2021
Funding Opportunity Announcement Issued:	Monday, August 09, 2021
Letter of Intent Due Date:	Monday, August 30, 2021
Application Due Date:	Tuesday, October 12, 2021
Award Notification Date:	Monday, January 03, 2022*
Start of Grant Budget Period:	Monday, February 14, 2022

*** Date Subject to Change**

Table of Changes		
Version	**Date**	**Change**
Ver. 1	July 12, 2021	Original
Ver. 2	July 14, 2021	• Office of Basic Energy Sciences: Updated program office overview • Topic 10, subtopic a: Corrected subtopic description • Topic 12, subtopic a: Corrected subtopic description • Topic 23, subtopic a: Updated Point of Contact • Topic 26: Updated Topic description • Topic 26, subtopic a: Updated subtopic description
Ver. 3	July 15, 2021	• Topic 1: Updated Topic description
Ver. 4	July 23, 2021	• Introduction to DOE SBIR/STTR Topics: Updated link online tutorials • Topic 21, subtopic d: Updated link for Reference #2 • Topic 31: Updated link for Reference #3
Ver. 5	September 15, 2021	• Topic 1, subtopic a: Added Point of Contact for Application Area 1

Return to Table of Contents

INTRODUCTION TO DOE SBIR/STTR TOPICS

This SBIR/STTR topics document is issued in advance of the FY 2022 DOE SBIR/STTR Phase I Release 1 Funding Opportunity Announcement scheduled to be issued on August 09, 2021. 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 either through a DOE-funded and selected contractor or through an awardee-funded and selected vendor(s).

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 Laboratory Contractor 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 Contractor 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 Laboratory Contractor and your project plan should reflect this.

How do I draft a subaward?
The technology transfer office of the collaborating university or DOE Laboratory will typically be able to assist with a suitable template.

Am I required to show I have a subaward with the university or National Laboratory Contractor 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 Laboratory Contractor via a subaward may help to accelerate the research or development effort. In those cases, the small business may wish to negotiate a subaward with the university or National Laboratory.

Is the university or National Laboratory Contractor required to become a subawardee if requested by the applicant?
No. Collaborations with universities or National Laboratory Contractors must be negotiated between the applicant small business and the research organization. The ability of a university or National Laboratory Contractor 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 an exclusive or non-exclusive license to the technology is available for negotiation. 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 granted 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 a no-cost, six month option to license the technology at the start of the Phase I award. 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 Laboratory Contractor 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.

Return to Table of Contents

How will applying for an SBIR or STTR grant associated with a TTO benefit me?

By leveraging prior research and patents from a university or National Laboratory Contractor 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.

Return to Table of Contents

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 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).

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

- Applied and Computational Mathematics to develop the mathematical algorithms, tools, and libraries to model complex physical and biological systems.
- High-performance Computing Science to develop scalable systems software and programming models, and to enable computational scientists to effectively utilize petascale and soon to be deployed exascale computers to advance science in areas important to the DOE mission.
- 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.
- Applied Computational Sciences Partnership to achieve breakthroughs in scientific advances via computer simulation technologies that are impossible without interdisciplinary effort.

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

In addition, applicants may consider to apply for Director's Discretionary allocation at the DOE's Open Science Computing facilities: the Oak Ridge Leadership Computing Facility (OLCF) [1], the Argonne Leadership Computing Facility (ALCF) [2], or the National Energy Research Scientific Computing Center (NERSC) [3]. Applicants who already have used the DOE facilities, may consider applying for the ALCC program [4]. ALCF has a site that includes everything an applicant may need to know to apply for allocation and get training: http://www.alcf.anl.gov/user-guides/how-get-allocation. Questions concerning allocations on the ALCF can be sent to David Martin at dem@alcf.anl.gov.

Descriptions of the allocation programs available at the OLCF are available at http://www.olcf.ornl.gov/support/getting-started/. Questions concerning allocations on the OLCF can be sent to Bronson Messer, bronson@ornl.gov.

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

References:

1. Oak Ridge Leadership Computing Facility, U.S Department of Energy, 2021, OLCF Director's Discretion Project Application, *Oak Ridge National Laboratory Leadership Computing Facility,* https://www.olcf.ornl.gov/for-users/documents-forms/olcf-directors-discretion-project-application/, (June 23,2021) Contact: Bronson Messer, bronson@ornl.gov
2. Argonne Leadership Computing Facility, U.S Department of Energy, 2021, Director's Discretionary Allocation Program, *Argonne Leadership Computing Facility,* https://www.alcf.anl.gov/science/directors-discretionary-allocation-program, (June 23, 2021) Contact: Katherine Riley, riley@alcf.anl.gov
3. NERSC, U.S. Department of Energy, Lawrence Berkeley National Laboratory, 2021, Apply For Your First NERSC Allocation, NERSC, https://www.nersc.gov/users/accounts/allocations/first-allocation/, (June 23, 2021) Contact: Richard Gerber, ragerber@lbl.gov
4. DOE ALCC Program, U.S Department of Energy, 2021, ASCR Leadership Computing Challenge (ALCC), U.S. Department of Energy Office of Science, https://science.osti.gov/ascr/Facilities/Accessing-ASCR-Facilities/ALCC, (June 23, 2021)

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 three 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 or Resham Kulkarni, resham.kulkarni@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 Earth and Environmental Systems Sciences Division (EESSD) 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.

Return to Table of Contents

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 Environmental System Science (ESS)[12] program.

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[13], 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 (ESS Science Focus Area programs at DOE labs and major 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[14] and several other recent reports[15-18]. To address the biogeochemistry and integrated water cycle grand challenges in the EESSD Strategic Plan, the ESS community generates 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 Sharing, Mining and Extracting Knowledge from Chemical and Geochemical Data

The Chemical Sciences, Geosciences, and Biosciences (CSGB) Division (reference 1) 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 impact and for attaining cleaner energy processes. Likewise, this knowledge leads to the discovery of new pathways for circular use or replacement of critical resources.

Measurement and computation of physicochemical phenomena leading to chemical transformations produce complex, non-uniform, unstructured and distributed data, and data models are typically not transferable outside the specific chemical system(s) used to generate the data. The broadly dispersed and diverse databases typically contain synthesis protocols, compositional, structural, reactivity, and spectroscopic information, and are not general enough to encourage data sharing beyond narrow communities.

Recent reports (reference 2) pinpoint the opportunities to increase impact of fundamental research on applied technology by developing multimodal approaches that encourage integration across types of data as well as techniques, for example by integrating models derived from disperse, heterogonous chemical information data with models derived from physical principles.

In particular, AI/ML tools are needed to facilitate the integration of highly heterogonous chemical data of diverse provenance, to promote data sharing for model fine tuning and generalization, extrapolation to data-poor regions, or to extend fundamental theories to complex many-parameter systems. Tools are needed to mine and extract key features from 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 surrogate models or augment physics-derived models. Such hybrid models should be capable of predicting dynamic behavior of chemical systems, so as to be of value for the design and development of novel separation, reaction, and transport processes.

Principal investigators are encouraged to identify and consider multiple sources of chemical information, including the literature, multiple experimental and computational techniques, and diverse and distributed research groups, in order to demonstrate the capability and versatility of the tools developed. Applicants should refer to the reports mentioned in reference 2 to identify a priority research opportunity and the type of chemical system targeted by the application.

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

References: General:

1. U.S. Department Energy, 2021, DOE Exascale Requirements Review, Exascaleage, https://exascaleage.org/, (June 23, 2021)

References: Application Area 1:

1. U.S. Department Energy, 2019, Genomic Science Program, *Genomic Science Program, Systems Biology for Energy and the Environment,* https://genomicscience.energy.gov/index.shtml, (June 23, 2021)
2. Arkin, Adam, Bader, David C., Coffey, Richard, et al, 2016, Biological and Environmental Research Exascale Requirements Review. An Office of Science review sponsored jointly by Advanced Scientific Computing Research and Biological and Environmental Research, *U.S. Department of Energy Office of Scientific and Technical Information*, https://www.osti.gov/biblio/1375720/, (June 23, 2021)
3. U.S. Department of Energy, 2021. *Biological Systems Science Division Strategic Plan*, DOE/SC-0205, https://genomicscience.energy.gov/2021bssdstrategicplan/, (June 23, 2021)

References: Application Area 2:

1. U.S Department of Energy, 2017, Grand Challenges for Biological and Environmental Research: Progress and Future Vision, *Report from the Biological and Environmental Research Advisory Committee,* DOE/SC-0190, https://genomicscience.energy.gov/BERfiles/BERAC-2017-Grand-Challenges-Report.pdf, (June 23, 2021)
2. U.S. Department of Energy, 2021, Environmental Molecular Sciences Laboratory (EMSL), U.S. DOE Office of Science, https://science.osti.gov/ber/Facilities/User-Facilities/EMSL, (June 23, 2021)
3. U.S. Department of Energy, 2021, Joint Genome Institute User Facility, *U.S. Department of Energy, Office of Science*, https://science.osti.gov/ber/Facilities/User-Facilities/JGI, (June 23, 2021)
4. U.S. Department of Energy, 2021, Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE), *U.S. Department of Energy, Office of Science,* http://ess-dive.lbl.gov/, (June 23, 2021)

5. U.S. Department of Energy, 2021, Systems Biology Knowledgebase (KBase), *U.S. Department of Energy, Office of Science,* http://kbase.us/, (June 23, 2021)
6. U.S. Department of Energy, 2021, AmeriFlux Network, *Biological and Environmental Research (BER), Earth and Environmental Systems Sciences Division,* https://ameriflux.lbl.gov/, (June 23, 2021)
7. U.S. Department of Energy, 2021, Worldwide Hydrobiogeochemical Observation Network for Dynamic River Systems (WHONDRS) Network, *U.S. Department of Energy, Pacific Northwest National Library*, https://www.pnnl.gov/projects/WHONDRS, (June 23, 2021)
8. AQUA-MER Database, 2018, U.S. Department of Energy, Biological and Environmental Research (BER), Earth and Environmental Systems Sciences Division, https://aquamer.ornl.gov/, (June 23, 2021)
9. U.S. Department of Energy, 2018, Earth and Environmental Systems Sciences Division Strategic Plan, *Environmental System Science Program,* DOE/SC-0192, Office of Biological and Environmental Research, p. 19-20, https://ess.science.energy.gov/eessd-strategic-plan/, (June 23, 2021)
10. U.S. Department of Energy, Office of Biological and Environmental Research, 2019, Bioimaging Science Program, *2020 PI Meeting Proceedings*, https://science.osti.gov/-/media/ber/bioimaging-technology/pdf/2020/Bioimaging_Science_PI_Meeting2020.pdf?la=en&hash=9361687676C0133A7EF11F959C691D02507B881F, (June 23, 2021)
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-DOE Joint Genome Institute*, https://jgi.doe.gov/user-programs/program-info/ficus-overview/emsl/, (June 23, 2021)
12. U.S. Department of Energy, Environmental System Science Program, 2021, Environmental System Science Program, Biological and Environmental Research (BER), Earth and Environmental Systems Sciences Division, https://ess.science.energy.gov/, (June 23, 2021)
13. U.S. Department of Energy, Office of Biological and Environmental Research, 2020, Data Management Policy, *Environmental Molecular Sciences Laboratory,* https://www.emsl.pnnl.gov/emslweb/emsl-data-management-policy, (June 23, 2021)
14. 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, (June 23, 2021)
15. 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, (June 23, 2021)
16. 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://www.bing.com/search?q=Technologies+for+Characterizing+Molecular+and+Cellular+Systems+Relevant+to+Bioenergy+and+Environment%2C+DOE%2FSC-0189&cvid=b7384d6bdb5c4ea5891e9bb947db0ab5&aqs=edge..69i57.363j0j4&FORM=ANAB01&PC=U531, (June 23, 2021)
17. 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, (June 23, 2021)
18. U.S. Department of Energy, 2021, Biological System Sciences Division Strategic Plan, *Office of Biological and Environmental Research*, https://genomicscience.energy.gov/2021bssdstrategicplan/, (June 23, 2021)

References: Application Area 3:

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

1. U.S. Department of Energy, 2021, Chemical Sciences, Geosciences, & Biosciences (CSGB) Division, *U.S. DOE Office of Science,* https://science.osti.gov/bes/csgb, (June 23, 2021)
2. U.S. Department of Energy, 2021, Community Resource Reports, *U.S. DOE Office of Science,* https://science.osti.gov/bes/Community-Resources/Reports,(June 23, 2021)

See, for example, “Basic Research Needs Workshop for Transformative Manufacturing”, “Basic Energy Sciences Roundtable on Producing and Managing Large Scientific Data with Artificial Intelligence and Machine Learning”, “Basic Energy Sciences Roundtable on Liquid Solar Fuels”, “Basic Energy Sciences Roundtable on Chemical Upcycling of Polymers”, “Basic Research Needs Workshop for Catalysis Science”.

2. ACCELERATING THE DEPLOYMENT OF ADVANCED SOFTWARE 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 Science (SC) Office of Advanced Scientific Computing Research (ASCR) has spent decades on, and invested millions of dollars in, the development of HPC software that operates efficiently on large, heterogeneous supercomputers. Today, this hardware (e.g., CPUs, GPUs, TPUs, ASICs) has permeated society at large, finding its way into everything from smart phones to cloud computers. However, many of the software packages and libraries that can take advantage of this heterogeneity have remained solely within the HPC ecosystem.

Work proposed under this topic must critically depend on one or more ASCR-funded software packages. Proposals should include a reference (webpage or other citation) to show that the relevant software has been supported by ASCR. Relevant software packages include, but are not limited to:

- Mathematical Libraries: SuperLU (https://portal.nersc.gov/project/sparse/superlu/), STRUMPACK (https://portal.nersc.gov/project/sparse/strumpack/), HYPRE (https://www.llnl.gov/casc/hypre/), Trilinos (https://trilinos.github.io/), PETSc (https://www.mcs.anl.gov/petsc/), SUNDIALS (https://computing.llnl.gov/projects/sundials), MFEM (https://mfem.org/).
- Programming Models: Kokkos (https://github.com/kokkos/kokkos), RAJA (https://github.com/LLNL/RAJA), Umpire (https://github.com/LLNL/umpire), Legion (https://legion.stanford.edu/)
- I/O: ADIOS2 (https://github.com/ornladios/ADIOS2), Parallel NetCDF (https://parallel-netcdf.github.io/), HDF5 (https://www.hdfgroup.org/)
- Compilers and Runtimes: LLVM (https://llvm.org/), Argobots (https://www.argobots.org/)
- MPI: OpenMPI (https://www.open-mpi.org/), MPICH (https://www.mpich.org/)
- Package Management: Spack (https://spack.io/)
- Software Stacks and SDKs: E4S (https://e4s-project.github.io/), xSDK (https://xsdk.info/)

See the references for an additional, partial listings of available software packages. Proposals without a critical dependence on one or more ASCR-funded software packages are out of scope.

ASCR understands that a diverse community of stakeholders contributing to the maintenance and evolution of a software package lowers the long-term risks associated with commercialization of that software. Accordingly, ASCR encourages contributing fixes for defects in the ASCR-funded software, changes needed to make the ASCR-funded software function on generally-available platforms, and other non-proprietary enhancements of general utility to the ASCR-funded software back to the project in a manner consistent with any applicable licensing requirements and other project policies. While not required, applicants are encouraged to provide letters of support from at least one developer of each ASCR-funded software package that plays a significant role in the proposed work. This letter should outline the mutually-understood procedure via which any relevant contributions will be reviewed for acceptance into the project and briefly outline any anticipated prerequisites to initiating that procedure (e.g., the future execution of a Contributor License Agreement (CLA)).

a. Deployment of ASCR-Funded Software

Accelerating the deployment and use of advanced, ASCR-funded software technologies, packages, and libraries can significantly improve the performance, reliability, and stability of commercial applications while lowering the cost of developing new capabilities. While many ASCR-supported software packages are open source, they are often complicated to use, distributed primarily in source-code form targeting common HPC systems, and potential adopters lack options for purchasing commercial support, training, and custom-development services. The expertise required to install and use these software packages poses a significant barrier to many organizations due to the levels of complexity built into them to facilitate scientific discovery and research. Moreover, without a commercial interest in broadly marketing the capabilities of the software, possibly including in markets beyond HPC, adoption is limited by a lack of exposure within the wider technology ecosystem. Providing simpler interfaces targeted for specific markets, or offering a spectrum of commercial services around the underlying open-source software, would make these software packages more usable for commercial, industrial, and non-scientific applications.

Grant applications are sought to take one or more ASCR-funded software packages and make them easier to use by a wide variety of industries or in commercial venues by developing commercial offerings based on those ASCR-funded software packages. This may include design, implementation, and usability testing of Graphical User Interfaces (GUIs), web interfaces, or interfaces for alternative programming languages (e.g., using Python, R, or Julia); porting to other platforms (e.g., cloud, mobile); simplification of user input; decreasing complexity of the code by stripping out components not required; hardening the code to make it more robust; adding new capabilities; adding user-support tools or services; or other ways that make the code more widely useable to industrial applications.

Questions – Contact: Hal Finkel, hal.finkel@science.doe.gov and/or William Spotz, William.Spotz@science.doe.gov

b. Integration of ASCR-Funded Libraries

Adopting and integrating advanced, ASCR-funded libraries into commercial products can lower the cost of developing new capabilities while simultaneously providing improved performance, reliability, and stability. The advanced mathematical and computational algorithms, and support for state-of-the-art hardware, can be leveraged by commercial software internally, thereby providing important capabilities without users interacting directly with the capabilities provided by the underlying ASCR-funded libraries. These commercial applications need not be targeted at HPC systems, but rather, may integrate and adapt the relevant ASCR-funded libraries for use in cloud, mobile, or other computing environments.

Grant applications are sought to take one or more ASCR-funded libraries and integrate them into existing, commercially-supported software products to provide unique, transformative capabilities. Applicants may choose to strip out code components, harden them, or perform any other tasks necessary to meet deployment requirements in the context of the envisioned commercial product.

Questions – Contact: Hal Finkel, hal.finkel@science.doe.gov and/or William Spotz, William.Spotz@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.

Questions – Contact: Hal Finkel, hal.finkel@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, (June 23,2021)
2. U.S. Department of Energy, 2020, SciDAC Feature, *Scientific Discovery through Advanced Computing (SciDAC), U.S. Department of Energy*, http://www.scidac.gov, (June 23, 2021)
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, (June 23, 2021)
4. U.S. Department of Energy, 2020, Exascale Computing Project, *U.S. DOE,* https://www.exascaleproject.org, (June 23, 2021)
5. U.S. Department of Energy, 2020, DOE CODE, *U.S. Department of Energy, Office of Scientific and Technical Information.* https://www.osti.gov/doecode/, (June 23, 2021)

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; ransomware; blockchain; enterprise; deception; virtualization; out-of-band; cyber-physical; data centers; database; basic research; natural language processing; collaborative computing; 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,* https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/ASCR_Cybersecurity_20_Research_Pathways_and_Ideas_Workshop.pdf, (July 12, 2021)
2. DOE Workshop Report: "The 2015 Cybersecurity for Scientific Computing Integrity Workshop," https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/ASCR_Cybersecurity_For_Scientific_Computing_Integrity_Report_2015.pdf, (July 12, 2021)
3. Campbell, S., Mellander, J., 2011, Experiences with Intrusion Detection in High Performance Computing, Lawrence Berkeley National Laboratory, National Energy Research Scientific Computing Center, https://cug.org/5-publications/proceedings_attendee_lists/CUG11CD/pages/1-program/final_program/Monday/03B-Mellander-Paper.pdf, (June 23, 2021)
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, (June 23, 2021)

4. 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 subtopic 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, *ACM Computing Surveys*, https://dl.acm.org/doi/10.1145/3182660 (June 23, 2021)
2. Liu, Z., Kettimuthu, R., Leyffer, S.. et al, 2017, A Mathematical Programming- and Simulation-Based Framework to Evaluate Cyberinfrastructure Design Choices, *2017 IEEE 13th International Conference on e-Science (e-Science), Auckland, 2017,* pp. 148-157, doi: https://doi.org/10.1109/eScience.2017.27 (June 23, 2021)
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.bing.com/search?q=Elastic+Data+Transfer+Infrastructure+for+a+Dynamic+Science+DMZ+Kettimuthu&cvid=587ca719e9ec4023a0af740ca57361ab&aqs=edge..69i57j69i59i450l6.462j0j1&pglt=2083&FORM=ANNTA1&PC=U531, (June 23, 2021)
4. Liu, Z., Kettimuthu, R., Balaprakash, P., Rao, N. S. V., 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, 2018, Paris, France*, https://link.springer.com/chapter/10.1007%2F978-3-030-19945-6_5?utm_medium=affiliate&utm_source=commission_junction&utm_campaign=3_nsn6445_brand_PID100357191&utm_content=de_textlink, (June 23, 2021)

References: Subtopic a:

1. Z. Liu, P. Balaprakash, R. Kettimuthu, and I. Foster, 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://dl.acm.org/doi/10.1145/3078597.3078605, (June 23, 2021)
2. Z. Liu, R. Kettimuthu, I. Foster and Y. Liu, "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, doi: 10.1109/ICDCS.2018.00180 https://ieeexplore.ieee.org/document/8416443
3. Rao, N. S. V., Liu, Q., Sen, S., et al, 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://ieeexplore.ieee.org/document/8038432, (June 23, 2021)
4. Liu, Z., Kettimuthu, R., et al, 2018, Toward a Smart Data Transfer Node, Future Generation Computing Systems, 2018, https://www.sciencedirect.com/science/article/abs/pii/S0167739X18302346, (June 23, 2021)

References: Subtopic b:

1. Allcock, W. GridFTP: Protocol Extensions to FTP for the Grid. Global Grid ForumGFD-R-P.020, 2003. https://www.ogf.org/documents/Drafts/GF5%20Drafts/gridftp_intro_gf5.pdf
2. Allcock, W., Bresnahan, J., Kettimuthu, R., et al, 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, (June 23, 2021)
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, (June 23, 2021)
4. Papadimitriou, G., Kiran, M., Wang, C., Mandal, A., and Deelman, E., 2019, Training Classifiers to Identify TCP Signatures in Scientific Workflows, International Workshop on Innovating the Network for Data Intensive Science (INDIS), Nov 2019, https://www.bing.com/search?q=Training Classifiers to Identify TCP Signatures in Scientific Workflows Papadimitriou&qs=n&form=QBRE&sp=-1&pq=training classifiers to identify tcp signatures in scientific workflows papadimitriou&sc=0-85&sk=&cvid=3E7530B8E95042FBB60D1BC293ED5CB0, (June 23, 2021)
5. Kiran, M., Mohammed, B., N. Krishnaswamy, DeepRoute: Herding Elephant and Mice Flows with Reinforcement Learning, International Conference on Machine Learning for Networking (MLN'2019), Paris, France, December 3-5, 2019, https://link.springer.com/chapter/10.1007/978-3-030-45778-5_20?utm_medium=affiliate&utm_source=commission_junction&utm_campaign=3_nsn6445_brand_PID100357191&utm_content=de_textlink, (June 23, 2021)
6. Dijkhuizen, N.V., Ham, J.V.D, 2018, A Survey of Network Traffic Anonymisation Techniques and Implementations, ACM Computing Surveys, Volume 51, Issue 3, https://doi.org/10.1145/3182660, (June 23, 2021)

5. TRANSPARENT OPTICAL QUANTUM 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 technologies to support the development long-distance optical quantum networks. The vision and requirements of these networks are outlined in the workshop report of quantum networks for open science [6].

Grant applications are sought in the following subtopics:

a. Photonic Quantum Light Sources

Quantum networks need clocked, pulsed, deterministic quantum light sources (for example, squeezed or multi-photon entangled cluster states, single photons, etc.). The sources should be tunable over the telecommunications C-band and operate at ambient; Low noise optical detectors that do not use cryogenics such as time-resolved homodyne and novel forms of discrete single photon detectors need to be developed to measure such non-classical states of light;

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

b. Quantum Buffers

Limited capacity memory to temporally delay quantum photons in transparent optical quantum communication networks components such as quantum repeaters, routers, switches, and quantum photonic sources. These buffers should be able operate at room temperature.

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

c. Optical Quantum Multiplexers/De-Multiplexers

Optical quantum multiplexers/De-Multiplexers for grooming large number of entangled states with hybrid continuous and discrete variable (Hybrid CV/DV) ending;

These devices are the first generation optical quantum networks devices intended to support research activities, pilot projects, and demonstration of optical quantum networks efforts. Applicants are encouraged to familiarize themselves with ongoing optical quantum networks research at university, National Labs, government, and industry as will like be potential target market for their resulting devices.

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

Out of Scope

Quantum devices not directly related to long-distance quantum networks will be automatically considered out of scope and will not be reviewed. The burden is on the applicant to ensure that the proposed effort addresses specific long-distance quantum networks functions**. Topics that will be considered out of scope include to the following**:

- Quantum computing devices
- Quantum materials
- Optical communication devices and technologies
- Classical network technology devices and software

References:

1. Weedbrook, C., 2011, Gaussian Quantum Information, p. 51, https://arxiv.org/pdf/1110.3234.pdf, (June 23, 2021)
2. Andersen, U.L., Neergaard-Nielsen, J.S., Van Loock, P., and Furusawa, A., 2015, Hybrid Discrete- and Continuous-variable Quantum Information, *Nature Physics*, Vol. 11, p. 713–719.https://www.nature.com/articles/nphys3410, (June 23, 2021)
3. Dias, J., and Ralph, T.C., 2017, Quantum Repeaters using Continuous-variable Teleportation, *Physical Review A,* Vol. 95, 022312, p. 11. https://arxiv.org/pdf/1611.02794.pdf, (June 23, 2021)
4. Huang, K., 2015, Optical Hybrid Quantum Information Processing, arXiv, https://www.researchgate.net/publication/261512563_Optical_Hybrid_Quantum_Information_Processing, (June 23, 2021)
5. Takeda, S., Fuwa, M., Van Loock, P., and Furusawa, A., 2014, Entanglement Swapping between Discrete and Continuous Variables, *Physical Review Letters, Vol. 114*, 100501, p. 9. https://arxiv.org/pdf/1411.1310.pdf, (June 23, 2021)
6. U.S. Department of Energy, 2018, DOE Workshop on Quantum Networks for Open Science, Office of Advanced Scientific Computing Research, p. 41, https://info.ornl.gov/sites/publications/Files/Pub124247.pdf, (June 23,2021)

6. 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. 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

Return to Table of Contents

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 Department of Energy (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. For additional information on BES user facilities, click here. The link to each facility webpage leads to detailed descriptions of the experimental facilities and the listing of available experimental techniques.

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. Here is a tool from DOE Office of Technology Transitions to discover and partner with DOE's National Labs. The DOE SBIR/STTR site also contains a resource to explore collaboration with the National Labs.

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.

7. MANUFACTURING OF ULTRA-HIGH QUALITY 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

This topic seeks the development of surface finishing techniques for manufacturing of coherence-preserving reflective optics that are used at Free-Electron Laser (FEL) and diffraction-limited storage ring X-ray light sources. In diffraction limited optics, the height errors from an ideal shape at high- and mid-spatial frequencies are especially detrimental to preserving the coherent X-ray beam wavefront, degrading beam properties such as the focused peak intensity. Advanced polishing techniques are required in order to achieve surface finishes with sub 1-nm root-mean-square (rms) height error on meter-scale mirrors. Such polishing techniques are often implemented iteratively, with corrective input coming from existing metrology capabilities. Both the proposed finishing technique and the associated metrology shall be capable of producing not only flat, but also curved figure surfaces on mirrors of substantial thicknesses. Another important goal in the mature phase of this development is the ability to apply the polishing technique and the associated metrology to the production of meter-long mirrors.

Grant applications are sought in the following subtopics:

a. Development of Deterministic Surface Finishing Techniques

In this subtopic, the development of surface finishing techniques is sought to produce long X-ray mirrors having substantially lower characteristic tool signature than is currently feasible using the state-of-the-art capabilities. Deterministic surface finishing techniques, such as ion beam figuring, sub-aperture polishing, magnetorheological finishing, or combinations of those techniques, are capable of producing high quality surfaces of arbitrary profiles by controlling the height errors at very high spatial frequencies, and should be further improved to meet the following requirements:

i. The iterative polishing technique shall rely on existing metrologies and be capable of producing two-dimensional surfaces with less than 0.3 nm rms deviation from the ideal profile in the spatial range of 200 nm to 0.5 mm, and less than 1 nm rms deviation in the range from 0.5 mm to 1/2 of the length of the mirror.
ii. Demonstrate the ability to fabricate mirrors with a tangential slope error less than 100 nrad in the spatial range from 0.5 mm to 100 mm.
iii. Capable of processing mirrors made from a silicon substrate with a thickness of up to 50 mm.
iv. Capable of producing flat, spherical, or elliptical surface figures, with curvature as short as 10 m radius when approximated to the nearest sphere.
v. Demonstrating the surface finishing technique over optics that are at least 200 mm in length and 20 mm in width.
vi. Having proven the ability to expand the technique to 1 m long mirrors.

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. U.S. Department of Energy, 2013, X-ray Optics for BES Light Source Facilities, *Report of the Basic Energy Sciences Workshop on X-ray Optics for BES Light Source Facilities* (2013), https://science.osti.gov/-/media/bes/pdf/reports/files/X-ray_Optics_for_BES_Light_Source_Facilities_rpt.pdf, (July 9, 2021)
2. Shi, X., Assoufid, L., and Reininger, R., 2016, How to Specify Super-Smooth Mirrors: Simulation Studies on Nano-Focusing and Wavefront Preserving X-ray Mirrors for Next-generation Light Sources, *Proc. SPIE 9687, 968703 (2016),* https://doi.org/10.1117/12.2241139, (July 8, 2021)
3. T. Pardini, D. Cocco, and S. P. Hau-Riege, 2015, Effect of Slope Errors On The Performance of Mirrors for X-ray Free Electron Laser Applications*, Opt. Express 23, 31889 (2015),* https://doi.org/10.1364/OE.23.031889, (July 9, 2021)
4. C. Maloney and W. Messner, 2019, Extending Magnetorheological Finishing to Address Short Radius Concave Surfaces and Mid-Spatial Frequency Errors, *Proc. SPIE 11175, 111750N (2019)*, https://doi.org/10.1117/12.2536920, (July 9, 2021)
5. T. Wang, L. Huang, K. Tayabaly, and M. Idir, 2019, Study on the Performances of Dwell Time Algorithms in Ion Beam Figuring, *Proc. SPIE 11175, 111750M (2019*), https://doi.org/10.1117/12.2536869, (July 9, 2021)
6. M. Sanchez del Rio, D. Bianchi, D. Cocco *et. al.*, 2016, DABAM: an open-source database of X-ray mirrors metrology", *J. Synchrotron Rad. 23, 665 (2016),* https://doi.org/10.1107/S1600577516005014, (July 9, 2021)

7. S. G. Alcock, I. Nistea, and K. Sawhney, 2016, Nano-metrology: The Art of Measuring X-ray Mirrors with Slope Errors < 100 nrad, *Rev. Sci. Instrum. 87, 051902 (2016),* https://doi.org/10.1063/1.4949272, (July 9, 2021)
8. G. Ghosh, A. Sidpara, and P. P. Bandyopadhyay, 2018, Review of Several Precision Finishing Processes for Optics Manufacturing", *J. Micromanufacturing 1, 170 (2018),* https://doi.org/10.1177%2F2516598418777315 , (July 9, 2021)
9. H. Yamaguchi, R. E. Riveros, I. Mitsuishi *et al.*, 2010, Magnetic field-assisted finishing for micropore X-ray focusing mirrors fabricated by deep reactive ion etching", *CIRP Annals 59, 351 (2010),* https://doi.org/10.1016/j.cirp.2010.03.115, (July 9, 2021)

8. STRAIN-FREE PROCESSING AND MOUNTING OF ULTRA-THIN DIAMOND CRYSTALS FOR APPLICATIONS AT NEXT GENERATION X-RAY SOURCES

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 seeks the development of damage-free and strain-free processing and mounting of ultra-thin diamond crystals for high-impact scientific applications at synchrotron and Free-Electron Laser (FEL) X-ray sources. Diamond crystal X-ray optics are essential for tailoring X-rays to meet the most challenging needs of pioneering research at next generation light source facilities. Numerous applications in this field require ultra-thin, yet nearly perfect diamond single crystals, just a few micrometers to a few tens of micrometers thick, that can properly function under Bragg diffraction conditions and with minimal wavefront distortions. These ultra-thin diamond crystals are required, in particular, for X-ray beam multiplexing monochromators at FEL and synchrotron radiation facilities, monochromators for self-seeding X-ray FELs, outcoupling from cavity-based X-ray FELs, X-ray beam splitters, and low-absorption wavefront-preserving windows, etc. While ultra-high quality diamond crystals are becoming available, processing capabilities are lacking in the US. Such processing capabilities include thinning/polishing and holding/mounting of these ultra-thin crystals without inducing crystal damage or introduction of lattice strain.

Grant applications are sought in the following subtopics:

a. Development of Damage-free and Strain-free Processing and Mounting of Ultra-thin Diamond Crystal Plates

In this subtopic applications are sought to develop processing and mounting methods for ultra-thin diamond crystals. These methods should be capable of manufacturing crystal plates as thin as 10 micrometers over an area of a few mm^2, and with a surface cut in different crystal orientations, such as the diamond (100), (111), (110), etc. These ultra-thin crystals should be mounted strain-free with specific Bragg-plane slope errors of no more than 200 $nrad/mm^2$, and mechanically stable in crystal holders with efficient thermal transport. The processed and mounted crystals should properly function under Bragg diffraction conditions and introduce minimal X-ray wavefront distortions. The ultra-thin diamond crystal plates can be manufactured and mounted either as separate plates or as drumhead crystals, which are monolithic crystal structures composed of a thin membrane furnished with a surrounding solid collar. The applicant must propose practical solutions to achieve these goals along with quantitative approaches to measure the lattice damage and strain.

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. U.S. Department of Energy, 2014, LCLS-II Conceptual Design Report, SLAC National Accelerator Laboratory Library, (2014), SLAC-R-1092, http://slac.stanford.edu/pubs/slacreports/reports09/slac-r-1092.pdf, (July 9, 2021)
2. P. F. Tavares, S. C. Leemann, M. Sjostrom, and A. Andersson, 2014, Diffraction-limited Storage Rings, *J. Synchrotron Rad. 21, 862 (2014),* https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4181638/pdf/s-21-00862.pdf, (July 9, 2021)
3. Yu. Shvyd'ko, 2019, Output Coupling from X-ray Free-Electron Laser Cavities with Intracavity Beam Splitters*, Phys. Rev. Accel. Beams 22, 100703 (2019),* https://link.aps.org/doi/10.1103/PhysRevAccelBeams.22.100703, (July 9, 2021)
4. J. Amann, W. Berg, V. Blank, V., F.-J. Decker, Y. Ding, P. Emma, Y. Feng, J. Frisch, D. Fritz, J. Hastings, *et al*., 2021, Demonstration of Self-Seeding in a Hard X-ray Free-Electron Laser, *Nature Photonics 6, 693 (2012),* https://www.nature.com/articles/nphoton.2012.180.pdf, (July 9, 2021)
5. Y. Feng, R. Alonso-Mori, T.R.M, Barends, V. D. Blank, S. Botha, M. Chollet, D. S. Damiani, R. B. Doak, J. M. Glownia, J. M. Koglin, *et al*., 2015, Demonstration of Simultaneous FEL Experiments Using Thin Crystal Multiplexing at the Linac Coherent Light Source", *J Synchrotron Rad. 22, 626 (2015),* https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4416679/pdf/s-22-00626.pdf, (July 9, 2021)
6. K.-J. Kim, Y. Shvyd'ko, and S. Reiche, 2008, A Proposal for an X-Ray Free-Electron Laser Oscillator with an Energy-Recovery Linac, *Phys. Rev. Lett. 100, 244802 (2008),* https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.100.244802, (July 9, 2021)
7. T. Kolodziej, P. Vodnala, S. Terentyev, V. Blank, and Yu. Shvyd'ko, 2016, Diamond Drumhead Crystals for X-ray Optics Applications, *J. Appl. Cryst. 49, 1240 (2016),* http://dx.doi.org/10.1107/S1600576716009171, (July 9, 2021)
8. H. P. Freund, P. J. M. van der Slot and Yu. Shvyd'ko, 2020, An x-ray regenerative amplifier free-electron laser using diamond pinhole mirrors*, New Journal of Physics 21, 093028 (2019)*, [1905.06279] https://arxiv.org/abs/1905.06279 (July 9, 2021)
9. P. Pradhan, M. Wojcik, X. Huang, E. Kasman, L. Assoufid, J. Anton, D. Shu, S. Terentyev, V. Blank, K.-J. Kim and Y. Shvyd'ko, 2020), Small Bragg-plane slope errors revealed in synthetic diamond crystals", *J. Synchrotron Rad. 27, 1553 (2020),* https://doi.org/10.1107/S1600577520012746, (July 9, 2021)

9. NOVEL MANUFACTURING CAPABILITIES FOR HIGH RESOLUTION X-RAY GRATINGS

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

To fully utilize DOE's high brightness and diffraction-limited X-ray sources, there is an urgent need for a quantum leap forward in the manufacturing capabilities of X-ray gratings that are required for a wide range of very high throughput ultra-high resolution spectroscopic methods. These applications call for the use of current and next generation grating systems, including blazed reflection gratings (i.e., grating with sawtooth profile groves), with lines that have better than 10 nm root-mean-square (rms) absolute position accuracy over the entire length of the optic. To sustain the power generated by these high brightness X-ray sources, the gratings should be realized directly on silicon substrates. To achieve such a high placement accuracy, the grating production should rely on fast techniques to minimize drifts arising from prolonged processing that is typical of serial writing methods.

Lengthy writing methods, such as the classical serial writing scheme used for mechanically ruled grating, are prone to high sensitivity to thermal and mechanical drifts. These methods, therefore, cannot be considered in the quest for achieving a sub-10 nm rms groove placing accuracy.

Grant applications are sought in the following subtopics:

a. Holographic, Lithographically Recorded and Parallelly Written Gratings Schemes

In this subtopic applications are sought for the development of grating production techniques using holographic methods, lithographic masks or parallelly written schemes for producing blazed gratings with the following requirements:

i. Having a shallow blaze angle down to, at least, 0.3° and arbitrary groove density variation patterns.
ii. The process shall either directly record the grating pattern onto the silicon substrate or the pattern may be generated on an intermediate layer and then transferred onto the silicon.
iii. The gratings shall have a minimum length of 200 mm and a width of no less than 20 mm.
iv. The groove density shall be as low as 50 lines/mm and as high as 2400 lines/mm.
v. Absolute placement accuracy of the grooves shall be better than 10 nm rms in the mature version of this technology, with the intermediate requirement for achieving a 50 nm rms placement accuracy.
vi. Having minimal density of structural defects such as breaks or pits.

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. U.S. Department of Energy, 2013, X-ray Optics for BES Light Source Facilities, 2013, *Report of the Basic Energy Sciences Workshop on X-ray Optics for BES Light Source Facilities,* (2013), https://science.osti.gov/-/media/bes/pdf/reports/files/X-ray_Optics_for_BES_Light_Source_Facilities_rpt.pdf, (July 9, 2021)
2. D. Voronov, E. Gullikson, and H. Padmore, 2017, Large area nanoimprint enables ultra-precise x-ray diffraction gratings, *Opt. Express 25, 23334 (2017),* https://www.osapublishing.org/oe/fulltext.cfm?uri=oe-25-19-23334&id=372814, (July 9, 2021)
3. D. L. Voronov, P. Lum, P. Naulleau, E. M. Gullikson, A. V. Fedorov, and H. A. Padmore, 2016, X-ray diffraction gratings: Precise control of ultra-low blaze angle via anisotropic wet etching, *Appl. Phys. Lett. 109, 043112 (2016),* https://doi.org/10.1063/1.4960203, (July 9, 2021)

10. HOLLOW-CORE FIBER BASED ULTRAFAST HIGH-POWER LASER BEAM DELIVERY SYSTEM

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 hollow-core fiber based ultrafast high-power laser beam delivery system used for demanding applications such as particle accelerators. In many laser applications in the accelerator facilities, lasers are operating in a burst-mode with high peak power to reduce the required laser average power. Due to the radiation concern, lasers are usually located outside of the accelerator tunnel and the laser beam is delivered to the beamline through a free-space transport line. The free space laser transport line suffers from numerous technical challenges including laser pointing stability control, radiation induced damage on optics surfaces, and maintenance difficulty due to the limited access, which significantly affect the light transmission efficiency and laser beam quality. Micro-structured hollow-core fibers guide the laser beam mostly (>99.9%) inside a hollow core (air, gas, or vacuum), enabling high power handling and drastically reduced nonlinear effects and catastrophic damage that would arise in conventional glass fibers. Today, ultrafast pulses with several 100 µJ energy and 100s of MW peak power can be transmitted in quasi single mode fashion with micro-structured hollow core fibers. Hollow-core fiber based high-power laser beam transport technology has been used in many industrial micromachining applications with great success and high reliability recently. Delivering high-energy laser pulses to the highly hostile environments such as particle accelerators with high stability, high reliability, and high transport efficiency would make many demanding and impactful applications a reality.

Grant applications are sought in the following subtopics:

a. Development of Hollow-Core Fiber based High-Power Laser Beam Delivery System

In this subtopic, we seek proposals for the development of a highly stable, efficient and radiation resistant ultrafast laser beam transport system using hollow core fibers. Design should prioritize low loss, high transport efficiency, and high beam quality. Possible solution for achieving low loss is using Nested Antiresonant Nodeless Fiber (NANF) with highly regular structures over the entire length of the fiber. In order to efficiently couple the laser output to the fiber and maintain beam quality, a special beam launching unit to the fiber will be required. This includes focusing and aligning the laser beam at the fiber tip with the required spot size and maintaining the beam position at the fiber tip with the fraction of the spot size. It is also highly desirable to integrate a beam pointing compensation system in the beam launching unit. This is to overcome the slow drift of the laser beam position at the source to ensure efficient coupling of the laser beam to the fiber. Reducing nonlinear effects due to high laser pulse energy (or high peak power) can be accomplished by enclosing the volume of the fiber core by pressurized dry air, gas, or by evacuation. This will also protect the hollow-core from dust particles and moisture. A mounting support to the fiber cable can be interfaced with the beam launching unit to ensure high repeatability, mechanical stability, and robustness of the system. The beam delivery system should be highly adaptable to work with high-energy ultrafast lasers particularly burst-mode laser systems. Key requirements include:

i. Laser wavelength range: NIR (1.0 – 1.1 um) or green (510 – 532 nm)
ii. Laser micro-pulse width: 1 – 100 ps
iii. Micro-pulse peak power: 2 – 20 MW
iv. Micro-pulse energy: 0.25 – 1 mJ
v. Micro-pulse repetition rate: 402.5 MHz
vi. Burst duration: 0.1 – 1 ms
vii. Burst-mode repetition rate: 10 – 60 Hz
viii. Macro-pulse energy: 10 – 40 J
ix. Beam transport loss: (dB/m): 0.003 – 0.01
x. Fiber bend loss at 20 cm radius (dB/m): < 0.02 (IR), < 0.5 (green)
xi. Laser beam quality M^2: < 1.2
xii. Laser polarization: linear (extinction ratio: > 50:1)
xiii. Fiber length: 50 – 70 m
xiv. Air pressure in fiber: ambient – 10^{-4} mbar

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. J. C. Knight, 2003, Photonic Crystal Fibres, *Nature 424, 847 (2003),* https://doi.org/10.1038/nature01940, (July 9, 2021)
2. B. Debord, et al., 2014, Multi-meter fiber-delivery and pulse selfcompression of milli-Joule femtosecond laser and fiber-aided laser-micromachining", *Opt. Exp. 22, 10735 (2014),* https://doi.org/10.1364/OE.22.010735, (July 9, 2021)
3. L. Olanterä *et al.*, 2013, Gamma irradiation of minimal latency hollow-core photonic bandgap fibres", *J. Instrum. 8, C12010 (2013),* https://doi.org/10.1088/1748-0221/8/12/C12010, (July 9, 2021)
4. H. Sakr, Y. Chen, G. T. Jasion, et al., 2020, Hollow core optical fibres with comparable attenuation to silica fibres between 600 and 1100 nm, *Nat. Commun. 11, 6030 (2020),* https://doi.org/10.1038/s41467-020-19910-7, (July 9, 2021)

11. SUPERCONDUCTING UNDULATOR WITH HIGH HEAT-LOAD LIMIT

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 seeks the development of superconducting undulator (SCU) which can be operated at higher temperature than 4.2 K with higher stability and 10x higher thermal load than previously utilized. Future electron storage rings for synchrotron radiation require insertion devices with much smaller vacuum chamber dimensions. Coupled with shorter electron bunches, the expected heat load on a small gap inner diameter vacuum chamber is more than an order of magnitude higher than what is measured in the current storage rings. For example, at one of the future upgrade lattices for NSLS-II, 4 mm gap vacuum chamber is expected to receive approximately 40 W/m just from resistive wall (RW) impedance. Besides RW impedance, there are other sources of heat load on the chamber, such as electron cloud multipacting, injection beam loss, geometric impedance contribution, and synchrotron radiation heating, especially due to the steering error. The steering error exacerbates for a lower energy ring, which has larger fan angle for the radiation from upstream magnets.

Nb_3Sn wire has instability issue with low on-conductor magnetic field in undulators. Magnesium Diboride superconductor was discovered in 2001, having critical temperature of 39 K. Unlike other high temperature superconducting materials, it is suitable to be made in wire form and its cost is not prohibitive. Recently, second-generation MgB_2 wire has been developed which has vast improvements in performance compared to the first-generation wire. MgB_2 wire can be stable in 2-3 T on-conductor field range and can withstand more heat load than Nb_3Sn wire.

Grant applications are sought in the following subtopics:

a. Development of Superconducting High Heat-load Undulator
In this subtopic, the development of a MgB_2-based 0.3 m long prototype is expected to be designed and constructed, and its heat load tolerance measured. Successful proposals will include detailed quench analysis, plan for magnetic measurement, and capability to deliver 2 m long SCU constructed and operated in a medium-energy storage ring. The expected parameters of the SCU are as follows:

i. Undulator period 12-15 mm
ii. Coil current density 1500A/mm^2 or greater
iii. Pole gap less than 5 mm

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. J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitani, and J. Akimitsu, 2001, Superconductivity at 39 K in magnesium diboride", *Nature 410, 63 (2001),* https://doi.org/10.1038/35065039, (July 9, 2021)
2. A. V. Zlobin, E. Barzi, D. Turrinoni, Y. Ivanyushenkov, and I. Kesgin, 2018, Advantage and Challenges of Nb_3Sn Superconducting Undulators," *Conference: 9th International Particle Accelerator Conference*, WEPML025, 2734 (2018), https://accelconf.web.cern.ch/ipac2018/papers/wepml025.pdf, (July 9, 2021)
3. H. W. Weijers, K. R. Cantrell, A. V. Gavrilin, E. L. Marks, and J. R. Miller, 2007, Assembly Procedures for a Nb3Sn Undulator Demonstration Magnet, *IEEE Transactions on Applied Superconductivity 17, 1239 (2007),* https://doi.org/10.1109/TASC.2007.899988, (July 9, 2021)
4. F. Wan, M. D. Sumption, M. A. Rindfleisch, C. J. Thong, M. J. Tomsic and E. W. Collings, 2017, High performance, advanced-internal-magnesium-infiltration (AIMI) MgB_2 wires processed using a vapor-solid reaction route," *Superconductor Science **33**, 094004 (2020),* https://doi.org/10.1088/1361-6668/ab9ef1, (July, 9, 2021)
5. T. Baig et al, 2017, "Conceptual designs of conduction cooled MgB_2 magnets for 1.5 and 3.0 T full body MRI systems", *Supercond. Sci. Technol. 30, 043002 (2017)*, https://doi.org/10.1088/1361-6668/aa609b, (July 9, 2021)

12. VISIBLE WAVELENGTH-TUNABLE PHOTOCATHODE DRIVE LASER

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 seeks the development of wavelength-tunable laser systems in the visible wavelength range for photocathode drive applications. Photoinjector drive lasers typically involve an oscillator, an amplifier, and harmonic frequency conversion, combined with spatial and temporal pulse shaping. These systems are heavily optimized to deliver exact pulse specifications at fixed wavelengths. However, the drive laser wavelengths that are available are predetermined by oscillator harmonics and the lasing medium rather than by design consideration of the wavelength that is optimal for generating the highest quality beam of electrons. A wide variety of semiconductor materials have been studied for use as cathodes at accelerator-driven light sources which require low-emittance, high average current, and long lifetimes with a wide range of wavelengths. Alternatively stated, the performance of photocathodes is normally optimal at wavelengths that are different from those readily available using current laser technologies making systematic study of a wide range of materials with a single laser source challenging.

a. Development of Wavelength-Tunable Visible Laser System

This subtopic seeks proposals for the development of a tunable-wavelength laser system that can deliver up to 100 μJ per pulse at a maximum repetition rate of 1 MHz, with optional pulse down-selection down to a single shot. The wavelength range of interest is 500 - 600 nm. This range is particularly interesting; materials studied have exhibited very low intrinsic emittance and quantum efficiency recovery leading to long lifetimes and robust operations. Closely examining semiconductor materials with photons near the effective work function (electron bandgap plus affinity) has shown that such a cathode can operate in optimal emissivity mode (high QE) or optimal mean transverse energy mode (low emittance) based on the wavelength of the laser. The baseline requirement of the intensity envelope is to be approximately 20 - 30 ps Gaussian full-width-at-half-maximum (FWHM), irrespective of whether it is a narrowband or broadband pulse. As per the transverse beam qualities, the baseline requirement is a Gaussian transverse mode with M2 ≤ 1.2.

Pulse powers in the regime of 50 μJ over the range of 500 - 600 nm will be sufficient for many high QE semiconductor photocathodes to generate adequate bunch charge for most photoinjector applications, which suffer from transport losses. For instance, this wavelength range is well suited to drive a 'standard' cathode like NaKSb near threshold. A wavelength-tunable drive laser system will also allow exploration of different types of photocathodes as well as for regularly making adjustments to accommodate photocathode QE and work function variability amongst samples or with aging.

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. Dowell, D. H., et al., 2010, Cathode R&D for future light sources, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 622, 685 (2010), https://www.sciencedirect.com/science/article/abs/pii/S0168900210006868?via%3Dihub, (July 9, 2021)
2. L. Cultrera, et al., 2015, Cold electron beams from cryocooled, alkali antimonide photocathodes, Physical Review Special Topics-Accelerators and Beams 18, 113401 (2015), https://journals.aps.org/prab/pdf/10.1103/PhysRevSTAB.18.113401, (July 9, 2021)
3. L. Cultrera, et al., 2013, Growth and characterization of rugged sodium potassium antimonide photocathodes for high brilliance photoinjector, Appl. Phys. Lett. 103, 103504 (2013), https://aip.scitation.org/doi/10.1063/1.4820132, (July 9, 2021)
4. J. Maxson, et al., 2015, Measurement of the tradeoff between intrinsic emittance and quantum efficiency from a NaKSb photocathode near threshold. Appl. Phys. Lett. 106, 234102 (2015), https://aip.scitation.org/doi/10.1063/1.4922146, (July 9, 2021)

Return to Table of Contents

13. ULTRA-HIGH RESOLUTION ELECTRON MONOCHROMATOR FOR APPLICATIONS IN TEM, STEM, AND LEEM

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

The development of advanced electron-optical characterization methods is critical for the design and understanding of advanced materials and structures, and in particular for quantum information science materials. State-of-the-art transmission (TEM) and scanning (STEM) transmission electron microscopes offer atomic-scale spatial resolution and analytical capabilities. However, the energy spread of the electron source limits the spectral resolution of the electron spectrometers used in conjunction with TEMs and STEMs, such as electron energy loss spectrometers (EELS). The energy spread of the electron source also places limitations on the resolution of spectroscopic and imaging techniques that employ lower probe energies, such as low energy electron microscopy (LEEM), which collects electrons that are reflected from the sample surface at near-zero energies at nm spatial resolution. Highly monochromatic beams will further benefit "quantum" (multi-pass) electron microscopes. The task of this call is to develop an ultra-high resolution electron monochromator that will advance electron spectroscopy and enhance imaging for improved characterization of structure, chemical composition and behavior of samples utilized in quantum information science.

Grant applications are sought in the following subtopics:

a. Development of Ultra-high Resolution Electron Monochromators

In this subtopic, we seek proposals for the development of electron monochromators that will be able to produce and manipulate highly coherent electron beams with ultralow energy spreads, high beam currents and with beam energies suitable for TEM/STEM and LEEM applications, in a compact format. Requirements for these tools include:

i. Energy spread in the range of 1 to 5 meV.
ii. Beam current in the range of 1 to 10 pA at 1 meV and > 100 pA at 5 meV energy spread.
iii. In the mature stage of the development, to be scaled for applications with beam energies ranging from 5 to 300 keV.
iv. Compact size up to 500 mm.

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. E. Bauer, 2020, Surface microscopy with low energy electrons: LEEM, *Journal of Electron Spectroscopy and Related Phenomena 241, 146806 (2020),* https://www.sciencedirect.com/science/article/pii/S0368204818301737, (July 9, 2021)
2. J. A. Hachtel, A. R. Lupini, J. C. Idrobo, 2018, Exploring the capabilities of monochromated electron energy loss spectroscopy in the infrared regime, *Nature Scientific Reports 8, 5637 (2018),* https://www.nature.com/articles/s41598-018-23805-5.pdf, (July 9, 2021)

3. J.C. Idrobo, 2020, A New Resolution Odyssey in Electron Microscopy, *arXiv: Materials Science, (2020),* https://arxiv.org/pdf/2009.05471.pdf, (July 9, 2021)
4. O. Krivanek, *et al.*, 2019, Progress in ultrahigh energy resolution EELS, *Ultramicroscopy 203, 60 (2019),* https://www.sciencedirect.com/science/article/abs/pii/S0304399118303668?via%3Dihub, (July 9, 2021)
5. P. Kruit, *et al*., 2016, Designs for a quantum electron microscope, *Ultramicroscopy 164, 31 (2016),* https://www.sciencedirect.com/science/article/pii/S0304399116300146, (July 9, 2021)

Additional information:
The five Nanoscale Science Research Centers (NSRCs) are DOE's premier user centers for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. Each center has particular expertise and capabilities in selected theme areas, such as synthesis and characterization of nanomaterials; catalysis; theory, modeling and simulation; electronic materials; nanoscale photonics; soft and biological materials; imaging and spectroscopy; and nanoscale integration. These laboratories contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other instruments not generally available except at major user facilities. NSRC resources and capabilities are available to the international academic, industry and government research community for successfully peer-reviewed research projects.
For more information see:
https://science.osti.gov/bes/suf/User-Facilities/Nanoscale-Science-Research-Centers
NSRC Portal: https://nsrcportal.sandia.gov/

14. THEORETICAL TOOLS TO ACCELERATE DISCOVERY AND IMPROVE CONTROL OF MULTI-MODAL AUTONOMOUS CORRELATIVE NANOSCALE MEASUREMENTS

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

With the advent of relatively inexpensive edge computing hardware, such as the NVIDIA Jetson, it is increasingly possible to not only perform 'live' data-analytics during experimentation, but also control these experiments actively to achieve autonomous experimentation, with multi-modal feedback [1,2]. Such a feedback could incorporate analysis from multiple different kinds of measurements performed on the same (or similar) material samples. Nanoscience facilities have multiple complementary characterization tools that probe different material properties. Specifically, imaging microscopy probes (STM, STEM, 4D-STEM, nano-ARPES, EELS, etc.) that can also operate in diffraction and spectroscopic modes, allow us to obtain the atomic and electronic landscape with resolutions both at the atomic level as well as the mesoscale, with measurements possible in operando. This is invaluable to understand how electron, spin, orbital, and lattice degrees of freedom couple at the atomistic scale to not only give rise to a specific material property but to generate a specific material response to an external stimulus which eventually determines its functionality at the meso and macroscales. Such new multi-modal nanoscale capabilities open the door for improved hypothesis testing, allowing accelerated discovery of new fundamental concepts and phenomena, pushing our boundaries of understanding the flow of matter and energy across multiple length and time scales.

To fully harness this emerging paradigm of multimodal nanoscale measurements for accelerated discovery and control, one requires predictive theory in the loop. This is not trivial, given that the size of the datasets from such measurements can be several terabytes for single experiments and sample, that are possibly correlated in a very high-dimensional space. Potential scientific discovery requires separating out sample-specific measurements from intrinsic material property and response, by analyzing this multi-dimensional correlation to enable both new scientific discoveries as well as improved capabilities for autonomous experiments. The challenge lies in developing theoretical tools that can identify pertinent signatures of the intrinsic physical phenomena in the highly correlated measurement space, that allow rapid detection of interesting anomalies – observations that go against prior knowledge pioneering potential discoveries, while at the same time bridging the multiple-length, time, and spectral ranges inherent in the data to provide a more holistic platform to enable accelerated discovery and improved control.

Grant applications are sought in the following subtopics:

a. Open-Source Software Framework for Multi-Scale Modeling – Theoretical and Computational Tools

Grant applications are sought for open-source cross-platform (Windows, Mac, Linux) software framework that allow us to bridge simulations across multiple length and timescales for a given material system. Scalable python-based workflows are needed that can interface to different first-principles and/or atomistic-MD simulation packages that scale well on DOE supercomputers (e.g., VASP, Quantum Espresso, GPAW, LAMMPS, GAMESS and similar) and can drive different types of atomistic calculations of 2d or 3d structural models and use this data to develop reduced models such as reactive force-fields and/or tight-binding DFT-models and/or continuum models. The workflow should integrate with popular computational databases (Materials Project, NOMAD, OQMD, JARVIS, C2DB and similar) and also be able to generate new structural models using scalable evolutionary search algorithms (genetic algorithms, particle swarm optimization and other similar approaches). Workflows and evolutionary algorithms should target vdW and molecular solids, as well as heterostructures formed from them. Proposals that target only bulk compounds or molecules or monolayer systems will not be considered responsive to this subtopic. Structure search algorithms should also allow archiving of this data to open-source databases in JSON format, specifically those in national-labs (such as Materials Project, NOMAD, OQMD, C2DB, DataFed at ORNL, JARVIS at NIST and others). Development of reactive force-fields and/or tight-binding models and/or continuum models, must embrace an active learning paradigm. The reduced models must be transferable to simulate different atomic structures incorporating structural heterogeneities (defects, grain boundaries, etc.). Non-reactive force-fields and tight-binding models not transferable to a wide range of coordination chemistries or heterogeneous structures will not be considered responsive to this subtopic. A GUI frontend job-manager and scheduler should allow seamless integration to multiple types of computing platforms (HPC, PC, cluster, graphics processors, etc.) via secure protocols. The software should be operable on a laptop computer and allow interactive visualization of computed signatures via open-source visualization tools (VMD, Ovito, Avogadro and similar). Expectation is that popular material simulation and visualization codes as listed above will be included in this computational software framework as a ‘black box’ so that the program is easily accessible even with a rudimentary understanding of the different methods underlying the software. Software stacks should be suitable for deployment within a multi-tool and multi-user scientific research facility (in particular, the DOE Nanoscale Science Research Centers).

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

b. AI/ML Framework for Correlative Multi-modal Analysis and Fingerprint Matching for Anomaly Detection and Knowledge Extraction – Theoretical and Computational Tools

Grant applications are sought to develop an AI/ML software that can generate a wide range of representations of atomic/electronic/phase-information from open-source simulation databases mentioned above and find correlations between multimodal signatures in nanoscale measurements and the underlying representations to generate fingerprints for novel properties, responses and physical phenomena enabling knowledge extraction. The software must target fingerprinting nanoscale measurements at DOE NSRC facilities, such as Raman, magneto-optics, STM, 4D-STEM, nano-ARPES, momentum-resolved EELS, vibrational-EELS, etc.

obtained from 2D materials, and their heterostructures, including those obtained from Moiré lattices. The fingerprints are expected to inform which experiments should be prioritized and be used to detect regions in a sample of interest that needs to be probed thereby better informing autonomous experimental control systems. Measurements that generate new fingerprints should also enable anomaly detection. The program should utilize GPU-acceleration both on extreme-edge devices, such as NVIDIA Jetson, where they can be loaded in control systems for anomaly detection, as well as connect to the cloud where knowledge extraction will be performed. The AI/ML surrogate models on the edge should be actively updated with those that reside in the cloud as measurements are made. The software should provide customization of what algorithms, materials, properties, responses are to be used that can be customized by users and utilized during data acquisition.

Approaches that do not use modern AI/ML methods will not be considered as responsive to this topic.

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

c. Electron Energy Loss Spectroscopy (EELS) Toolkit – Theoretical and Computational Tools

Advances in electron microscopes are leading to large increases in the size and quality of spectrum images with nano- to atomic-scale resolution and 10 – 100 meV energy resolution that can reveal subtle chemical and dynamical details in materials. First-principles computational methods, such as density functional theory (DFT), can provide much needed interpretation of such measurements [1]. Furthermore, the same methods can predict interesting spectral features that can be searched for directly in measurements [2,3]. However, the application of such methods is technically challenging, slowing their adoption by the larger community, despite many recent theoretical advances [4,5,6,7]. Many studies would benefit from an interactive, user-friendly toolkit to both build representative models and to generate spectra measurable using electron energy loss spectroscopy (EELS), which probes materials properties through fundamental excitations of core electrons, plasmons, optical excitations, phonons, etc. The same toolkit would also be applicable to synchrotron X-ray measurements and could be added to the tools of computational scientists worldwide. Coupling to existing materials databases would be desirable, and machine learning (ML) approaches to accelerate calculations are strongly encouraged.

Examples of public EELS data sets can be found here:

- https://eels.info/atlas
- https://eelsdb.eu/
- http://muller.research.engineering.cornell.edu/sites/WEELS/

The Materials Project provides X-ray absorption spectra (analogous to EELS) for listed materials: https://materialsproject.org/

Solutions must contain all of the following:

- Interface/API to existing visualizers and environments, e.g., ASE, Avogadro, VESTA, etc.
- Graphical user interface to build/visualize atomic/molecular models and their electronic structure with associated spectral calculations
- User-friendly interactive structural manipulation and associated spectral evolution (enhanced by ML), possibly connected to molecular dynamics sampling
- Programmable (notebook/workflow) functionality via python interface
- Common interface (I/O) for multiple computational engines (localized orbitals or plane waves)

The deliverables that will define success are:

1) A flexible platform to connect computational software and simulation results with spectroscopy and microscopy measurements through interactive visual cues related to atomic and electronic structure. (required)
2) A user-friendly interface that can identify and characterize spectral features accessing a database of measurements and/or simulations for relevant materials and associated atomic structure. (required)
3) Tools to educate the user on atomic detail in measured spectra and/or propose experiments on materials that might display interesting spectral features. (optional but desirable)
4) An interactive tool that would automatically direct measurements by identifying regions of chemical interest based on spectral cues, prompting collection of additional data in these regions. (optional but desirable)

Open source software solutions are strongly encouraged.

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: Subtopics a and b:

1. University of Toronto, 2020, AI For Discovery and Self-Driving Labs, *The Matter Lab, University of Toronto, Department of Chemistry,* https://www.matter.toronto.edu/basic-content-page/ai-for-discovery-and-self-driving-labs, (July 9, 2021)
2. Kalinin, S.V., et al, 2021, Automated and Autonomous Experiment in Electron and Scanning Prob Microscopy, *arXiv: 2103. 12165v1*, https://arxiv.org/abs/2103.12165, (July 9, 2021)

References: Subtopic c:

1. Pascal, T.A., et al, 2014, Finite temperature effects on the X-ray absorption spectra of lithium compounds: First-principles interpretation of X-ray Raman measurements, *J. Chem. Phys. 140, 034107 (2014),* https://dx.doi.org/10.1063/1.4856835, (July 9, 2021)
2. Pascal, T.A., et al, 2015, X-ray Spectroscopy as a Probe for Lithium Polysulfide Radicals, *Phys Chem Chem Phys 17, 7743 (2015),* https://dx.doi.org/10.1039/C4CP05316H, (July 9, 2021)
3. Drisdell, W.S., et al, 2013, Probing Adsorption Interactions In Metal-Organic Frameworks Using X-ray Spectroscopy, *J. Am. Chem. Soc. 139, 035104 (2013),* https://dx.doi.org/10.1021/ja408972f, (July 9, 2021)
4. Liang, Y., et al, 2017, Accurate X-Ray Spectral Predictions: An Advanced Self-Consistent-Field Approach Inspired by Many-Body Perturbation Theory, *Phys. Rev. Lett. 118, 096402 (2017),* https://dx.doi.org/10.1103/PhysRevLett.118.096402, (July 9, 2021)
5. Roychoudhury, S., et al, 2020, Deciphering the Oxygen Absorption Pre-edge: a Caveat on its Application for Probing Oxygen Redox Reactions in Batteries, Energy & Environmental Materials accepted (2020), https://doi.org/10.1002/eem2.12119, (July 9, 2021)
6. Eichhorn, J., et al, 2020, Revealing Nanoscale Chemical Heterogeneities in Polycrystalline Mo-BiVO4 Thin Films, *Small 2001600 (2020),* https://doi.org/10.1002/smll.202001600, (July 9, 2021)
7. Wang, H., et al, 2019, A combined multi-reference pump-probe simulation method with application to XUV signatures of ultrafast methyl iodide photodissociation, *J. Chem. Phys. 151, 124106 (2019),* https://doi.org/10.1063/1.5116816, (July 9, 2021)

Additional information:
The five Nanoscale Science Research Centers (NSRCs) are DOE's premier user centers for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. Each center has particular expertise and capabilities in selected theme areas, such as synthesis and characterization of nanomaterials; catalysis; theory, modeling and simulation; electronic materials; nanoscale photonics; soft and biological materials; imaging and spectroscopy; and nanoscale integration. These laboratories contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other instruments not generally available except at major user facilities. NSRC resources and capabilities are available to the international academic, industry and government research community for successfully peer-reviewed research projects.
For more information see:
https://science.osti.gov/bes/suf/User-Facilities/Nanoscale-Science-Research-Centers
NSRC Portal: https://nsrcportal.sandia.gov/

15. FAIR DATA MANAGEMENT SOFTWARE TOOLS FOR USER FACILITIES

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

FAIR data principles multiply the impact of scientific datasets by emphasizing Findability, Accessibility, Interoperability, and Reuse. There remain numerous technical challenges limiting more widespread adoption of FAIR principles in facilities hosting a diversity of scientific measurement tools. Scientific user facility scientists need software tools that reduce the burden for organizing, annotating, and releasing datasets of experimental measurements of materials. We solicit technical solutions which leverage artificial intelligence and machine-learning (AI/ML) methods to dramatically simplify the task of managing microscopy image datasets of material surfaces, in particular data collected on optical/Raman microscopes, scanning probe microscopes, and electron microscopes. Tools must be optimized to assist with these scientific image datasets, especially to organize, annotate, and distribute in keeping with the principles of FAIR and open data. Tools should leverage AI/ML to implement the following features: automatic searching and indexing of existing data stored in filesystems; suggestions of links between data, papers, scientific taxonomies, and material databases (especially Materials Data Facility, Zenodo, Dryad, Materials Cloud, and Dataverse); automated clustering and metadata suggestion; discovery of trends within datasets; and streamlined submission of datasets to repositories. Technical development should result in the delivery of an extensible software system suitable for deployment within a multi-tool and multi-user scientific research facility (in particular, the DOE Nanoscale Science Research Centers). NSRC collaborations are not required for this topic, however applicants interested in accessing relevant data repositories to design and test their solutions should contact an NSRC and state this collaboration in their application.

Grant applications are sought in the following subtopics:

a. Microscopy Tools – Theoretical and Computational Tools
The integrated solution must:
- Run on an on-site network-attached server.
- Be able to index network-accessible storage systems.
- Respect user-specified access and distribution rules (while connecting to external resources for comparison and uploading).
- Expose a web-based user interface for browsing, organizing, and annotating image data.

- Automatically sort and classify two-dimensional image data that may be single-channel (greyscale) or multi-channel (e.g., hyperspectral).
- Perform data classification and tagging by combining deep learning methods for extracting image signatures (e.g., via autoencoders), and natural language processing methods (such as those based on word2vec) that operate in a semantic latent embedding space.
- Provide tools for users to visualize and explore the AI/ML latent spaces, and export associated signatures into downstream analysis tools.
- Have good performance for realistic dataset sizes. In particular, new datastores containing tens of thousands of images should be indexed within hours, and the index should update within seconds upon addition of new images.
- Have sufficient performance for user-interactive tasks, such as enabling rapid (within seconds) user querying for a datastore containing millions of images.

Approaches that do not use modern AI/ML methods will not be considered for this topic.

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. Kramer, M.A, 1991, Nonlinear principal component analysis using autoassociative neural networks, *AIChE Journal. 37 (2): 233–243,* https://aiche.onlinelibrary.wiley.com/doi/10.1002/aic.690370209, (July 9, 2021)
2. Goodfellow, I., et al, 2016, Deep Learning, *MIT Press. ISBN 978-0262035613,* https://www.deeplearningbook.org/, (July 9, 2021)
3. Welling, M., et al, 2019, An Introduction to Variational Autoencoders, *Foundations and Trends in Machine Learning, 12 (4): 307–392. arXiv:1906.02691,* https://arxiv.org/abs/1906.02691, (July 9, 2021)
4. Mikolov, T., et al, 2013, Efficient Estimation of Word Representations in Vector Space, *arXiv:1301.3781,* https://arxiv.org/abs/1301.3781, (July 9, 2021)
5. Mikolov, T., 2013, Distributed representations of words and phrases and their compositionality, *Advances in Neural Information Processing Systems*, *arXiv:1310.4546* https://arxiv.org/abs/1310.4546, (July 9, 2021)
6. Goldberg, Y., Levy, O., 2014, word2vec Explained: Deriving Mikolov et al.'s Negative-Sampling Word-Embedding Method, *arXiv:1402.3722,* https://arxiv.org/abs/1402.3722, (July 9, 2021)

Additional information:

The five Nanoscale Science Research Centers (NSRCs) are DOE's premier user centers for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. Each center has particular expertise and capabilities in selected theme areas, such as synthesis and characterization of nanomaterials; catalysis; theory, modeling and simulation; electronic materials; nanoscale photonics; soft and biological materials; imaging and spectroscopy; and nanoscale integration. These laboratories contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other instruments not generally available except at major user facilities. NSRC resources and capabilities are available to the international academic, industry and government research community for successfully peer-reviewed research projects.

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

16. LOW COST, SOLUTION PROCESSIBLE PEROVSKITE MATERIALS FOR HIGH PERFORMANCE X-RAY IMAGING

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

X-ray imaging is a non-destructive approach with application in medical imaging, material structure characterization, and security screening [1,2]. Historically, x-ray detection has been a limiting factor for x-ray imaging, with no cost-effective detectors available that can achieve both high quantum yield and high resolution. A direct-conversion x-ray detector utilizing a semiconductor to directly convert x-ray photons to charge carriers potentially offers the best spatial and energy resolution [3].

The ideal properties for an efficient x-ray imaging detector include a) high atomic number (Z) for efficient photon absorption; b) high carrier mobility and long lifetime; c) low trap density to minimize dark noise. Amorphous Selenium (a-Se) has been used to build imaging detectors [4], however, the poor degree of crystallinity of a-Se causes charge accumulation, which blurs image quality. Other semiconductors like Ge and CdTe have been investigated, but the cost to fabricate at sufficient scale is still too high.

Recently, metal-halide perovskite materials containing high Z elements have been demonstrated as promising semiconductors for x-ray imaging detectors [5-10]. Perovskites have excellent carrier mobility and lifetime and are free of deep trap states. Perovskites can also be processed from solution – these characteristics together address the shortcomings of classical semiconductors for low-cost x-ray imaging detectors.

Grant applications are sought for developing a pixelated x-ray imager using low-cost metal halide perovskite semiconductors (examples are: methylammonium lead triiodide (bromide), formamidinium lead triiodide, bismuth-based perovskites). The targeting x-ray energy range is 10 - 100 keV, for x-ray crystallography and medical imaging. Other absorber materials such as metal oxides or organic semiconductors will not be considered; other indirect detection techniques like scintillator-based imager will not be considered.

Grant applications are sought in the following subtopics:

a. Low-Cost Pixelated X-Ray Imager
Develop a low-cost pixelated x-ray imager combining a polycrystalline perovskite x-ray absorber (processed from low temperature, solution-based methods) with a silicon thin film transistor panel. The detection sensitivity should be more than 100 $\mu C\ Gy_{air}^{-1}cm^{-2}$ and the pixel size should be below 100-micrometers.

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

b. Pixelated Circuits on a Single Crystal Perovskite Wafer
Develop pixelated circuits on a single crystal perovskite wafer with large lateral dimension (5 cm by 5 cm) and develop read out electronics for imaging. The targeting sensitivity should be better than 1000 $\mu C\ Gy_{air}^{-1}cm^{-2}$. The number of pixels built on each crystal should be more than 100 with pixel sizes below 200 micrometers.

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. Ballabriga, R. *et al*, 2020, Photon Counting Detectors for X-ray Imaging with Emphasis on CT. *IEEE Transactions on Radiation and Plasma Medical Sciences*, 1-1, (2020), https://ieeexplore.ieee.org/xpl/RecentIssue.jsp?punumber=7433213, (July 9, 2021)
2. Delpierre, P. *et al*, 2001, X-ray pixel detector for crystallography, *IEEE Transactions on Nuclear Science 48, 987-991, (2001),* https://ieeexplore.ieee.org/abstract/document/958710, (July 9, 2021)
3. Kasap, S. O., Zahangir Kabir, M. & Rowlands, J. A., 2006, Recent advances in X-ray photoconductors for direct conversion X-ray image detectors, *Current Applied Physics 6, 288-292, (2006),* https://www.sciencedirect.com/science/article/abs/pii/S1567173905002415, (July 9, 2021)
4. Huang, H., Abbaszadeh, S., 2020, Recent Developments of Amorphous Selenium-Based X-Ray Detectors: A Review, *IEEE Sensors Journal 20, 1694-1704, (2020),* https://ieeexplore.ieee.org/document/8886491, (July 9, 2021)
5. Kim, Y. C*., et al.*, 2017, Printable organometallic perovskite enables large-area, low-dose X-ray imaging, *Nature 550, 87-91, (2017),* https://www.nature.com/articles/nature24032, (July 9, 2021)
6. Liu, J., *et al.*, 2019, Flexible, Printable Soft-X-Ray Detectors Based on All-Inorganic Perovskite Quantum Dots, *Advanced Materials 31, 1901644, (2019),* https://onlinelibrary.wiley.com/doi/abs/10.1002/adma.201901644, (July 9, 2021)
7. Pan, W.*, et al.*, 2017, Cs2AgBiBr6 single-crystal X-ray detectors with a low detection limit, *Nature Photonics 11, 726-732, (2017),* https://www.nature.com/articles/s41566-017-0012-4, (July 9, 2021)
8. Tsai, H., *et al.*, 2020, A sensitive and robust thin-film x-ray detector using 2D layered perovskite diodes, *Science Advances 6, eaay0815, (2020),* https://advances.sciencemag.org/content/6/15/eaay0815, (July 9, 2021)
9. Wei, H. *et al.*, 2016, Sensitive X-ray detectors made of methylammonium lead tribromide perovskite single crystals, *Nature Photonics 10, 333-339, (2016),* https://www.nature.com/articles/nphoton.2016.41, (July 9, 2021)
10. Zhuang, R. *et al.*, 2019, Highly sensitive X-ray detector made of layered perovskite-like (NH4)3Bi2I9 single crystal with anisotropic response, *Nature Photonics 13, 602-608, (2019),* https://www.nature.com/articles/s41566-019-0466-7, (July 9, 2021)

Additional information:

The five Nanoscale Science Research Centers (NSRCs) are DOE's premier user centers for interdisciplinary research at the nanoscale, serving as the basis for a national program that encompasses new science, new tools, and new computing capabilities. Each center has particular expertise and capabilities in selected theme areas, such as synthesis and characterization of nanomaterials; catalysis; theory, modeling and simulation; electronic materials; nanoscale photonics; soft and biological materials; imaging and spectroscopy; and nanoscale integration. These laboratories contain clean rooms, nanofabrication resources, one-of-a-kind signature instruments, and other instruments not generally available except at major user facilities. NSRC resources and capabilities are available to the international academic, industry and government research community for successfully peer-reviewed research projects.
For more information see:

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

17. 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 facilities where users conduct research on the structure and dynamics of materials, chemical and biological systems. 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 the capabilities for research employing neutron scattering, including advances that will impact clean energy research. Grant applications should define the instrumentation need for the facilities and outline the research that will lead to innovative capabilities for the facilities. 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 of the research for the new instrumentation and tools by providing a letter of support from the user facility staff scientist or a successful user.

A successful user is defined as someone at a research institution who has recently performed neutron scattering measurements at the facilities and published results in peer reviewed 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: New and active DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply for computational time at the DOE National Energy Research Scientific Computing Center (NERSC), a primary scientific computing facility for the DOE. 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 measurements. 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 and operando research. Sample environments may enable conditions appropriate for in situ materials synthesis and operando assessment of materials and chemistries in energy and advanced manufacturing/chemical processing environments, and support innovative approaches to incorporate diagnostic and characterization tools that complement neutron scattering data.

Development of steady state high field magnets: The steady-state high-field magnets currently are limited to a maximum field of 16 tesla at US neutron scattering facilities. This limits research on materials and other systems at higher magnetic fields [5-7]. To address this gap, development is needed for high field magnets with appropriate geometries, based on new technologies (e.g., high temperature superconductors) suitable for neutron scattering research at the current and future neutron scattering facilities such as SNS Second Target Station.

Development of neutron transparent sample environments for in-situ studies: Neutron scattering measurements to measure changes in samples in-situ and operando conditions are of increasing importance to the neutron scattering user community. As such, sample environments that allow scattering measurements on samples maintained at conditions relevant to the sample's synthesis, processing, or property are of interest. Tools are needed for precision control of parameters such as temperature and humidity or solvent partial pressure (e.g., Peltier-driven relative humidity chamber and control system [8]) that allow simultaneous characterization of the same sample by neutron scattering measurements in coordination with other techniques such as Raman spectroscopy [9], FTIR spectroscopy [10], or light scattering [11].

Development of advanced sample positioning, manipulation, and containment devices: Neutron scattering experiments frequently involve measurements of multiple samples in extreme conditions or measurement of scattering from a sample of complex geometry in many different positions and orientations. Experiments of this nature would be greatly facilitated by compact programmable sample manipulators capable of positioning a sample or sample environment device at a precise position and orientation within a beam. Examples of this would include a sample mounting arm that can move a sample of complex geometry and mass ranging from a few grams to tens of kilograms on a predefined trajectory through the neutron beam with positional accuracy of better than 0.1 mm and angular accuracy better than 0.1 degrees, an automated sample changer capable of selecting samples at elevated or cryogenic temperatures and placing them in the measurement position in the beam within the sample environment, and a sample loader capable of removing a highly radioactive sample from storage and placing it in a sample environment for measurement and then returning it to safe storage after the measurement.

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

b. 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], advanced neutron beam choppers for neutron energy selection [17], and spin state selection and control devices [18].

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

c. Situation-responsive Experiment Planning and Optimizations Tools

As demands increase for neutron scattering facilities, there are needs to perform scattering measurements with higher efficiency and improved use and quality of data in subsequent analyses. Savings in measurement times for a given sample at required resolution can directly lead to more experiments to be conducted at the facilities. This could be achieved with innovative protocols based on artificial intelligence (AI) for autonomous experimentation controlled by machine learning (ML) algorithms.

ML-based on-the-fly analysis and dynamic control of diffraction experiments at synchrotron beam lines have already shown significant benefits [19-23]. Previous examples of fully-automated closed-loop measurements have demonstrated reduction in overall number of experimental cycles by an order of magnitude through the use of Bayesian optimization algorithms. Successful projects will develop software tools and protocols to significantly speed up the measurement and data collection processes.

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

d. Advanced Choppers

Advances over the last decades have led to short-pulse sources with brightest neutron beams. While neutron choppers capable of extracting short bursts of these high-brightness neutrons have benefitted from magnetic bearing technology, they are still limited by the payload or rotating neutron selecting component. New developments in chopper design, particularly in the type known as Fermi choppers that incorporate thin absorbing materials in a housing spun at high speeds, are needed for the current and future high brightness neutron sources such as SNS Second Target Station under construction at ORNL. Incorporating neutron reflecting mirrors into the payload, something known as a "magic" chopper, is a challenge but it will allow a single device to cover a wide range of wavelengths and stay well matched to the source characteristics [24].

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

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 topic descriptions above.

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

References:

1. U.S. Department of Energy, Neutron Scattering Facilities, Office of Science, https://science.osti.gov/bes/suf/User-Facilities/Neutron-Scattering-Facilities, (July 9, 2021)
2. United States 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, (July 9, 2021)
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, (July 9, 2021)
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, (July 9, 2021)
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, (July 9, 2021)
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, (July 9, 2021)

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, (July 9, 2021)
8. Heller, W. T., Waring, A. J., Lehrer, R. I., Harroun, T. A., Weiss, T. M., Yang, L., and Huang, H. W., 2000, Membrane Thinning Effect by the Beta-Sheet Antimicrobial Protegrin, Biochemistry 39: 139-145 (2000), https://pubmed.ncbi.nlm.nih.gov/10625488/, (July 9, 2021)
9. 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, (July 9, 2021)
10. 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, (July 9, 2021)
11. 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, (July 9, 2021)
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, (July 9, 2021)
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/, (July 9, 2021)
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, (July 9, 2021)
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, (July 9, 2021)
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, (July 9, 2021)
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, (July 9, 2021)
18. Sarenac, D., J. Nsofini, I. Hincks, M. Arif, Charles W. Clark, D. G. Cory, M. G. Huber, and D. A. Pushin. "Methods for preparation and detection of neutron spin-orbit states." *New Journal of Physics 20, no. 10 (2018): 103012.* https://iopscience.iop.org/article/10.1088/1367-2630/aae3ac, (July 9, 2021)
19. A. Gilad Kusne, et al., 2014, "On-the-fly machine-learning for high-throughput experiments: search for rare-earth-free permanent magnets," *Scientific Reports 4, 6367 (2014).* https://www.nature.com/articles/srep06367, (July 9, 2021)
20. A. Gilad Kusne, et al., 2020, On-the-fly Closed-loop Autonomous Materials Discovery via Bayesian Active Learning, *Nature Communications 11, 5966 (2020).* https://www.nature.com/articles/s41467-020-19597-w, (July 9, 2021)

21. Noack, Marcus M., et al. 2019, A kriging-based approach to autonomous experimentation with applications to x-ray scattering. *Scientific reports 9, 1 (2019).* https://www.nature.com/articles/s41598-019-48114-3, (July 9, 2021)
22. Noack, Marcus M., et al. 2020, Advances in kriging-based autonomous x-ray scattering experiments. *Scientific reports 10, 1 (2020).* https://www.nature.com/articles/s41598-020-57887-x, (July 9, 2021)
23. Rakita, Yevgeny, et al., 2020, Active Reaction Control of Cu Redox State Based on Real-Time Feedback from In Situ Synchrotron Measurements, *Journal of the American Chemical Society 142, 18758 (2020),* https://pubs.acs.org/doi/10.1021/jacs.0c09418, (July 9, 2021)
24. 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, (July 9, 2021)

18. MEMBRANES FOR ELECTROCHEMICAL ENERGY STORAGE 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, increased mechanical strength, 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.

Electricity itself is difficult to store on any scale. Electrochemical devices that can convert electrical current from carbon-free sources of energy – solar, wind, or geothermal – into chemical energy that can be stored are therefore important in the future clean energy landscape. 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, redox flow batteries, solar fuel generators, and electrolyzer cells. 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, non-solar driven electrolyzer cells, or aqueous all-vanadium redox flow batteries do not fall within this topic and will not be considered. Electrochemical applications focused on power generation (e.g., fuel cells) or on 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 Rechargeable Batteries

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. In many cases, the new chemistry or cell architecture being explored involves differences in operating voltage, working ions, interfacial environments, or charge transport requirements that necessitate development of new electrolytes which are not compatible with commercial Li-ion membranes. Poor performance (e.g., wetting) of a commercial Li-ion membrane when used in a non-traditional electrolyte developed for a new battery technology can lead to difficulties demonstrating the commercialization potential of the underlying new battery chemistry or architecture.

To ensure that compatible electrolyte-membrane combinations exist for technology development of advanced electrochemical energy storage beyond Li-ion batteries, grant applications for this subtopic should address one of the following three areas:

- Non-aqueous redox flow batteries utilizing organic redox active materials – Development of highly ion-selective membranes that resist swelling and fouling in organic solvents, are mechanically robust, and prevent unwanted crossover of redox active materials could greatly accelerate the development of non-aqueous flow batteries for grid storage applications.[3] Included are membranes with high ion-selectivity derived by physical, chemical, or combined means to prevent unwanted crossover in the non-aqueous redox flow battery architecture.

- Advanced electrochemical energy storage using multivalent working ions – Development of highly ion-selective membranes for use with non-traditional liquid electrolytes is needed for advanced rechargeable batteries using magnesium, aluminum, zinc, or other multiply-charged cations as the working ion. Non-traditional liquid electrolytes include organic, aqueous, ionic liquid-based, highly concentrated, and/or inhomogeneous compositions that are specifically designed for multivalent battery chemistry.

- Advanced electrochemical energy storage using dense 3D arrays of nanoscale battery components (e.g., nano-electrodes) – Development of precise nanoscale structures that serve as separators between individual nanoscale electrodes in a novel battery architecture are needed to advance beyond today's 2D, planar structures towards fully 3D, densely packed arrays of nanoscale components.[4] Included are novel solid-state electrolytes which serve both as a conformal membrane separator and electrolyte in such battery architectures and which can be readily deposited with nanoscale precision for a battery architecture beyond a 2D thin-film structure. Improvements to well-known solid-state electrolytes such as lithium phosphorus oxynitride (LiPON) will not be considered if applied only to thin-film batteries or similar battery architectures with planar "2D" electrodes.

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 require non-traditional electrolytes. The focus is to be on membrane development, although limited development of the non-traditional electrolyte may be required due to the nature of early stage research and development. The following characteristics and advanced functionality are also desired and should be demonstrated if possible:

- Membranes that have an ion transference number approaching unity for the relevant working ions;
- Membranes that can be used with highly conducting, novel electrolytes designed for ultrafast (>6C) charge/discharge rate;
- Membranes with inherent resistance to fouling, swelling, and other time-dependent changes in relevant properties;
- Membranes that self-heal, self-repair, or otherwise mitigate unwanted degradation of performance while in operation.

The goal of any proposed work under this subtopic should be to develop a battery membrane material with improved, selective ion transport and a sufficient lifetime to support commercialization of the underlying 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. 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, (July 9, 2021)
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, (July 9, 2021)
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, (July 9, 2021)
4. Ashby, D. S., Choi, C. S., Edwards, M.A., Talin, A. A., White, H. S., and Dunn, B. S., 2020, High-Performance Solid-State Lithium-Ion Battery with Mixed 2D and 3D Electrodes, *ACS Appl. Energy Mater. 2020, 3, 9, 8402–8409. DOI: 10.1021/acsaem.0c01029.* https://pubs-acs-org.proxy.scejournals.org/doi/10.1021/acsaem.0c01029, (July 9, 2021)

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, (July 9, 2021)
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/, (July 9, 2021)
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, (July 9, 2021)

19. DESIGN OF COLOR CENTERS FOR SPIN QUBIT DEVICES

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

The performance of quantum information and optics, navigation and geoscience probes, and nano-sensing in condensed-matter physics, depends strongly on the quality of materials integrated into them. Color centers with a particular concentration and orientation of optically active defect spins, to produce highly efficient quantized optical transitions and long spin coherence times, are the key to advancing spin qubit devices. Clean, reliable, and reproducible implementation of these atom-like impurities and defects, and having their properties be decoupled from the host materials, allows optimization of optical and spin properties. Of particular interest in this topic is the design of color centers, by control of vacancies in high-quality diamond (e.g., NV centers), or defects in other wide bandgap semiconductors and oxides, for advancing applications of high-resolution quantum sensors or long-distance quantum networks.

Applicants with collaborations for measurements or demonstrations that require access to DOE sites, National Laboratories, or universities must include letters of support from the relevant collaborator, field site manager, or equivalent. Technologies whose applications are biologically related will not be considered.

Grant applications are sought in the following subtopics:

a. Synthesis of High-Quality Color Centers

Applications must effectively address each of the following four research areas, to undergo merit review.

1. Express the idea for a specific color center design, aimed for a particular improved application.
2. Describe the materials growth capabilities for producing high-purity host materials with clean/large surfaces, with the ability to incorporate low-strain and localized defects at atomically controlled depths and arrangements.
3. Explain the aim for optimal coherence yield on the designer color centers, by integrating optical and spin property measurements and local nanoscale characterizations, to demonstrate narrow and stable optical lines.
4. Show the capability to produce a prototype device based on the long-lived and localized spins, for either nanoscale measurements or telecom wavelength networks.

Questions – Contact: Athena S. Sefat, Athena.Sefat@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 designer color centers interfaced with high-resolution quantum sensors or long-distance quantum networks applications. Applicants to this subtopic are strongly encouraged to confirm the responsiveness of their proposed innovation with the contact provided below, before making submissions.

Questions – Contact: Athena S. Sefat, Athena.Sefat@science.doe.gov

References:

1. U. S. Department of Energy, 2016, Quantum Sensors at the Intersections of Fundamental Science, Quantum Information Science & Computing, https://science.osti.gov/-/media/hep/pdf/Reports/DOE_Quantum_Sensors_Report.pdf, (July 9, 2021)
2. U. S. Department of Energy, 2017, Opportunities for Basic Research for Next-Generation Quantum Systems, https://science.osti.gov/-/media/bes/pdf/reports/2018/Quantum_systems.pdf, (July 9, 2021)

20. 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) enable the deployment of advanced reactors to help meet the Administration's energy security and clean energy goals; (3) develop sustainable nuclear fuel cycles; and (4) maintain US leadership in nuclear energy technology.

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: Stephen Kung, Stephen.Kung@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, 2021, Office of Nuclear Energy Strategic Vision, https://www.energy.gov/ne/downloads/office-nuclear-energy-strategic-vision, (July 9, 2021)
2. U.S. Department of Energy, 2021, Fuel Cycle Technologies, Office of Nuclear Energy, Science and Technology, http://www.energy.gov/ne/nuclear-reactor-technologies/fuel-cycle-technologies, (July 9, 2021)
3. U.S. Department of Energy, 2021, Nuclear Reactor Technologies, Office of Nuclear Energy, Science and Technology. http://www.energy.gov/ne/nuclear-reactor-technologies, (July 9, 2021)
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, (July 9, 2021)
5. U.S. Department of Energy, 2017, Technology and Applied R&D Needs of Molten Salt Chemistry (2017), https://www.ornl.gov/sites/default/files/Molten%20Salt%20Workshop_Final_092917.pdf, (July 9, 2021)

21. 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

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 oil and gas supplies. The subsurface can also serve as a reservoir for energy storage for power produced from intermittent generation sources, such as wind and solar. As such, understanding and effectively harnessing subsurface resources while mitigating impacts of their development and use are critical pieces of the Nation's forward energy strategy.

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.

For this topic, the National Energy Technology Laboratory is not eligible to act as a subawardee.

Grant applications are sought in the following subtopics:

a. Geothermal

This subtopic focuses on critical aspects of wellbore integrity needed for widespread commercialization of geothermal technologies which directly supports the Biden Administration's goals for a clean energy future. In order to advance the state of the art of well integrity and well failure mitigation, the Department of Energy's Office of Basic Energy Sciences and Geothermal Technologies Office have teamed together to support R&D in the subtopic below. The goal of this topic is to advance innovation in the geothermal industry by integrating practices from subsurface focused sectors (geothermal, oil and gas, mining, etc.) that may substantially improve geothermal well completion, stimulation, and/or operations via improved understanding and prevention of wellbore impairment.

Applications of interest under this subtopic should focus on the challenges related to improving technologies related to geothermal energy development in conditions with elevated temperatures (> 390°F or approximately 200°C) and crystalline lithologies. Specifically of interest are advances to the state-of-the-art for characterization, prevention, and/or remediation of downhole well integrity failures that cause significant non-productive time or impaired well performance.

Applications of interest may include, but are not limited to novel materials or technologies that could be integrated with the well completion process that would provide geothermal operators the ability to detect and monitor well integrity issues; e.g., well completion methods and/or sensors that incorporate monitoring capabilities without operators being required to re-enter the well following completion. They could include innovative diagnostics systems for continual monitoring of geothermal well conditions such as temperature, pressure, flow, phase, chemistry, etc. (borehole or surface based). Innovative telemetry methods, systems for signal acquisition, and/or data analysis methods that integrate new sensing approaches for well integrity surveillance would be of interest. Applications could also include novel, targeted remediation technologies that can be deployed without the use of a drilling rig, or new materials that enable improvements in targeted remediation approaches.

Addressing these items would be beneficial to operators as the incremental costs to remediate these issues could ultimately be lowered by development of advanced detection and by higher accuracy with respect to diagnosing the problem. Advancement in remediation and/or prevention technologies could then be developed and deployed more appropriately.

A Phase I application should focus on proof of concept via engineering design, materials development, modeling, and/or laboratory scale testing (as applicable). Phase I efforts should be scalable to subsequent Phase II development including model validation, prototype development, and/or pilot or field-scale testing (as applicable).

Proposed projects with modeling or analysis components 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. Applications must be responsive to the subtopic of improving understanding of well integrity via innovative methods. Applications focusing on updated cement formulations, chemical or mechanical diverters, or proposing conventional well remediation technologies (rig-based and/or not operable at the specified temperature) will be deemed non-responsive.

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

b. Turning Oilfield Waste into a Feedstock: Technologies for Realizing Value from Produced Water

Produced water is a large volume byproduct stream associated with oil and gas exploration and production. Approximately 21 billion barrels (1 barrel (bbl) = 42 U.S. gallons) of produced water are generated each year in the United States from about 900,000 wells.[1] This is equivalent to a volume of 2.4 billion gallons per day. The cost of managing produced water is a significant factor in the profitability of oil and gas production. Generally speaking, the volume of water production relative to oil and gas production increases as a well ages. When managing produced water (collecting, treating, transporting, and disposing of the water) exceeds the value of the hydrocarbon produced from the well, the well is usually shut in and any oil or gas remaining to be produced is lost or its production delayed until oil or gas prices rise to the point that production is once again profitable.

Water produced from conventional wells varies in terms of the level of salinity and other constituents such as naturally occurring radioactive materials (NORM), dissolved minerals, dissolved hydrocarbons, metal ions, sulphur, and other trace elements. Salinity is typically the greatest barrier to reuse; the saltier the brine the more energy must be expended to remove the salt to the point where the reduced salinity water can be reused. Generally, the cost of removing the salt from oilfield brine is greater than the value of the water, given other options for water supply in areas where oilfield produced water is available.

Large volumes of produced water are flowed back from hydraulic fracturing of unconventional shale gas and tight oil wells, and this water can exhibit very high salinity as well as high concentrations of fracturing fluid additives. For the most part, however, operating and service companies have found ways to remove most of the contaminants other than the salt and then employ additives that render the brine reusable as hydraulic fracturing makeup water. A certain percentage of the water treatment process output still must be disposed of in deep disposal wells.

Over the past decade the U.S. Department of Energy's (DOE) Office of Fossil Energy (FE) has funded new research and development (R&D) projects aimed at reducing the cost of treating and reusing produced water with an overall goal of transforming this waste to a resource. DOE has previously invested approximately $100 million into produced water projects and continues to collaborate with industry, universities, state governments, other federal agencies, and non-governmental organizations.[2] The objective of finding transformational technologies for low-cost desalination of oilfield produced brine remains, but DOE believes that there may by niche markets where a combination of factors may make it possible for novel technologies to provide a pathway for value to be extracted from produced water.

Accordingly, DOE is seeking proposals for the development and testing of technologies that rely on some combination of the following features to achieve economic feasibility in a specific producing basin or region:

- Lower salinity produced water (e.g., some Rocky Mountain brines are relatively fresh),
- Co-location of stranded gas (e.g., flared associated gas, shallow low pressure gas) that can be utilized as a low cost (or no-cost) source of power,
- Co-location with disposal options (e.g., deep wells) for process outputs of no value,
- Possibility of integration of renewable (e.g., solar, geothermal or wind) power into the process,
- Presence of higher value constituents within a specific produced water stream (e.g., lithium, minerals, rare earth elements),
- Nearby markets for water treated to a suitable level of salinity (e.g., power plant cooling water or possibly agricultural use),

- Nearby markets for products generated from the water stream (e.g., crystal salt, hydrogen from renewable powered electrolysis), and
- Potential for smaller-scale, modular, skid-mounted process units that can be reused to spread capital investments across a wider area of use.

While the number of places where such combinations of technologies can be effective may be small, DOE hopes to illuminate how a path to commercial produced water reuse can be feasible if all options for energy savings and marketable products are examined.

Proposals for technology development and testing should include at least a cursory evaluation of the potential economics of an operating process with reasonable estimates of product values and process costs at the selected location.

Although the focus of this solicitation is on proving concepts and developing and testing technologies capable of being scaled up to field level prototypes, proposals for detailed feasibility studies could be acceptable if they are aimed at providing a better understanding of the basic science behind a novel process, that could lead to a breakthrough in its economic application.

Letters of industry support for the proposed process or the inclusion of industry partners on the proposal team are encouraged.

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

c. Novel Concept for Underground Gas Storage Reservoir Management

Natural gas storage facilities are a critical component of our energy supply and distribution chain, allowing elasticity in gas supply to accommodate daily to seasonal demand fluctuations. As evident by the 2015 Aliso Canyon Gas Storage facility incident, a loss of well integrity (SS#25) resulted in significant consequences, including the prolonged shutdown of the entire facility. The high visibility of the event has led to increased scrutiny of the safety of natural gas storage and raised broader concerns about energy reliability for natural gas and hydrogen storage throughout the country. In addition, gas storage operators are facing increased and more complex responsibilities for managing energy storage operations. Low- cost methods that improve the accuracy of cushion and base gas inventory verification are needed to optimally manage stored natural gas. Migration of injected base or cushion natural gas out of the storage reservoir has not been well documented. Hydraulic communication with adjacent formations or migration of gas out of the storage reservoir due to unknown faults, poor reservoir traps or abandoned production wells can lead to unaccounted for volumes of natural gas losses. The SBIR study will address the scope of unaccounted for gas which may have been due to migration. Information on working gas, base/cushion gas, operating capacity, injection, withdrawal volumes, current and non-current revenues, gas losses, storage field demographics and reservoir types is contained among the available data bases -FERC Form 2, EIA Form 191, AGA and FERC Jurisdictional databases. The objective would be to assess and model the leak/migration pathways of subsurface methane in Underground Gas Storage settings. The research would provide additional information for the Administration's support for long term geologic storage of CO2 and hydrogen.

Questions – Contact: Christopher Freitas, christopher.freitas@hq.doe.gov

d. Machine Learning (ML)/Artificial Intelligence (AI) to Create Innovative and Productive Use of Carbon Storage Datasets Available Within EDX

Continued advances in machine learning (ML), artificial intelligence (AI), sensing capabilities, and other innovations are likely to benefit the research community [1]. The carbon storage program has a vast repository of project data and tools gained from over 20+ years of research and development. Several carbon storage tools are actively being used to enable project decisions ranging from assessing storage capacity (CO2-Screen, by DOE-NETL) and optimizing integrated CCS infrastructure decisions (SimCCS, by LANL) to modeling subsurface multiphase fluid flow and transport (STOMP, by PNNL) [2]. Leveraging these tools and data beyond their current applications can be beneficial for private and public use as the full potential of end uses and applications is currently unknown.

Grant applications are sought to catalyze machine learning/artificial intelligence innovations that would use the vast resources of available carbon storage and subsurface data from past and ongoing DOE-funded carbon storage projects. Applicants can reference 927 gigabytes of existing data on Energy Data Exchange (EDX) [3] and are encouraged to think creatively for new applications of these data. The intent is to foster innovation and enable more productive public uses of available carbon storage data and tools which may be underutilized. Repurposing available data could benefit broader subsurface research including storage capacity estimations incorporating spatial constraints such as fault proximity and municipal boundaries, characterization of non-technical risks and restrictions, plume detection, and detection of legacy wells – however these topics are not all inclusive and a wide range of ideas for innovative uses are welcomed.

Questions – Contact: Sarah Leung, sarah.leung@hq.doe.gov

e. Turnkey Service to Enable a Passive Seismic Monitoring Network During Carbon Storage Site Characterization

The carbon storage program is focused on developing site selection processes and tools that can accurately and affordably assess seismicity risk prior to the CO_2 injection phase of a commercial-scale CCS operation (>1 million metric tons per year). At the initial phase of a project, there is a strong need to understand natural seismicity risks prior to any CO_2 injection, preferably prior to making large investments in developing the storage project. Current processes to understand seismicity risks are highly specialized, labor intensive, time constrained, and expensive. The level of naturally occurring seismic noise also creates an apparent threshold and substantial potential error in identifying and detecting the first motion of seismic events. A balance is sought between a fit-for-purpose number and placement of sensors along with the sensitivity, frequency range, and types of sensors for accurate seismic detection of very small seismic events ($M < 0$) to deploy over months to years, while also creating an intelligent level of processing and interpretation that is streamlined and does not create a burdensome task for carbon storage project developers and operators. Because seismicity assessment remains an important factor across the project lifecycle (prior to, during, and after CO_2 injection), an additional consideration should be placed on the robust and rugged nature of the system design with an outlook that the system could be updated or upgraded for use in later phases of the project.

Grant applications are sought for systems that facilitate easier, better, higher-resolution data acquisition and interpretation of seismicity and the risks posed to the carbon storage project, especially during the site characterization phase, for a broad set of stakeholders. To enable this step increase, the goal is to develop a turnkey service that will deliver a passive seismic monitoring network by using seismic or subsurface acoustic sensor data, coupled with a tailored level of processing and right-sized data storage and archiving.

Questions – Contact: Sarah Leung, sarah.leung@hq.doe.gov

f. CO_2 Use to Enhance Biochar for Soils or Agricultural Carbon Products

The use of biochar is considered to be a 2,000 year-old practice that converts agricultural waste into a soil enhancer [1]. Biochar is a fine-grained, highly porous charcoal that helps soils retain nutrients and water [1]. The positive attributes of biochar application are carbon storage, improved food security, increased soil biodiversity, and minimized deforestation [1]. It is maintained that biochar can be an essential tool to increase food security and cropland diversity in areas with severely depleted soils, scarce organic resources, and inadequate water and chemical fertilizer supplies [1]. More nutrients stay in the ground through biochar instead of leaching into groundwater and causing pollution [1]. Furthermore, it is noted that the carbon in biochar resists degradation and can hold carbon in soils for hundreds to thousands of years [1]. Biochar is produced from pyrolysis or gasification thermal conversion processes.

It is widely known the acidic soil is an increasing global problem. In Australia, almost half of the 100 million ha of agricultural soils are acidic with a pH below 5.5 [2]. Suppose the biochar contains a substantial amount of pH-increasing species, such as calcium and magnesium. In that case, it may have enhanced benefits beyond that of carbon, which is resistant to degradation for many years, e.g., neutralizing acidic soils. For example, it is noted that animal bone char is another form of biochar that, under controlled thermal conditions, produces a phosphorus (P) rich product [3]. The bone char produced from animal bones, which is the result of partial calcination or the pyrolysis of meat industry waste, is mainly composed of hydroxyapatite (HAP) [$Ca_{10}(PO_4)_6(OH)_2$] and carbon [3]. It has been reported as a promising adsorbent for fluoride ions in water [3]. Thus, biochar may also have an additional benefit besides carbon. Biochar may be beneficial for neutralizing acidic soils if it can uptake CO_2 from flue gas wastes streams by forming carbonates, e.g., calcium and magnesium. This can be an additional source to neutralize acidic soils besides the widely known benefits of using fly ashes, especially calcium-rich types [4, 5] while reducing CO_2 emissions. Therefore, biochar that has undergone a process to uptake CO_2 and form carbonates may enhance its use for soil applications' performance.

The DOE is currently supporting multiple small- and large-scale R&D projects to demonstrate the technical and economic feasibility of Carbon Capture and Use (CCU). The benefits of biochar and high calcareous fly ashes are already proven for soil improvement applications. Proposals are sought to use CO_2 to enhance biochar. Proposals are sought that investigate technologies that optimize, or preferably maximize, CO_2 adsorption within biochar and/or fly ash. Proposals should then validate improved soil amendment capabilities of the CO_2-enhanced species compared to traditionally produced biochar additives. The proposal should use CO_2 waste streams from power plants, industrial furnaces, or direct air capture (DAC) to provide the carbon dioxide source. The proposal should seek to validate the performance of a carbon product from renewable biomass for agriculture carbon applications (see the following Ref. [6]).

Questions – Contact: Aaron Fuller, aaron.fuller@hq.doe.gov and Amishi Kumar, amishi.kumar@hq.doe.gov

References: Subtopic a:

1. U.S. Department of Energy, 2021, Geothermal Technologies Office, https://energy.gov/eere/geothermal, (July 9, 2021)
2. U.S. Department of Energy, 2021, GeoVision: Harnessing the Heat Beneath our Feet, *Geothermal Technologies Office,* https://www.energy.gov/eere/geothermal/geovision, (July 9, 2021)
3. U.S. Department of Energy, 2021, Subsurface Science, Technology, Engineering, and R&D Crosscut (SubTER), https://www.energy.gov/subsurface-science-technology-engineering-and-rd-crosscut-subter, (July 9, 2021)

References: Subtopic b:

1. Aqwatec, 2021, About Produced Water (Produced Water 101), Aqwatec, http://aqwatec.mines.edu/produced_water/intro/pw/, (July 9, 2021)
2. U.S. Department of Energy, 2020, Produced Water: From a Waste to a Resource, *Office of Fossil Energy and Carbon Management,* https://www.energy.gov/fe/articles/produced-water-waste-resource, (July 9, 2021)

References: Subtopic c:

1. United Energy Development Consultants. Work, 1998, Underground Natural Gas Storage Reservoir Management Phase II, Final Report June 1, 1995 to March 30, 1996, Performed Under Contract No.: DE-AC21-94MC31113, https://digital.library.unt.edu/ark:/67531/metadc705920/m1/1/, (July 9, 2021)

References: Subtopic d:

1. National Petroleum Council, 2019, Meeting the Dual Challenge: A Roadmap to At-Scale Deployment of Carbon Capture, Use, and Storage, Chapter Seven – CO2 Geologic Storage, December 2019, https://dualchallenge.npc.org/files/CCUS-Chap_7-030521.pdf, (July 9, 2021)
2. National Energy Technology Laboratory, 2021, DOE-NETL EDX Carbon Storage Tools. https://edx.netl.doe.gov/dataset/?type=tool&q=carbon+storage, (July 9, 2021)
3. National Energy Technology Laboratory, 2021, DOE-NETL EDX Carbon Storage Open Database. https://edx.netl.doe.gov/group/carbon-storage-open-database, (July 9, 2021)

References: Subtopic e:

1. Ground Water Protection Council and Interstate Oil and Gas Compact Commission, 2021, Potential Induced Seismicity Guide: A Resource of Technical and Regulatory Considerations Associated with Fluid Injection, March 2021, 250 pages, https://www.gwpc.org/sites/gwpc/uploads/documents/publications/FINAL_Induced_Seismicity_2021_Guide_33021.pdf, (July 9, 2021)
2. NRAP, 2021, Passive Seismic Monitoring Tool (PSMT), https://edx.netl.doe.gov/nrap/passive-seismic-monitoring-tool-psmt/, (July 9, 2021)
3. NRAP, 2021, Short-Term Seismic Forecasting Tool (STSF), https://edx.netl.doe.gov/nrap/short-term-seismic-forecasting-stsf/, (July 9, 2021)
4. NRAP, 2021, DRAFT Recommended Practices for Managing Induced Seismicity Risk Associated with Geologic Carbon Storage, https://edx.netl.doe.gov/dataset/draft-rec-practices-for-managing-is-risk-associated-with-geologic-carbon-storage, (July 9, 2021)
5. Los Alamos National Laboratory, 2019, Monitoring for Faults at a Critical State of Stress, 2019 Carbon Capture, Utilization, Storage, and Oil and Gas Technologies Integrated Review Meeting August 26-30, 2019, https://netl.doe.gov/sites/default/files/netl-file/Chen-2019CO2review.pdf, (July 9, 2021)

References: Subtopic f:

1. International Biochar initiative. Biochar. [May 26, 2021]; Available from: https://biochar-international.org/biochar/, (July 9, 2021)
2. Ukwattage N.L., et al, 2013, The use of coal combustion fly ash as a soil amendment in agricultural lands (with comments on its potential to improve food security and sequester carbon), *Fuel 2013;109:400–8,* https://www.sciencedirect.com/science/article/abs/pii/S001623611300104X, (July 9, 2021)

3. Alkurdi S.S.A., et al, 2019, Biochar versus bone char for a sustainable inorganic arsenic mitigation in water: What needs to be done in future research? Environment international 2019;127:52–69, https://www.sciencedirect.com/science/article/pii/S016041201833085X, (July 9, 2021)
4. Ram L.C., et al, 2010, An appraisal of the potential use of fly ash for reclaiming coal mine spoil. Journal of environmental management 2010;91(3):603–17, https://pubmed.ncbi.nlm.nih.gov/19914766/, (July 9, 2021)
5. Jala S, Goyal D., 2004, Fly ash as a soil ameliorant for improving crop production--a review. Bioresource technology 2006;97(9):1136–47, https://pubmed.ncbi.nlm.nih.gov/16551534/, (July 9, 2021)
6. National Carbon Technologies, 2021, Industry-Leading Carbon Production: Agricultural Carbon Products. Bioenergy Carbon Products. [May 26, 2021]; Available from: https://national-carbon.com/bioenergy-carbon/, (July 9, 2021)

22. ADVANCED FOSSIL ENERGY AND CARBON MANAGEMENT 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

The Office of Fossil Energy and Carbon Management (FECM) Research, Development, Demonstration, and Deployment (RDD&D) program conducts research that focuses on early-stage technologies that help to ensure clean and affordable energy for all Americans, facilitate the transition towards a carbon-pollution-free economy, rebuild a U.S critical minerals (CM) supply chain, and retain and create good paying jobs with a free and fair chance to join a union and collectively bargain. FECM's priorities include: Reduce Methane Emissions; Accelerate Carbon-Neutral Hydrogen (H2): Develop Low-Carbon Supply Chains for Industries; Advance Carbon Dioxide Removal Technologies; Invest in Thoughtful Transition Strategies to a net-zero carbon economy in coal and fossil-based power plant communities; Demonstrate and Deploy Point Source Carbon Capture and Storage to meet net-zero emissions goals by 2050; Advance CM, Rare Earth Elements (REE), Coal Waste to Products and Mine Remediation; Increase Efficient Use of Big Data and Artificial Intelligence (AI); Address the Energy Water Nexus.

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/.

For this topic, the National Energy Technology Laboratory is not eligible to act as a subawardee.

Grant applications are sought in the following subtopics:

a. Production of "Blue Hydrogen" using Novel Membrane Technologies
R&D efforts have significantly increased to transition to a reliable, and low-carbon hydrogen economy as part of their global efforts toward combating the climate change. The U.S has a roadmap toward a lower carbon economy by 2035. Delivering 90 percent clean electricity, removing atmospheric CO_2 on a large scale, development of the EV-charging stations and hydrogen transport and storage infrastructure are some of the landmarks that need to be achieved by 2035 to remain consistent with the 1.5℃ of warming proposed by IPCC.[1]

Hydrogen can be used as an energy carrier or as an alternative fuel in the industrial, residential, and transportation sectors. Today, the majority of the hydrogen in the US is produced through steam methane reforming, an energy intensive process with significant carbon footprint. Furthermore, storage and transport of hydrogen from the production sites to the end-use locations are other challenges that contribute significantly to the finished cost of hydrogen delivered. Metallic membranes, due to their modular nature and high permeability and selectivity toward hydrogen may be used to address some of these challenges.[2]

The Office of Fossil Energy and Carbon Management is seeking novel applications that address the production, separation, and purification of hydrogen through coal or biomass gasification using membrane technologies. A successful application should address the fundamental problems associated with hydrogen production using metallic membranes and proposals should tackle challenges such as membrane embrittlement due to hydrogen diffusion[3], pinhole development, and membrane failure due to numerous cooling/heating cycles[4]. In addition, a successful application must have a robust plan for decarbonizing the entire process.

A strong and comprehensive techno-economic analysis (TEA) must be considered in the proposal and the finished cost of delivering blue hydrogen must be compared against the alternative approaches such as conventional steam reforming, water electrolysis, and plasma technologies.

In order for the application to be considered for funding, the PI must consider the use of computational and simulation packages developed by DOE's Simulation Based Engineering (SBE) team, more specifically Institute for the Design of Advanced Energy Systems (IDAES) and/or Multiphase Flow with Interphase eXchanges (MFiX).

Questions – Contact: Kourosh Kian, kourosh.kian@hq.doe.gov

b. Low-Cost High-Performance Regenerative Fuel Cells (RFCs) for Fossil-Integrated Hydrogen Energy Storage

Co-location of energy storage with fossil fuel power plants helps to improve plant flexibility, promote efficient plant operations, and increase plant lifetime. The Advanced Energy Storage Program[1-3] initiated by the DOE's Office of Fossil Energy and Carbon Management (FECM) is focused on advancing a variety of energy storage technologies and integrating them with fossil-fueled assets. This subtopic is specifically focused on hydrogen energy storage systems, so non-hydrogen energy storage technologies will be considered non-responsive. Hydrogen energy storage offers the potential for long-term, seasonal storage of off-peak electricity. RFCs produce hydrogen via electrolysis in charging mode to store excess electrical energy and generate power in fuel cell discharging mode. Unitized RFCs that combine electrolyzer and fuel cell operations in a single stack offer the potential for significantly reduced cost and overall system simplification; therefore, system designs based on unitized RFCs are preferred but not required.

The DOE's FECM solicits proposals focused on developing system designs for integrating RFC based hydrogen storage technologies with large-scale fossil assets in an efficient and cost-competitive way. Phase I applications must provide how the proposed system would reduce overall capital cost, increase durability, and improve performance compared to other competing storage technologies. They should also address any key barriers for integrating RFCs with fossil assets. Phase II effort should include system-level demonstration of the energy storage system with either unitized or discrete RFCs, analysis of cost and performance benefit, and detailed plans for integration with at least one fossil asset class.

Questions – Contact: Mani Gavvalapalli, nagamani.gavvalapalli@hq.doe.gov

c. Decision Support Tools for Decarbonization through Hybrid Systems

Decarbonization of the electricity sector by 2035 will require significant investments in new technologies over the next 20 years. Hybrid energy systems that combine one or more primary energy sources with energy storage technologies and carbon capture offer potential benefits, including greater flexibility and reduced cost under various decarbonization scenarios. Similar flexibility and cost benefits could arise from hybrid systems capable of producing more than one product (e.g., electricity and hydrogen).

The U.S. Department of Energy and National Energy Technology Laboratory (NETL) have created an advanced, open source, integrated computational platform through the Institute for the Design of Advanced Energy Systems (IDAES) [1], [2], which supports multi-scale optimization of new energy technologies and hybrid systems. Recent efforts have included the use of IDAES to enable the optimal design of hybrid systems that are tightly coupled with the electricity grid [3].

Proposals are sought to develop and apply a decision support tool that directly utilizes the capabilities of IDAES. Applicants must specify the target hybrid energy system application under investigation that is relevant to fossil energy and/or carbon management, including (but not limited to) any combination of assets such as fossil-based dispatchable power, carbon capture, carbon storage, energy storage, renewables, etc.

It is hoped that a user-friendly, decision support tool and visualization capability will help enable the widespread use of models and simulations for expansion planning to inform future investments for decarbonization. Initial prototype of the decision support tool should enable rapid quantitative evaluations of several technology options, process configurations, and scales after optimizing their design and interactions with the bulk power system and/or gas pipeline infrastructure while properly valuing characteristics like operational flexibility, reliability, and resiliency. The target end user for the decision support tool includes utilities and regulators, to aid in the evaluation of different decarbonization scenarios and technologies to inform policy and investments.

Questions – Contact: Kylee Underwood, mary.underwood@netl.doe.gov

References: Subtopic a:

1. National Academies of Sciences, Engineering, and Medicine, 2021, Accelerating Decarbonization of the US Energy System. (2021), https://www.nationalacademies.org/our-work/accelerating-decarbonization-in-the-united-states-technology-policy-and-societal-dimensions, (July 9, 2021)
2. Liguori, Simona, et al., 2020, Opportunities and challenges of low-carbon hydrogen via metallic membranes, *Progress in Energy and Combustion Science 80 (2020): 100851,* https://www.sciencedirect.com/science/article/pii/S0360128520300617, (July 9, 2021)
3. Philpott, J. E., 1985, Hydrogen diffusion technology, *Platinum Metals Review 29.1 (1985): 12-16,* https://www.technology.matthey.com/article/29/1/12-16/, (July 9, 2021)
4. Guazzone, F. et al, 2007, Leak growth mechanism in composite Pd membranes prepared by the electroless deposition method, *AIChE journal 54.2 (2008): 487-494,* https://aiche.onlinelibrary.wiley.com/doi/abs/10.1002/aic.11397, (July 9, 2021)

References: Subtopic b:

1. U.S. Department of Energy, 2020, *Energy Storage Grand Challenge (ESGC)* https://www.energy.gov/energy-storage-grand-challenge/energy-storage-grand-challenge, (July 9, 2021)
2. U.S. Department of Energy, 2020, *Energy Storage For Fossil Fuel Energy Systems*, 2020. https://netl.doe.gov/coal/crosscutting/energy-storage, (July 9, 2021)

3. 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, (July 9, 2021)

References: Subtopic c:

1. National Energy Technology Laboratory, 2021, *Institute for the Design of Advanced Energy Systems*. Accessed: May 28, 2021. [Online] Available: https://idaes.org/, (July 9, 2021)
2. Lee, A., Ghouse, J.H., et. al., 2021, The IDAES process modeling framework and model library – Flexibility for process simulation and optimization," J. of Advanced Manufacturing and Processing, (2021). DOI: https://doi.org/10.1002/amp2.10095, (July 9, 2021)
3. U.S. Department of Energy, 2021, *Design Integration and Synthesis Platform to Advance Tightly Coupled Hybrid Energy Systems*. Accessed May 28, 2021. [Online] Available: https://gmlc-dispatches.github.io, (July 9, 2021)

23. RARE EARTH ELEMENTS AND CRITICAL MINERALS

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 offshore markets. When viewed in their entirety, the rare earth element (REE) and critical minerals (CM) supply chains consist of mining, separation, refining, alloying, and ultimately manufacturing devices and components. A major issue with respect to REE development in the U.S. is the lack of refining, alloying, and fabricating capacity that could process any domestically produced REE and/or CM [1].

Efforts conducted under DOE-NETL's Feasibility of Recovering Rare Earth Elements (REE) program between 2014 and 2020, successfully demonstrated the very first step for the utilization of coal and coal-based resources to produce rare earth elements needed for our commodity and defense industries. This achievement was marked by demonstrating the technical feasibility and processing capability to extract and separate REE from domestic coal-based resources (i.e., run-of-mine coal, coal refuse (mineral matter that is removed from coal prior to shipment), clay/sandstone over/under-burden materials, ash (coal combustion residuals), and aqueous effluents such as acid mine drainage (AMD), and associated solids and precipitates resulting from AMD treatment), and recovery of these materials as mixed rare earth oxides or salts (MREO/MRES) at levels of 96-98% purity (960,000-980,000ppm) in three, first-of-a-kind, domestic, small pilot-scale facilities.

Currently, under DOE-NETL's RD&D program, state-of-the-art, conventional extraction/separation/recovery process concepts are being assessed for near-future production of 1-3 tonnes/day of high-purity MREO in engineering-scale prototype facilities. Conversion of the MREO/MRES into individually separated, high purity REO/RES, and subsequently conversion to metals (MREM/MRES) will be essential for alloying and/or incorporation of these materials into intermediate products (i.e., magnets; etc.) or into manufactured end-products (i.e., wind turbines; fuel cells; etc.).

Building on the accomplishments achieved in DOE-NETL's Feasibility of Recovering Rare Earth Elements program, efforts in 2019 were additionally directed to co-production of critical minerals (CM), as cobalt (Co), manganese (Mn), lithium (Li), and potentially aluminum (Al), zinc (Zn), germanium (Ge), and gallium (Ga) from domestic, coal-based, REE-containing feedstock materials. This expansion aligned with DOE-NETL's effort to support Executive Order 13817 [2], which led to changing the name of DOE-NETL's program in 2020 to Critical Minerals Sustainability.

For this topic, the National Energy Technology Laboratory is not eligible to act as a subawardee.

Grant applications are sought in the following subtopics:

a. Advanced Alloy Development

As part of the DOE-NETL rare earths (REE) and critical minerals (CM) program, REE and CM are being produced in small pilot-scale extraction/separation/recovery facilities (100-200 gm/day), and are being planned for near future-term production in larger engineering-scale prototype systems (1-3 tonnes mixed rare earth oxides/salts (MREP/MRES)/day). These dual-use materials, when produced in larger quantities, will be available for use in the manufacture of metals, alloys, superalloys, ceramics, catalysts, batteries, phosphors, and so on, for the commercial and defense industries, and additionally will provide a means for use in the development of "new" and advanced materials.

Applicants will address:

- Annual domestic and international production of metals, alloys, superalloys including first and second-generation single crystals, and intermetallic materials.
- Annual domestic supply requirements (i.e., quantity and purity) of REE and/or CM from off-shore producers to meet the various U.S. metal, alloy, superalloy, and intermetallic supply chain needs.
- Identification of advanced metal, alloy, superalloy, and intermetallic compositions containing REE and/or CM for enhanced performance (i.e., high temperature strength, oxidation resistance, ductility, creep resistance, durability, etc.); Address industrial applications that would benefit from having these advanced materials be made available for use in advanced component and/or equipment development (i.e., advanced alloys containing scandium for aerospace industry, etc.).
- If theoretical modeling is used to establish advanced material compositions, describe methodology and rationale of approach, and provide projected enhanced materials performance results.

Questions – Contact: Heather Hunter, heather.hunter@netl.doe.gov

References:

1. Humphries, M., 2013, *Rare Earth Elements: The Global Supply Chain*, Congressional Research Service Washington, DC., 2013. https://fas.org/sgp/crs/natsec/R41347.pdf, (July 9, 2021)
2. Executive Order 13817, 2017, A Federal Strategy to Ensure Secure and Reliable Supplies of Critical Minerals, December 20, 2017. List of Critical Minerals posted in Federal Register/Vol. 83, No. 97/Friday, May 18, 2018/Notices, https://www.federalregister.gov/documents/2018/05/18/2018-10667/final-list-of-critical-minerals-2018, (July 9, 2021)
3. Brothers, E., 2019, NioCorp produces aluminum-scandium master alloy, with significant potential uses in defense, aerospace, and other applications, *Aerospace Engineering and Design, August 20, 2019,* https://www.intelligent-aerospace.com/commercial/article/14037964/aluminumscandium-alloy-for-military-and-aerospace-applications, (July 9, 2021)
4. Schmidtke, K., et al, 2011, Process and Mechanical Properties: Applicability of a Scandium modified Al-alloy for Laser Additive Manufacturing, *Physics Procedia, Volume 12, Part A, 2011, p. 369-374.* https://www.sciencedirect.com/science/article/pii/S187538921100126X, (July 9, 2021)
5. Perry, A.J., 1977, The Constitution of copper-hardened samarium-cobalt permanent magnets*, Journal of Less Common Metals, Volume 1, Issue 1, January 1977, p. 153-162.* https://www.sciencedirect.com/science/article/abs/pii/0022508877901825, (July 9, 2021)

Return to Table of Contents

6. Giamei, A.F., 2013, *Development of Single Crystal Superalloys: A Brief History,* Advanced Materials and Processes, September 2013, p. 26-30. https://www.asminternational.org/documents/10192/6019788/amp17109p26.pdf/3def4e97-ace9-47e4-8661-2d7bc8f71f84, (July 9, 2021)

24. 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. Split Laser Sensor for Harsh Environment Sensing Applications

This Technology Transfer Opportunity seeks to license and commercialize a split laser measurement technology (U.S. Patent 8,786,840, [1]) developed and patented by U.S. Department of Energy's National Energy Technology Laboratory (NETL). The technology is low-cost, portable, and ready to be deployed in a wide variety of remote, harsh environment sensing applications that are relevant to fossil energy and carbon management, including (but not limited to) [2]: long-term CO2 sequestration monitoring, characterization of rare earth elements, contaminant monitoring and remediation, natural gas reservoir detection, water treatment and filtration systems, etc.

The base technology [3, 4] can support i) laser induced breakdown spectroscopy (LIBS) and/or Raman measurements of solids and liquids, and/or, ii) LIBS measurements of gases with appropriate laser safety accommodations. The technology involves the use of a diode pumped passively Q-switched solid-state laser that is remotely fiber pumped to produce high peak power nanosecond scale output pulses. The use of a passive Q-switch allows for the removal of the high voltage active Q-switch and also allows for the fusing of the remainder of the optical components that comprise the laser head into a monolithic unit which eliminates the need for alignment and any worries of misalignment. Low peak power pumping light is delivered via the optical fiber to the laser medium where a train of high peak power pulses are produced as long as the pumping light is applied. The output can be focused to produce sparks in air, on solid surfaces, or inside liquids.

Applicants must leverage this technology for a fossil-based energy and/or carbon management system.

The split laser system is adaptable with base functionality that may be extended and customized to support a wide variety of end use applications that are relevant to fossil-based energy systems. The ability of the probe to be sealed allows for usage in separations processes and/or other industrial process where critical element concentrations are needed for control and optimization. The probe also has the ability to be deployed into the subsurface to measure concentrations of various elements at rates up to 20 Hertz (in its existing configuration). In addition, the use of the optical fiber allows for versatile deployment capability of the laser into areas that would not normally accommodate a laser system. The technology can easily be attached to a robotic manipulator for interrogation of remote sites or areas of interest. Lastly, the end probe of the measurement system has been specifically designed to be low cost and rugged so that it is easily repaired or replaced if damaged, while keeping the sensitive upstream system components at a safe distance.

Licensing Information:
NETL Technology Transfer Office
Contact: Jessica Lamp (412)-386-7417
License Type: Exclusive or Non-exclusive
Patent Status: U.S. Patent 8,786,840
Publication date: July 22, 2014
Filing date: January 26, 2012

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

References:

1. Woodruff, S.D., McIntyre, D.L., Jain, J.C., 2007, Method and device for remotely monitoring an area using a low leak power optical pump (U.S. Patent No. 8,786,840), *US Patent and Trademark Office,* https://www.epa.gov/sites/production/files/2018-08/documents/gd-52v.2.pdf, (July 9, 2021)
2. National Energy Technology Laboratory, 2012, A Unique Split Laser System for Environmental Monitoring, https://www.netl.doe.gov/node/458, (July 9, 2021)
3. Hartzler, D.A., Jain, J.C., McIntyre, D.L., 2019, Development of a subsurface LIBS sensor for in situ groundwater quality monitoring with applications in CO2 leak sensing in carbon sequestration, *Scientific Reports, (2019) 9:4430, DOI: 10.1038/s41598-019-41025-3* https://www.nature.com/articles/s41598-019-41025-3, (July 9, 2021)
4. Hartzler, D.A., Bhatt, C.R., Jain, J.C., McIntyre, D.L., 2019, Evaluating laser induced breakdown spectroscopy sensor technology for rapid source characterization of rare earth elements, *ASME Journal of Energy Resources Technology, DOI: 10.1115/1.4042747*, https://asmedigitalcollection.asme.org/energyresources/article-abstract/141/7/070704/725825/Evaluating-Laser-Induced-Breakdown-Spectroscopy?redirectedFrom=fulltext, (July 9, 2021)

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, visit https://science.osti.gov/ber/Research.

25. TECHNOLOGIES FOR SOIL AND WATER PHOSPHORUS MEASUREMENTS IN TERRESTRIAL-AQUATIC INTERFACES

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, https://ess.science.energy.gov/) 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 terrestrial-aquatic interfaces, defined as the broad zones where the land margin meets the fresh and/or salt-water environment. For field observations and experiments, TAIs such as coastal or inland wetlands and riparian zones represent a major knowledge gap in understanding and scaling. This is because TAIs 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.

Terrestrial-aquatic interfaces are characterized by steep environmental and process gradients at plot and landscape scales and are subject to wide ranges of forcing and environmental conditions. 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.

Phosphorus (P) abundance, availability, and transport are important aspects of the biogeochemistry and ecosystem ecology of TAIs. As a key nutrient in freshwater and estuarine TAIs as well as adjacent terrestrial ecosystems, the ability to accurately measure the amount and form of P across the TAI at multiple process-relevant scales is critical for understanding hydro-biogeochemical function, nutrient retention, and transport dynamics within the TAI as well as upstream and downstream within integrated watersheds (Reference 3). The input and export of P in TAIs is influenced by variable hydrologic conditions from local to watershed scales, as well as internal cycling within the water, soils, and vegetation that both control and respond to the form and reactivity of P. Phosphorus is found in dissolved, particulate, and soil-bound fractions of both inorganic and organic forms, with P solubility and bioavailability influenced by physical conditions (e.g., pH, redox, etc.) and biological activity of microbial growth and metabolism, plant root uptake and detrital inputs, and animal trophic dynamics.

Quantifying available and bound organic and inorganic P within surface water and soils is crucial for understanding local TAI ecosystem processes as well as mobility and transport to/from adjacent ecosystems to better incorporate TAI dynamics into integrated watershed and regional predictive models However, there are several challenges inherent in obtaining the measurements necessary to do so. These would ideally be In situ continuous measurements that could be sustained over long time periods (e.g. seasonal). Many current technologies are extractive, requiring disturbance and synoptic sampling, and/or dependent upon considerable sample processing and P extraction, which imposes considerable expense and effort on extensive sampling and compromises the ability to fully capture and characterize P dynamics at system-relevant spatial scales. Therefore, the development of new non-destructive technologies for more continuous, in situ measurement that can be hardened against the strong environmental gradients and potential destructive forces of the TAI environment are required to advance the understanding of P biogeochemistry in TAIs.

Grant applications submitted to this topic must emphasize development of technologies that will help address these measurement challenges in TAIs. Applications should (1) demonstrate performance characteristics of the proposed technology, and (2) show a capability for deployment at field scales ranging from experimental plot size (meters to a hectare) to nominal dimensions of TAI ecosystems and watersheds (hectares to kilometers). Phase I projects must perform feasibility and/or field tests of proposed technologies 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 subtopic:

a. Technologies for In situ Measurement of Soil Pore Water and Aquatic Phosphorus in Terrestrial-Aquatic Interfaces

Sensitive, accurate, and in situ characterization and monitoring of soil and surface water phosphorus (P) is needed for terrestrial-aquatic interfaces, e.g., freshwater or saltwater wetlands, stream or riverine riparian zones, and lake or ocean shorelines. Current sensors and approaches lack the feasibility and resolution needed for adequate scalable in situ measurement of P chemistry (e.g., orthophosphate, soluble P, etc.), particularly at low concentrations in both soil and aquatic environments. (Reference 4-9). Sensors and technologies developed under this topic should be rugged, portable, and low concentration sensitive in situ devices capable of continuous or repetitive high-precision measurements. Additionally, these technologies should be cost-effective for field deployment in remote locations that often have little to no power available, may be under heavy vegetation cover with thick organic soil or sediment, and subject to daily-to-seasonal surface water inundation, high humidity, and/or corrosive (saline) water/environments. Applications should consider the following aspects:

Phosphorus chemistry	Sensors or other systems developed under this topic should measure the concentration of soluble reactive phosphate (orthophosphate; 0.25 mg P/L), though the capability to measure additional forms as well is encouraged (e.g., inorganic P (µg P/L), organic P (mg P/L), total P (mg P/L), etc.). Measurements should be robust with sufficient measurement accuracy and precision for high resolution of differences in surface water and soil pore water concentration; sensitivity for detecting rapid changes; and detection limits/calibration ranges suitable for natural system conditions (Note: other applications for environmental hygiene or management such as wastewater, industrial effluent, etc. are secondary in scope to the focus on natural system conditions).
Environmental concerns and deployment considerations	The technology should be minimally invasive, rugged, UV resistant, and resistant to issues with biofilms/biofouling, water turbidity, long-term wet environments, animal impacts, temperature extremes, pH changes, and saline environments. The design should be able to collect measurements at a specific point and a known volume/depth.
Platform design	The technology should be deployable as an array (either multiple units, or multiple sensors per unit) to enable spatial characterization. Platform weight and size should be minimized as appropriate for the technology methodology (e.g., colorimetric assay, vacuum extraction, etc.) and be minimally invasive when installed. The technology should have low-power requirements with a contained power source or linkage to off-grid power sources (i.e., batteries, solar power). Data connection/ retrieval should be done on-board or via remote access such as a data logger or through other mechanisms (e.g., Bluetooth, cellular, etc.).
Sampling frequency	The technology should aim to take measurements at hourly or sub-hourly timescales.
Calibration	The technology should have minimal calibration drift that would enable extended deployments for at least 3 months.

Questions – Contact: Daniel Stover, Daniel.Stover@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: Daniel Stover, Daniel.stover@science.doe.gov or Brian Benscoter, Brian.Benscoter@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 on-board or centralized/remote data storage and download capability for extended unattended operation and data collection. 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. 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. 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 permitted 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, (June 23, 2021)
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, (June 23, 2021)
3. Reddy, K.R. et al, 1999, Phosphorous Retention in Streams and Wetlands: A Review, *Critical Reviews in Environmental Science and Technology,* Volume 29, Issue 1, pp 83-146, DOI: 10.1080/10643389991259182, https://www.tandfonline.com/doi/pdf/10.1080/10643389991259182, (June 23, 2021)
4. DeLaune, R.D., et al, 2013, Methods in Biogeochemistry of Wetlands, *Soil Science Society of America Book Series, Number 10, Soil Science Society of America,* Madison, WI, USA, https://books.google.com/books?hl=en&lr=&id=emDMDwAAQBAJ&oi=fnd&pg=PP12&dq=Methods+in+Biogeochemistry+of+Wetlands&ots=gB_H5hdAxE&sig=-0YMVatCYfxeOSD1TGfTB_OFyQ8 -v=onepage&q=Methods%20in%20Biogeochemistry%20of%20Wetlands&f=false, (June 23, 2021)
5. Griffiths, N.A. and Sebestyen, S.D., 2016, Dynamic Vertical Profiles of Peat Porewater Chemistry in a Northern Peatland, *Wetlands*, Volume 36, pp 1119-1130, https://www.fs.usda.gov/treesearch/pubs/53071, (June 23, 2021)
6. Pellerin, B.A. et al., 2016, Emerging Tools for Continuous Nutrient Monitoring Networks: Sensors Advancing Science and Water Resources Protection, *Journal of the American Water Resources Association*, Volume 52, pp 993-1008, https://onlinelibrary.wiley.com/doi/full/10.1111/1752-1688.12386, (June 23, 2021)
7. U.S. Environmental Protection Agency, 2008, Methods for Evaluating Wetland Condition: #18 Biogeochemical Indicators, *U.S. Environmental Protection Agency*, EPA-822-R-08-022, https://www.epa.gov/sites/production/files/documents/wetlands_18biogeochemical.pdf, (June 28, 2021)
8. Watson, S.J. et al., 2018, Phosphorus Forms in Sediments of River-Dominated Estuary, *Frontiers in Marine Ecology*, Volume 5:302. doi: 10.3389/fmars.2018.00302, https://www.frontiersin.org/articles/10.3389/fmars.2018.00302/full, (June 28, 2021)

9. Dunne, E.J. et al, 2010, Soil Phosphorous Flux from Emergent Marsh Wetlands and Surrounding Grazed Pasture Uplands, *Ecological Engineering*, doi:10.1016/j.ecoleng.2010.06.018, https://www.sciencedirect.com/science/article/abs/pii/S0925857410001722, (June 28, 2021)

26. 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 atmospheric variables and processes that are important to climate including aerosol formation, chemical composition, and optical properties; cloud and precipitation formation, microphysical, and optical properties; details of atmospheric structure and variability including turbulence, temperature, trace gas, wind, vertical velocity, and water vapor profiles that affect aerosol, cloud, and precipitation formation or the Earth's energy balance; boundary layer processes that affect aerosol and cloud formation; and aerosol-cloud-precipitation-radiation interactions and feedbacks. 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 2-7).

This topic is specifically focused on developing technologies for robust and well-characterized robust and well-characterized measurements of atmospheric aerosol, cloud, turbulence, precipitation, temperature, trace gas, vertical velocity or water vapor properties that are relevant to atmospheric process and Earth system understanding. Proposed technologies must be suitable for deployment under realistic operating conditions at long-term ground-based measurement sites such as those operated by the Atmospheric Radiation Measurement (ARM) user facility (www.arm.gov and Reference 6), the Ameriflux program (https://ameriflux.lbl.gov/) , or on airborne research platforms (https://arm.gov/capabilities/observatories/aaf/; Reference 8). Therefore, applications must consider and discuss factors such as the size, weight, and power; data logging; calibration procedures; maintenance requirements; and/or other factors critical to successful operation of the proposed technology in realistic field conditions.

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 will not be considered. Applications that do not focus on measurement of one of the atmospheric variables/processes described above or that do not clearly describe relevance of the proposed measurement technology to the scientific goals of the EESSD division will not be considered. Applications focused primarily on technologies for air quality measurements will not be considered.

a. Automated Adaptive Sampling for Atmospheric Measurements

The atmosphere is highly variable and quantities such as aerosol, water vapor, or clouds that are important for studying climate-relevant atmospheric processes may vary substantially over short spatial scales or with changing meteorological conditions. Additionally, it is of interest to be able to track atmospheric features such as clouds or aerosol plumes as they are advected by the wind over a fixed observational site (References 9, 10). Many atmospheric measurement instruments have multiple modes of operating, with some modes more suitable for different atmospheric conditions. These different operating modes are generally programmed into a set sampling sequence, which may vary based on deployment location, or may be changed manually for different atmospheric conditions. For example, scanning radars may be programmed to perform one sequence of elevation and azimuthal scans in a location that typically experiences low-level stratocumulus clouds and a different sequence of scans in a location with frequent deep convective clouds (Reference 11). A wind lidar may alternate between modes focused on measuring turbulence, vertical profiles of mean wind speed, or wind shear (Reference 12). A cloud condensation nuclei counter scans through a range of supersaturations, with the details of the scans depending on the expected aerosol type at the measurement location (Reference 13).

The atmospheric community has developed some basic automated techniques to switch between instrument operational modes in atmospheric sampling. For example, an adaptive sampling technique has been developed for aerosol sun photometers in which they transition to “cloud mode” when they detect that clouds are completely blocking the sun (Reference 14). Similarly, the radar wind profilers operated by the ARM user facility have been adapted to operate only in precipitation mode when precipitating conditions are identified via real-time monitoring of the moments data (Reference 15). More sophisticated algorithms that use measurements from multiple sensors are beginning to be developed (Reference 16).

With advances in miniaturization of computing hardware (i.e., edge computing) and rapid analysis techniques (e.g., machine learning), it is now possible to develop more sophisticated smart sensors for atmospheric measurements – instruments that can use built-in computing resources to analyze real-time measurements and adapt their operating mode without manual intervention (References 6, 17). There is an opportunity and a need for more integrated instrument development that considers this type of adaptive sampling in the design of the measurement system itself.

This sub-topic seeks grant applications for development of atmospheric measurement systems that can adaptively change operating mode, sampling, or scanning strategy based on measured atmospheric conditions without manual intervention. Examples of applications of interest include, but are not limited to:

- Automatically switching operational parameters of a cloud condensation nuclei counter or other aerosol instrument based on measured aerosol characteristics; for example, scanning at higher supersaturation during nucleation events
- Automatically switching instrument operational parameters such as sampling frequency, resolution, scanning geometry, pulse characteristics, polarization, or averaging time, based on detection of a feature of interest (e.g., cloud, aerosol layer, precipitation, wind shear, turbulence) or the characteristics of the measurement (e.g., cloud height, cloud phase, wind speed, aerosol loading, particle size) or the desired uncertainty of the measurement (e.g., longer averaging times for lower concentrations or weaker features)
- Automatically switching operational mode to protect an instrument from measurements that might contaminate the data of interest or damage sensors; for example, protecting sensitive aerosol or chemical sensors from high local emissions from a ship stack or other point source
- Automatically tracking/following a feature of interest (e.g., cloud, aerosol plume, air mass)

Applications to this sub-topic must:

- Propose a complete measurement system that is suitable for field deployment, including a measurement sensor and the hardware, software, and computational processor needed to control the automated adaptive sampling
- Identify any auxiliary measurements needed for the adaptive sampling criteria and how they will be obtained (i.e., from the proposed instrument system itself or from other existing commercial instruments or readily available data)
- Propose adaptive sampling solutions that operate in real-time or near real-time to modify the operations of the measurement system
- Propose software that allows options for user input or modification of the adaptive sampling criteria (i.e., applicants should not propose completely black box solutions). Identify which data were sampled, which excluded, and how that decision was made to allow the user to tune the algorithm to the situation of interest.
- Focus on measurement of an atmospheric quantity of relevance to EESSD and clearly indicate how adaptive sampling of the proposed quantity is scientifically important and relevant to EESSD's interest in understanding climate-relevant atmospheric processes (References 1, 6, 18, 19).
- Clearly indicate how the proposed technology is an advance over existing commercial instrumentation for the measurement of interest.

Applications may:

- Focus on developing adaptive sampling techniques for an existing measurement system or develop a completely new system. Applications that focus on modifying an existing system from another vendor must either show commitment from the instrument vendor for the proposed solution or that the proposed solution can be easily integrated into an existing measurement system without direct involvement from the vendor (i.e., indicate how a software solution will integrate with the existing instrument software, data logger, etc).
- Propose solutions that consist of networks of sensors.

- Propose solutions that analyze only measurements from the proposed system itself (i.e., stand-alone) or that include auxiliary measurements from other commercial instruments or readily available data sources.
- Develop adaptable or expandable solutions that could integrate with a variety of different instruments. However, such applications must clearly describe the implementation for at least one specific measurement system.

Applications are encouraged to:

- Consider use of open source software.

Applications that propose software solutions alone without a clear description of how the software solution would be integrated into an existing or proposed measurement system or applications that only analyze data in post-processing and do not alter instrument operations in real-time are out of scope for this solicitation. Applications that do not clearly describe a realistic field-deployable measurement system are out of scope for this solicitation.

Questions – Contact: Sally McFarlane, Sally.McFarlane@science.doe.gov or Jeff Stehr, jeff.stehr@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: Sally McFarlane, Sally.McFarlane@science.doe.gov or Jeff Stehr, Jeff.Stehr@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, (June 28, 2021)
2. Stith, J. L., et al., 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, (June 28, 2021)
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, (June 28, 2021)
4. Wood R., Jensen, M. P., Wang, J., Bretherton, C. S., et al., 2016, Planning the Next Decade of Coordinated Research to Better Understand and Simulate Marine Low Clouds, *Bulletin of the American Meteorological Society*, Volume 97 Issue 9, https://journals.ametsoc.org/bams/article/97/9/1699/69544/Planning-the-Next-Decade-of-Coordinated-Research, (June 28,2021)
5. Shrivastava M., Cappa, C. D., Fan, J., Goldstein, A., et al., 2017, Recent Advances in Understanding Secondary Organic Aerosol: Implications for Global Climate Forcing, *Reviews of Geophysics*, Volume 55 Issue 2, https://agupubs.onlinelibrary.wiley.com/doi/full/10.1002/2016RG000540, (June 28, 2021)
6. Mather J., 2021, Atmospheric Radiation Measurement User Facility 2021 Decadal Vision, Ed, *U.S. Department of Energy, DOE/SC-ARM-20-014*, https://www.arm.gov/publications/programdocs/doe-sc-arm-20-014.pdf, (June 28, 2021)

7. National Academies of Sciences, Engineering, and Medicine, 2018, The Future of Atmospheric Boundary Layer Observing, Understanding, and Modeling: Proceedings of a Workshop, *Washington, DC: The National Academies Press*, https://doi.org/10.17226/25138, (June 28, 2021)
8. Schmid, B., Tomlinson, J. M., Hubbe, J. M., Comstock, J.M., et al., 2014, The DOE ARM Aerial Facility, *Bulletin of American Meteorological Society*, Volume 95 Issue 5, p. 723–742, https://doi.org/10.1175/BAMS-D-13-00040.1, (June 28, 2021)
9. Borque, P., Kollias, P., & Giangrande, S., 2014, First Observations of Tracking Clouds Using Scanning ARM Cloud Radars*, Journal of Applied Meteorology and Climatology*, Volume 53 Issue 12, p. 2732-2746, https://journals.ametsoc.org/view/journals/apme/53/12/jamc-d-13-0182.1.xml, (June 28, 2021)
10. Weekley, R. A., Goodrich, R. K., & Cornman, L. B., 2016, Aerosol Plume Detection Algorithm Based on Image Segmentation of Scanning Atmospheric Lidar Data*, Journal of Atmospheric and Oceanic Technology*, Volume 33 Issue 4, p. 697-712, https://journals.ametsoc.org/view/journals/atot/33/4/jtech-d-15-0125_1.xml, (June 28, 2021)
11. Kollias, P., Bharadwaj, N., Clothiaux, E. E., Lamer, K., et al., 2020, The ARM Radar Network: At the Leading Edge of Cloud and Precipitation Observations, *Bulletin of the American Meteorological Society,* Volume 101 Issue 5, p. E588-E607, https://journals.ametsoc.org/view/journals/bams/101/5/bams-d-18-0288.1.xml, (June 28, 2021)
12. Wang, H., Barthelmie, R. J., Clifton, A., & Pryor, S. C., 2015, Wind Measurements from Arc Scans with Doppler Wind Lidar*, Journal of Atmospheric and Oceanic Technology*, Volume 32 Issue 11, p. 2024-2040, https://journals.ametsoc.org/view/journals/atot/32/11/jtech-d-14-00059_1.xml, (June 28, 2021)
13. Uin J., 2016, Cloud Condensation Nuclei Particle Counter Instrument Handbook. Ed. by Robert Stafford, *DOE ARM Climate Research Facility*, DOE/SC-ARM-TR-168, https://armweb0-prod.ornl.gov/capabilities/instruments/ccn, (June 28, 2021)
14. Chiu J.C., Huang, C.H., Marshak, A., Slutsker, I., Giles, D.M., Holben, B.N., Knyazikhin, Y., and Wiscombe, W.J., 2010, Cloud optical depth retrievals from the Aerosol Robotic Network (AERONET) cloud mode observations, *Journal of Geophysical Research – Atmospheres*, Volume 115 Issue D14, D14202, 10.1029/2009jd013121, https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2009jd013121, (June 28, 2021)
15. Muradyan P. and Coulter, R., 2020, Radar Wind Profiler (RWP) and Radio Acoustic Sounding System (RASS) Instrument Handbook. Ed. by Robert Stafford, *U.S. Department of Energy,* DOE/SC-ARM/TR-044, http://www.arm.gov/publications/tech_reports/handbooks/rwp_handbook.pdf, (June 28, 2021)
16. Kollias, P., Luke, E., Oue, M., & Lamer, K., 2020, Agile Adaptive Radar Sampling of Fast-evolving atmospheric phenomena guided by satellite imagery and surface cameras, *Geophysical Research Letters*, Volume 45, e2020GL088440, https://doi.org/10.1029/2020GL088440, (June 28, 2021)
17. Beckman et al, 2020, 5G Enabled Energy Innovation: Advanced Wireless Networks for Science, Workshop Report, *U.S. Department of Energy,* doi:10.2172/1606538, https://science.osti.gov/-/media/ascr/pdf/programdocuments/docs/2020/5G-Science-Workshop-Brochure-2020.pdf?la=en&hash=37F873FAF5CFBF3B08B6E12A12756D87431484DD, (June 28, 2021)
18. U.S. Department of Energy, 2017, Grand Challenges for Biological and Environmental Research: Progress and Future Vision, *DOE/SC-0190*, https://science.osti.gov/-/media/ber/berac/pdf/Reports/BERAC-2017-Grand-Challenges-Report.pdf, (June 28, 2021)
19. U.S. Department of Energy, 2018, Scientific User Research Facilities and Biological and Environmental Research: Review and Recommendations, *A Report from the Biological and Environmental Research Advisory Committee*, https://science.osti.gov/-/media/ber/pdf/community-resources/2018/BERAC_UserFacilities_Report.pdf?la=en&hash=7567B911F08BA759D1CE94AB11C4CAFE5E77C6D8, (June 28, 2021)

27. 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 and imaging capabilities for researchers studying microbial or plant systems, or their components, 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, neutron or infrared beamline-based techniques and cryo-EM/ET 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. Additionally, tools for correlating different imaging and spectroscopic approaches will be considered. This could include detailed evaluation of the same sample with different techniques, or sequential, multi-scalar techniques for macromolecular or multicellular imaging followed by selection of targeted domains for high resolution analysis.

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, 2020, *BER Structural Biology Resources and Imaging Resources*, http://www.BERStructuralbioportal.org, (June 28, 2021)
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*, DOE/SC-0189, https://genomicscience.energy.gov/technologies/Technologies_highres.pdf, (June 28, 2021)
3. U.S. Department of Energy, Office of Biological and Environmental Research, 2021, *Biological Systems Science Division, Strategic Plan*, U.S Department of Energy, https://genomicscience.energy.gov/2021bssdstrategicplan/BSSD_Strategic_Plan_2021.pdf, (June 28, 2021)

28. 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 Bioimaging Science 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, cry electron microscopes, high resolution mass spectrometers), and can be easily deployed in public and private sector to make them accessible to the larger scientific community.

Note: 1) For 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.

2) Real or perceived device developments for medical imaging and/or applications including disease diagnostics or therapies in biological, animal and/or human systems are excluded.

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

b. New Quantum Enabled Bioimaging and Sensing Approaches For Bioenergy

Quantum science concepts pose interesting possibilities for imaging and sensing of biological processes in living biological systems non-destructively in real time. Quantum approaches should propose a comparative advantage over classical optical methods. Processes of interest to BER include but are not limited to measuring enzyme function within cells, tracking metabolic pathways in vivo, monitoring the transport of materials into and out of cells or across cellular membranes and, measuring signaling processes between cells and within plant-microbe and microbe-microbe interactions.

Current technical limitations and challenges associated with optical imaging and microscopy include: 1) depth imaging - light scattering and diffraction in biological tissue, a major barrier to imaging biological processes deep within tissue (plants or rhizosphere) - restricts optical microscopy to superficial layers, leaving many important biological questions unanswered; 2) photo-damage - classical high flux multiphoton optical imaging causes photo-damage to cellular viability and perturbation to molecular biology for in situ imaging of biological processes in living systems, rendering the sample useless for repeat imaging and measurement of dynamic processes to be performed within the same biological system over different time intervals; and 3) suboptimal stability, brightness and photo-bleaching of the fluorophore when used in combination with an optical imaging approach.

Under this subtopic, applications are sought to explore new quantum science-enabled imaging detectors and sensors envisioned to overcome the current challenges of in-depth imaging including associated scattering and diffraction problems, and suboptimal stability and photo-bleaching issues to enable prolonged imaging studies. Quantum science concepts such as quantum entanglement, where the quantum states of paired photons are linked but the number of photons and therefore overall intensity within the sample is low, have opened new opportunities for imaging of biological systems of interest to BER. Entangled photon absorption follows linear rather than the classical intensity dependence and can be observed at much lower photon fluxes, suggesting a potential for development of new imaging approaches. Quantum entanglement imaging could also be combined with quantum science-based probes for sensing and measurement. These probes can be tailor-made to have high multiphoton cross-sections, multiple chemical functionalities for protein binding and molecular tracking properties, spectrally tunable emission, and quantized absorption/emission states to enable high absorption of multiple entangled photons. Thus, quantum entangled pairs of single photon-emitting probes can potentially enable sub-diffraction limited functional imaging in situ. Such systems may offer substantial improvement in signal detection and spatial and spectral selectivity by utilizing non-classical properties of light under low excitation power without causing significant photo-damage to cell composition or perturbing the natural biological processes within the cell.

This subtopic for proposals seeks fundamental research towards development of new quantum science-enabled probes and sensors applicable for imaging of plant and microbial systems relevant to bioenergy and environmental research conducted within BER programs. These quantum approaches and imaging systems would need to visualize dynamic cellular processes, in real time, in a nondestructive manner, and at sufficient resolution to enable the validation of hypotheses of cellular function occurring in depth. Some research areas of major emphasis within BER include understanding plant metabolism impacting cell wall composition/decomposition, deconstruction of plant polymers (lignin, cellulose, hemicellulose) to monomers, engineered microbial pathways for conversion of plant biomass-derived substrates to fuels and chemicals, and signaling and interactions within environmental microbiomes.

This subtopic for Proposals encourages the development of new quantum-based imaging approaches and demonstration of their utility for imaging biological systems of relevance to bioenergy and environmental research. Potential proposals should address one or more of the topics according to examples outlined below, for prototype development:

- New quantum entanglement-based approaches for probes and sensors, to allow the observation and characterization of multiple complex biological processes occurring in depth within living plant and microbial systems nondestructively in real-time.
- New quantum entanglement enabled imaging devices with desirable photon intensities and wavelengths to overcome the problems of diffraction and scattering to allow the detection of image signals occurring in depth in a 3D volumetric composition within living plant and microbial systems.

EXCLUSIONS/RESTRICTIONS:

- Real or perceived developments for medical imaging and/or applications including disease diagnostics or therapies in biological, animal and/or human systems are excluded.
- Standalone development of quantum dots for routine or innovative biological imaging experiments is excluded.
- The use of commercially available quantum dots (QDs), probes, or sensors as standards for data calibration and to study instrument performance for optical imaging experiments as a part of research proposal, are excluded from consideration.

Questions – Contact: Paul Sammak, Paul.Sammak@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 for Subtopic a - Contact: Prem Srivastava, Prem.Srivastava@science.doe.gov
Questions for Subtopic b - Contact: Paul Sammak, Paul.Sammak@science.doe.gov

References: Subtopic a:

1. U. S. Department of Energy, 2020, Bioimaging Science Program, Principal Investigator Meeting Proceedings, *Office of Science*, https://science.osti.gov/-/media/ber/pdf/community-resources/2021/Bioimaging_Science_PI_Meeting2021.pdf, (June 28, 2021)
2. U. S. Department of Energy, 2020, Bioimaging Research to Develop Imaging Instrumentation and Approaches, *Office of Science, Biological and Environmental Research*, https://science.osti.gov/-/media/grants/pdf/foas/2021/SC_FOA_0002393.pdf, (June 28, 2021)

References: Subtopic b:

1. Lim, X., 2016, The Nanolight Revolution is Coming, *Nature*, Volume 531, p. 26-28, http://www.nature.com/news/the-nanolight-revolution-is-coming-1.19482, (June 28, 2021)
2. Downie, H., Holden, N., Otten, W., et al, 2012, Transparent Soil for Imaging the Rhizosphere, *PLoS ONE,* Volume *7* Issue 9, https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0044276, (June 28, 2021)

Return to Table of Contents

29. 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, (June 28, 2021)
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, (June 28, 2021)
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, (June 28, 2021)
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, (June 28, 2021)
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, (June 28, 2021)
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, (June 28, 2021)

30. 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 and/or microbial communities to increase biomass in large-scale bioenergy crop production. Projects should focus on direct manipulation of microbes or microbial communities that result in increases in biomass in terrestrial bioenergy crops (i.e., perennial grasses, sorghum, non-food oil crops, or trees) under non-stress and/or abiotic stress growth conditions, preferably in a natural setting. These microbes and/or microbial communities may be natural and/or synthetic. 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.

Note: Microbial communities are defined as a multispecies communities consisting of interacting microorganisms, including bacteria, viruses, fungi, etc. While macro-eukaryotes (insects, worms, etc.) are important members of the overall soil ecosystem, they should not be the focus of 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, *U.S. Department of Energy,* DOE/SC-0201, https://www.genomicscience.energy.gov/centers/BRC_Booklet_2020LR.pdf, (June 28, 2021)
2. U.S. Department of Energy, 2015, Lignocellulosic Biomass for Biofuels and Bioproducts: Workshop Report, *U.S. Department of Energy*, DOE/SC-0170, https://www.genomicscience.energy.gov/biofuels/lignocellulose/BioenergyReport-February-20-2015LR.pdf, (June 28, 2021)
3. U.S. Department of Energy, 2015, Basic Research Opportunities in Genomics Science to Advance the Production of Biofuels and Bioproducts from Plant Biomass*, U.S. Department of Energy,* DOE/SC-0177, https://www.genomicscience.energy.gov/biofuels/BER-Bioenergy-WhitePaper-Final.pdf, (June 28, 2021)
4. U.S. Department of Energy, 2018, Bioenergy Research Centers 10-Year Retrospective: Breakthroughs and Impacts 2007-2017 Report, *U.S. Department of Energy,* DOE/SC-0193, September 2018. https://www.genomicscience.energy.gov/centers/brcretrospective.pdf, (June 28, 2021)

References: Subtopic b:

1. U. S. Department of Energy, 2018, Systems Biology of Bioenergy-Relevant Microbes to Enable Production of Next-Generation of Biofuels and Bioproducts, *Office of Science, Biological and Environmental Research,* https://science.osti.gov/-/media/grants/pdf/foas/2018/SC_FOA_0001865.pdf, (June 28, 2021)
2. U.S. Department of Energy, 2015, Lignocellulosic Biomass for Biofuels and Bioproducts: Workshop Report, *U.S. Department of Energy,* DOE/SC-0170. https://www.genomicscience.energy.gov/biofuels/lignocellulose/BioenergyReport-February-20-2015LR.pdf, (June 28, 2021)
3. U.S. Department of Energy, 2011, Biosystems Design Report from the July 2011 Workshop, *U.S. Department of Energy,* DOE/SC-0141, https://www.genomicscience.energy.gov/biosystemsdesign/report/biosystemsdesignreport2012.pdf, (June 28, 2021)

References: Subtopic c:

1. U.S. Department of Energy, 2021, Biological Systems Science Division Strategic Plan: April 2021, *U.S. Department of Energy*, https://science.osti.gov/-/media/ber/pdf/bssd/BSSD_Strategic_Plan_2021_HR.pdf?la=en&hash=FA2B1022AEA759C046E751AED82C3347C0CF144D, (June 28, 2021)
2. U.S. Department of Energy, 2020, Bioenergy Research Centers: 2020 Program Updates, *U.S. Department of Energy,* https://genomicscience.energy.gov/centers/BRC_Booklet_2020HR.pdf, (June 28, 2021)
3. U. S. Department of Energy, 2020, Systems Biology Research to Advance Sustainable Bioenergy Crop Development, *Office of Science, Biological and Environmental Research,* https://science.osti.gov/-/media/grants/pdf/foas/2020/SC_FOA_0002214.pdf, (June 28, 2021)
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, (June 28, 2021)
5. U. S. Department of Energy, 2017, Biosystems Design to Enable Next-Generation of Biofuels and Bioproducts, *Office of Science, Biological and Environmental Research,* https://science.osti.gov/-/media/grants/pdf/foas/2017/SC_FOA_0001650.pdf, (June 28, 2021)

Return to Table of Contents

31. BIOLOGICAL APPROACHES AND TECHNOLOGIES FOR SYNTHETIC POLYMER UPCYCLING

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

Globally, more than 350 million metric tons of plastics or petroleum-based synthetic polymers are produced annually, and their production is anticipated to quadruple by 2050. Approximately 2% of total energy consumption in the United States is used to manufacture plastics, resins, and synthetic rubber. While plastic production consumes nearly 6% of global oil production, plastic consumables are largely only used once and then discarded into landfills and the environment. This suggests that a significant opportunity exists to recover both energy and carbon from plastic waste. DOE therefore seeks to support development of new methods to improve petroleum-based synthetic polymer recycling and upcycling technologies.

a. Biological Approaches and Technologies for Synthetic Polymer Upcycling

This topic addresses the need to develop biological solutions for petroleum-based synthetic polymer upcycling that may offer unique advantages over traditional recycling methods. Though petroleum-based synthetic polymers are typically considered to be highly recalcitrant to biological depolymerization, there is evidence that some plastics can be enzymatically deconstructed. Therefore, enzymatic pathways may exist or may be modified to breakdown polymers that currently cannot be recycled. With this topic, BER seeks projects that apply the principles of genome engineering and microbiome science to re-design metabolic pathways in established or emerging model organisms and/or within complex communities to deconstruct petroleum-based synthetic polymers and/or to convert polymer waste streams to usable monomers for new materials that have desirable performance and end-of-life characteristics. Projects should include identifying and developing novel biological mechanisms, enzymes, and pathways for petroleum-based synthetic polymer deconstruction and conversion focused on elucidating novel enzymes and biochemical pathways for petroleum-based synthetic polymer breakdown and/or designing new biosynthetic pathways for the conversion of polymers into new products or their precursors.

Applications on the environmental dimension of plastics pollution and/or degradation are not within scope. Primarily descriptive studies that aim only to survey strains, environments, enrichments, or consortia via metagenomic or transcriptomic sequencing are not encouraged. Studies that target human or environmental health aspects of polymers or their breakdown products are not within scope. Applications for research that would result in incremental advances in our current understanding or technology are not encouraged. Experimental studies should be focused on the biological conversion of polymers and synthetic biology. Studies that do not target petroleum-based synthetic polymers as substrates or are solely focused on just the chemical analogs or monomers for petroleum-based synthetic polymer breakdown products are not encouraged.

Questions – Contact: Dawn M. Adin (dawn.adin@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: Dawn M. Adin (dawn.adin@science.doe.gov)

References:

1. Ellen MacArthur Foundation, 2017, The New Plastics Economy: Rethinking the Future of Plastics & Catalysing Action, *Ellen MacArthur Foundation*, https://www.ellenmacarthurfoundation.org/assets/downloads/publications/NPEC-Hybrid_English_22-11-17_Digital.pdf, (June 30, 2021)
2. National Academy of Sciences, Engineering, and Medicine, 2020, Closing the Loop on the Plastics Dilemma: Proceedings of a Workshop–in Brief, *The National Academies Press*, https://doi.org/10.17226/25647
3. U.S. Department of Energy Office of Energy Efficiency and Renewable Energy (EERE), 2020, Plastics for a Circular Economy Workshop: Summary Report, *DOE/EE-2074*, https://www.energy.gov/eere/bioenergy/downloads/plastics-circular-economy-workshop-summary-report
4. REMADE Institute, 2019, REMADE Institute Technology Roadmap 2019, *REMADE Institute,* https://remadeinstitute.org/technology-roadmap
5. U.S. Department of Energy, 2019, Roundtable on Chemical Upcycling of Polymers, *U.S. Department of Energy,* https://science.osti.gov/-/media/bes/pdf/reports/2020/Chemical_Upcycling_Polymers.pdf
6. U.S. Department of Energy, 2019, Genome Engineering for Materials Synthesis: Workshop Report, U.S. Department of Energy, *DOE/SC-0198*, https://genomicscience.energy.gov/biosystemsdesign/gems/index.shtml
7. U.S. Department of Energy, 2019, Breaking the Bottleneck of Genomes: Understanding Gene Function Across Taxa Workshop Report, *DOE/SC-0199, U.S. Department of Energy Office of Science,* https://genomicscience.energy.gov/genefunction/
8. U.S. Department of Energy, 2021, Plastics Innovation Challenge Draft Roadmap, *U.S. Department of Energy*, https://www.energy.gov/sites/default/files/2021/01/f82/Plastics%20Innovation%20Challenge%20Draft%20Roadmap.pdf.
9. U.S. Energy Information Administration, 2017, 2014 Manufacturing Energy Consumption Survey, *U.S. Energy Information Administration*, https://www.eia.gov/consumption/manufacturing/data/2014/
10. U.S. Department of Energy, 2021, Systems Biology of Bioenergy-Relevant Microbes to Enable Production of Next-Generation of Biofuels and Bioproducts, *Office of Science, Biological and Environmental Research,* https://science.osti.gov/-/media/grants/pdf/foas/2021/SC_FOA_0002448.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. By producing and studying highly unstable nuclei that are now formed only in supernovae and neutron star mergers in sufficient numbers, scientists could better understand stellar evolution and the origin of the elements. 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.

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.

Return to Table of Contents

32. 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. The electron ion collider (EIC), undergoing design and 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 these facilities, 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 and/or the Office of Advanced Scientific Computing Research 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 or Advanced Scientific Computing Research).

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's 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.

Proposals are sought for:

- 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;
- (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);
- 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.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate for Software and Data Management: Gulshan Rai, Gulshan.Rai@science.doe.gov

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. Concurrently, 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. Such tools include the application of specific AI algorithms and techniques for the preparation and staging of large training sets. Sources of such data are described in Topic xx (Nuclear Instrumentation, Detection Systems and Techniques).
Proposals are sought to develop:

- ML and AI technologies 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.

Applicants are strongly encouraged to consult the references and open literature to best understand the tools already in use by the community. 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.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate for Software and Data Management: Gulshan Rai, Gulshan.Rai@science.doe.gov

c. Heterogeneous Concurrent Computing

Computationally demanding theory calculations as well as detector simulations and data analysis tasks are significantly accelerated through the use of general purpose Graphics Processing Units (GPUs). The use of FPGA based computing is also being explored by the community. The ability to exploit this hardware for concurrent computing has been significantly constrained by the effort required to port the software to these computing environments.

Proposals are sought to develop:

- Cross compilation or source-to-source translation tools 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 even though 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 nuclear physics. 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.

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.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate for Software and Data Management: Gulshan Rai, Gulshan.Rai@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 general description at the beginning of this topic.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate for Software and Data Management Gulshan Rai, Gulshan.Rai@science.doe.gov

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. USQCD: US Lattice Quantum Chromodynamics, *National Computational Infrastructure for Lattice Quantum Chromodynamics*, www.usqcd.org/
4. U.S. Department of Energy, 2009, SciDAC Scientific Discovery Through Advanced Computing SciDAC, *The Secret Life of Quarks*, https://www.osti.gov/servlets/purl/1062585
5. The Globus Alliance, Homepage, *University of Chicago and Argonne National Laboratory*, https://www.globus.org/
6. HTCondor: High Throughput Computing, *University of Wisconsin*, www.cs.wisc.edu/condor/
7. CERN VM Software Appliance, https://cernvm.cern.ch/appliance/
8. Open Science Grid (OSG), The Virtual Data Toolkit (VDT), *VDT Software Distribution*, http://vdt.cs.wisc.edu/index.html/
9. CERN, 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), 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. Event-Driven Architectures (EDA), *Wikipedia*, http://en.wikipedia.org/wiki/Event_driven_architecture
13. IEEE 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. Welcome to the XRootD Webpage, *XRootD*, http://xrootd.slac.stanford.edu/
15. Bellenot, B., Brum, R., Ganis, J., et al., CERN, PROOF (Parallel ROOT Facilities), *ROOT Data Analysis Framework*, https://indico.cern.ch/event/408139/contributions/979707/attachments/815576/1117520/CHEP06-098-ganis-paper.pdf
16. 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, 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., Streaming readout V, *Brookhaven National Laboratory,* https://www.bnl.gov/srv2019/
21. Armando Di Bello, F., et al., 2020, Towards a Computer Vision Particle Flow, *arXivLabs,* https://arxiv.org/abs/2003.08863
22. Cisbani, E., et al., 2019, AI-optimized detector design for the future Electron-Ion Collider: the dual-radiator RICH case, *arXivLabs,* https://arxiv.org/abs/1911.05797
23. 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, *arXivLabs,* https://arxiv.org/abs/2002.01427
24. Albertsson, K., et al., 2018, Machine Learning in High Energy Physics Community White Paper, *arXivLabs,* https://arxiv.org/abs/1807.02876
25. Bedaque, P., Boehnlein, A., Cromaz, M., et al., Report from the A.I. For Nuclear Physics Workshop, 2020, *arXivLabs,* https://arxiv.org/abs/2006.05422

33. 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 detectors described in Topic xx (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, from photons or neutral or charged particles, or extreme cryogenic temperatures.

All grant applications must explicitly show relevance to the 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 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 NP will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from the NP 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 NP Facilities and the wider NP community's 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, and minimal, or at least repeatable differential 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.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate(s) for Electronics and Circuits: Manouchehr Farkhondeh, Manouchehr.Farkhondeh@science.doe.gov

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. The proposed hardware must clearly advance in the state-of-the-art;
2) Two-dimensional high-channel-count circuits for small pixels combined with high-density, high-yield, and low-capacitance interconnection techniques. Layering these 2D ASICS via interconnects to increase functionality is also of interest;
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); and
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.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate(s) for Electronics and Circuits: Manouchehr Farkhondeh, Manouchehr.Farkhondeh@science.doe.gov

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 less than 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.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate(s) for Electronics and Circuits: Manouchehr Farkhondeh, Manouchehr.Farkhondeh@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 general description at the beginning of this topic.

Questions – Contact: Michelle Shinn, Michelle.Shinn@science.doe.gov or the NP SBIR/STTR Topic Associate(s) for Electronics and Circuits: Manouchehr Farkhondeh, Manouchehr.Farkhondeh@science.doe.gov

References:

1. sPHENIX, 2014, An Upgrade Proposal from the PHENIX Collaboration, p.243, http://www.phenix.bnl.gov/phenix/WWW/publish/documents/sPHENIX_proposal_19112014.pdf
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, http://inspirehep.net/record/1280344?ln=en#
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. 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, https://ieeexplore.ieee.org/document/1134244
12. IEEE, 2014, Complete Technical Program, IEEE Nuclear Science Symposium and Medical Imaging Conference, Seattle, WA, November 8-15, https://ieeexplore.ieee.org/xpl/mostRecentIssue.jsp?punumber=7422433
13. Polushkin, V., Wiley, J., 2004, Nuclear Electronics: Superconducting Detectors and Processing Techniques, 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. Physics with Integrated CMOS Sensors and Electron Machines (PICSEL), Institut Pluridisciplinaire Hubert Curien (IPHC), http://www.iphc.cnrs.fr/-PICSEL-.html
17. Omega Micro, Polytechnique, http://omega.in2p3.fr/
18. Large-Area Picosecond Photo-Detectors Project, PSEC, psec.uchicago.edu
19. 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://indico.cern.ch/event/124063/contributions/93075/attachments/73558/105465/LHCC_review_2011.pdf
22. Report from the A.I. For Nuclear Physics Workshop, 2020, arXivLabs, https://arxiv.org/abs/2006.05422
23. Purschke, M.L., et al., Streaming readout V, Brookhaven National Laboratory, https://www.bnl.gov/srv2019/
24. Lee, Y., Macchiavelli, A.O., Effects of magnetic fields on HPGe tracking detectors, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Vol 992, 2021, https://doi.org/10.1016/j.nima.2021.165017
25. Capra, S., Mengoni, D., Dueñas, J.A., et al., Performance of the new integrated front-end electronics of the TRACE array commissioned with an early silicon detector prototype, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, Vol 935 2019, Pages 178-184, https://doi.org/10.1016/j.nima.2019.05.039
26. Varner, G., Cao, J., Wilcox, M., Gorham, P., Large Analog Bandwidth Recorder and Digitizer with Ordered Readout (LABRADOR) ASIC, https://www.phys.hawaii.edu/~idlab/publications/LABRADOR.pdf .

34. 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 NP will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from NP 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 (HPC) 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 HPC 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, particulate-free bellows and gate valves and associated low-loss cryogenic beam line flange connections. Design for a common flange size, e.g., 2.75", with scalability to larger sizes;
2) techniques for removal of 1 µm and larger particulates in diameter from superconducting cavities to 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 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 Q_0 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) development of wide tuning (with respect to the center frequency of up to 10^{-4}) SRF cavities for acceleration and/or storage of relativistic heavy ions; and
3) devices and methods for accurate in-situ measurement of SRF cavity Q_o's at very high values, where an individual cavity's dynamic losses may be small compared to the static background;

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 nuclear physics 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 0.1□ 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 electron-cyclotron resonance (ECR) ion source injection region;
3) passivation techniques or other treatments to ECR components to reduce contamination from the alloys used in the source;
4) novel quench protection systems for Nb3Sn and high-temperature superconducting (HTS) 4th and 5th Generation ECR ion source combined function magnets (sextupole and solenoids); and
5) efficient continuous wave (cw) positron beam sources (polarized and unpolarized) motivated by the nuclear physics 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.

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

d. Polarized Beam Sources and Polarimeters

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

1) Associated components sought for significantly improving performance of high current CW polarized electron sources for delivering beams of ~1-10 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) absolute polarimeters for spin polarized 3He beams with energies up to 160 GeV/nucleon;
3) polarimeter concepts for bunch by bunch hadron polarimetry with a bunch spacing as short as 2 ns;
4) advanced electron or positron beam polarimeters such as those that operate in the energy range of 1-100 MeV, with average currents exceeding 100 uA, or with accuracies that are <1%; and
5) UHV ceramic insulators and cables suitable for a DC high voltage photo-gun operating 500 kV .

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.

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

e. Rare Isotope Beam Production Technology

Grant applications are sought to develop:

1) Radiation resistant stepper motor with radiation tolerance to 10^4 Gy (10^6 rad);
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;
3) Development of radiation hard tracking detector system for phase space diagnostics of ions. If possible, it should avoid the need for gases, as well as other utilities. Ideal conditions as follows: particle rates up to ~10^4 Hz, 30 cm by 20 cm detection region; ~1mm position resolution for ions with Z>10 [21];
4) A variable energy degrader system that allows adjusting the angle of a wedge-shaped degrader for rare isotope beams. The design should generate overall (center) thicknesses of 1 mm or less of aluminum. Similar systems with thicker wedges are described in [22,23];
5) Development of additive manufacturing technologies (3D printing) for construction of superconducting coils for Walstrom type [24] large aperture multipoles for fast rare isotope beam spectrometers; and
6) Development of alternative manufacture technologies (for example, hydroforming) for high power (up to 300 kW) beam dump for ~ 200 MeV/u heavy ion beam

(Additional needs for high-radiation applications can be found in subtopic e "Technology for High Radiation Environments" of Topic 35, 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.

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

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; and
3) devices/systems that measure the emittance of intense (>100 kW) CW ion beams

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.

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

g. Magnet Development for NP Facilities

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. In general, NP's other high beam power facilities have similar needs. 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; and more efficient, lower cost power supplies for such 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.

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

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, Argonne Tandem Linac Accelerator System (ATLAS), *Office of Science,* https://science.osti.gov/np/facilities/user-facilities/atlas/
3. U.S. Department of Energy, Labs at-a-Glance: Thomas Jefferson National Accelerator Facility, Future Science at Thomas Jefferson National Accelerator Laboratory, *Office of Science*, http://science.osti.gov/laboratories/thomas-jefferson-national-accelerator-facility/
4. U.S. Department of Energy, Relativistic Heavy Ion Collider (RHIC), *Office of Science*, https://science.osti.gov/np/facilities/user-facilities/rhic/
5. 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. 7th SRF Materials Workshop, 2012, *Thomas Jefferson National Accelerator Laboratory*, 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. Tesla, 2014, *TESLA Technology Collaboration Meeting*, KEK, Dec 2-5, 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. 17th International Conference on RF Superconductivity, SRF2015 Whistler, 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. Physics with Positron Beams at Jefferson Lab 12 GeV, 2019, *arXivLabs*, 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. Report from the A.I. For Nuclear Physics Workshop 2020, *arXivLabs*, 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. An Electron-Ion Collider Study, 2019, *Brookhaven National Laboratory*, https://wiki.bnl.gov/eic/upload/EIC.Design.Study.pdf
21. H. Kumagai, et al., 2013, Development of Parallel Plate Avalanche Counter (PPAC) for BigRIPS fragment separator, *Nucl. Instrum. Meth. B* p.717, https://www.sciencedirect.com/science/article/abs/pii/S0168583X13009932?via%3Dihub
22. Hwang, J., et al., Angle-tunable wedge degrader for an energy-degrading RI beamline, *PTEP*, Volume 2019, Issue 4, https://doi.org/10.1093/ptep/ptz028
23. Folger, H., et al., 1991, Targets and degraders for relativistic heavy ions at GSI, *NIM-A*, Volume 303, Issue 1, https://doi.org/10.1016/0168-9002(91)90759-J
24. Walstrom, P.L., 2004, Soft-edged magnet models for higher-order beam-optics map codes, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, Volume 519, Issues 1–2,p. 216–221, https://www.sciencedirect.com/science/article/pii/S0168900203030237?via%3Dihub

35. 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 Facility for Rare Isotope Beams (FRIB) nearing completion at Michigan State University, the Relativistic Heavy Ion Collider (RHIC), the Argonne Tandem Linac Accelerator System (ATLAS) at Argonne National Laboratory, and the future Electron-Ion Collider (EIC) at Brookhaven National Lab. 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 in 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 NP will be considered nonresponsive to this topic. Applicants are strongly encouraged to review recent SBIR/STTR awards from NP 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 NP Facilities and the wider nuclear physics community's 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 (HPC) 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 HPC 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:

- Large area Multigap Resistive Plate Chamber (MRPC) detectors with very high rate capability (≥200 kHz/cm^2) radiation (10 Mrad with 10^{15} n/cm^2),magnetic field tolerance (2-3 T), and high timing resolution< 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 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;
- 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/cm^2);
- 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 1H to 235U), 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; 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.

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

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.

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

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:

- Nonhygroscopic scintillator 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 nonhygroscopic scintillators with timing resolution better than 10 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.

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

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 be used in common radiation transport codes like GEANT4, 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.

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

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. Facility for Rare Isotope Beams (FRIB), *Michigan State University*, 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. Ahmed, M.W., et al, "A new cryogenic apparatus to search for the neutron electric dipole moment", *JINST* 14 P11017 (2019), https://doi.org/10.1088/1748-0221/14/11/P11017
4. Adare, A., Daugherity, M.S., Gainey, K., Isenhower, D., et.al., 2012, *sPHENIX: An Upgrade Proposal from the PHENIX Collaboration*, p. 200, http://www.phenix.bnl.gov/phenix/WWW/publish/dave/PHENIX/sPHENIX_MIE_09272013.pdf
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, http://inspirehep.net/record/1280344?ln=en#
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, Frontier Detectors for Frontier Physics: Proceedings of the 8th Pisa Meeting on Advanced Detectors, *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 Collaboration). 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. Rau, W., and Heusser, G., "^{222}Rn emanation measurements at extremely low activities", *Applied Radiation and Isotopes 53* (2000) 371-375, https://www.mpi-hd.mpg.de/biblio/preprints/2000:039.pdf

11. Heusser, G., "Low-Radioactivity Background Techniques", *Annu. Rev. Nucl. Part. Sci*. 1995.45:543-590, https://www.annualreviews.org/doi/pdf/10.1146/annurev.ns.45.120195.002551
12. Public database of material radio-purity measurements, https://www.radiopurity.org
13. sPHENIX, 2014, *An Upgrade Proposal from the PHENIX Collaboration*, p.243, http://www.phenix.bnl.gov/phenix/WWW/publish/documents/sPHENIX_proposal_19112014.pdf
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. 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
17. 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
18. Niinikoski, T.O., Abreu, M., Anbinderis, P., Anbinderis, T., et al., 2004, Section A--Accelerators, Spectrometers, Detectors and Associated Equipment, *Low-temperature Tracking Detectors, Nuclear Instruments and Methods in Physics Research*, Vol. 520, Issues 1-3, p. 87-92, https://www.sciencedirect.com/science/article/pii/S0168900203031310
19. Scintillator Properties Database, *Lawrence Berkeley National Laboratory*, http://scintillator.lbl.gov/
20. 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
21. 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
22. X Theoretical Design (XTD) Division, *Los Alamos National Laboratory*, MCNPX, http://mcnpx.lanl.gov/
23. CERN, INFN, 2010, *FLUKA*, Fluktuierende Kaskade, http://www.fluka.org/fluka.php
24. 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
25. 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
26. 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
27. 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
28. Armando Di Bello, F, et al., 2020 Towards a Computer Vision Particle Flow, *arXivLabs,* https://arxiv.org/abs/2003.08863
29. Cisbani, E., et al., (2019) AI-optimized detector design for the future Electron-Ion Collider: the dual-radiator RICH case, *arXivLabs,* https://arxiv.org/abs/1911.05797
30. 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, *arXivLabs,* https://arxiv.org/abs/2002.01427

31. Albertsson, K., et al., (2018) Machine Learning in High Energy Physics Community White Paper, *arXivLabs,* https://arxiv.org/abs/1807.02876
32. Report from the A.I. For Nuclear Physics Workshop (2020), *arXivLabs,* https://arxiv.org/abs/2006.0542
33. Aschenauer, E., et. al., *Electron-Ion Collider Detector Requirements and R&D Handbook*, http://eicug.org/web/sites/default/files/EIC_HANDBOOK_v1.1.pdf