



# U.S. Department of Energy

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

### Topics FY 2019 Phase I Release 1

Version 4, August 20, 2018

- 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 16, 2018
Funding Opportunity Announcement Issued:	Monday, August 13, 2018
Letter of Intent Due Date:	Tuesday, September 04, 2018
Application Due Date:	Monday, October 15, 2018
Award Notification Date:	Monday, January 07, 2019*
Start of Grant Budget Period:	Tuesday, February 19, 2019

\* Date Subject to Change

Table of Changes		
Version	Date	Change
Ver. 1	July 16, 2018	Original
Ver. 2	July 24, 2018	<ul style="list-style-type: none"> <li>• Entire Document: Added "Return to Table of Contents" link</li> <li>• Topic 30: Corrected Superscript and Subscript</li> <li>• Topic 31: Corrected Superscript and Subscript</li> <li>• Topic 32: Corrected Superscript and Subscript</li> </ul>
Ver. 3	August 8, 2018	<ul style="list-style-type: none"> <li>• Topic 1: Updated "References: Subtopic a" to "References: Application Area 1"</li> <li>• Topic 1: Updated "References: Subtopic b" to "References: Application Area 2"</li> <li>• Topic 1: Change "References: Subtopic c" to "References: Application Area 3"</li> <li>• Topic 1: Change "References: Subtopic d" to "References: Application Area 4"</li> <li>• Topic 1: Change "References: Subtopic e" to "References: Application Area 5"</li> <li>• Topic 3 Subtopic b: Changed Point of Contact</li> </ul>
Ver. 4	August 20, 2018	<ul style="list-style-type: none"> <li>• Removal of Topic 23 subtopic a "Technology Transfer Opportunity: Membraneless Seawater Desalination with a Bipolar Electrode"</li> </ul>

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## INTRODUCTION TO DOE SBIR/STTR TOPICS

This SBIR/STTR topics document is issued in advance of the FY 2019 DOE SBIR/STTR Phase I Release 1 Funding Opportunity Announcement scheduled to be issued in on August 13, 2018. 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.energy.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: <http://www.doesbirlearning.com/>. Please check out the tutorials--a series of short videos designed to get you up to speed quickly.

### **COMMERCIALIZATION**

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

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

### **TECHNOLOGY TRANSFER OPPORTUNITIES**

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

#### **What is a TTO?**

A TTO is an opportunity to leverage technology that has been developed at a university or DOE National Laboratory. Each TTO will be described in a particular subtopic and additional information may be obtained by using the link in the subtopic to the university or National Lab that has developed the technology. Typically the technology was developed with DOE funding of either basic or applied research and is available

for transfer to the private sector. The level of technology maturity will vary and applicants are encouraged to contact the appropriate university or Laboratory prior to submitting an application.

**How would I draft an appropriate project description for a TTO?**

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

**Am I required to show I have a subaward with the university or National Lab that developed the TTO in my grant application?**

No. Your project plan should reflect the most fruitful path forward for developing the technology. In some cases, leveraging expertise or facilities of a university or National Lab via a subaward may help to accelerate the research or development effort. In those cases, the small business may wish to negotiate with the university or National Lab to become a subawardee on the application.

**Is the university or National Lab required to become a subawardee if requested by the applicant?**

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

**Are there patents associated with the TTO?**

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

**Will the rights to the TTO be exclusive or non-exclusive?**

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

**If selected for award, what rights will I receive to the technology?**

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

**How many awards will be made to a TTO subtopic?**

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

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

By leveraging prior research and patents from a National Lab you will have a significant “head start” on bringing a new technology to market. To make greatest use of this advantage it will help for you to have prior knowledge of the application or market for the TTO.

**Is the review and selection process for TTO topics different from other topics?**

No. Your application will undergo the same review and selection process as other applications.

**PROGRAM AREA OVERVIEW: OFFICE OF SCIENCE**

The Office of Science’s mission is to deliver scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic and national security of the United States. The Office of Science is the Nation’s largest Federal sponsor of basic research in the physical sciences and the lead Federal agency supporting fundamental scientific research for our Nation’s energy future. For more information on the Office of Science mission please visit <https://science.energy.gov/>. The topic below is a collaborative topic among multiple programs in the Office of Science.

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

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$1,500,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

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
  - 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
- 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.)

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.

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.

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.

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

### **a. 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" and associated meta-datasets greatly exceeds the ability to interpret these data. Innovations in data integration approaches and new software 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 is needed. Solutions are needed to assist these science communities in managing and analyzing their data.

Questions – Contact: Ramana Madupu, [Ramana.Madupu@Science.doe.gov](mailto:Ramana.Madupu@Science.doe.gov)

**b. Application Area 2: Technologies for Managing and Analyzing Complex Data for Watersheds and Terrestrial Ecosystems**

BER's Environmental System Science (ESS) activity consists of the Subsurface Biogeochemical Research (SBR) and the Terrestrial Ecosystem Science (TES) programs. The SBR program has a “watershed science for energy” focus which seeks to advance a robust predictive understanding of how watersheds within the contiguous United States function as complex hydro-biogeochemical systems and how these systems respond to perturbations such as changes in contaminant loading, land use, weather patterns, and snow melt. The TES program seeks to improve the representation of terrestrial ecosystem processes in Earth system models focusing on ecosystems and processes that are globally important, climatically or environmentally sensitive, and comparatively understudied or underrepresented in Earth system models. Both SBR and TES investigators are encouraged to use a holistic systems approach to understand and capture in predictive models the coupled physical, chemical and biological interactions that control the functioning of watershed systems and terrestrial ecosystems, and that extend from bedrock to the top of the vegetative canopy and across a vast range of spatial and temporal scales. Investigators are encouraged to use an iterative approach to understand the structure and functioning of complex environmental systems using a hierarchy of models to drive experimentation and observations across relevant spatial and temporal scales. A key challenge for the SBR and TES scientific communities is dealing with the extreme complexity and variety of data that is generated from these watershed and terrestrial ecosystems experiments and observations, and facilitating the use of these complex data sets to test and further advance predictive models of the structure and functioning of watershed systems and terrestrial ecosystems. The watershed and terrestrial ecosystem simulation outputs are increasing in size and complexity as the model fidelity and the temporal and spatial bandwidths of the simulations increase.

Questions – Contact: David Lesmes, [David.Lesmes@science.doe.gov](mailto:David.Lesmes@science.doe.gov) or Jay Hnilo, [Justin.Hnilo@science.doe.gov](mailto:Justin.Hnilo@science.doe.gov) or Paul Bayer, [paul.bayer@science.doe.gov](mailto:paul.bayer@science.doe.gov)

**c. Application Area 3: Technologies and Tools to Integrate and Analyze Data from Multiple Instruments and Data Systems**

A 2017 workshop report on Grand Challenges from BER's Advisory Committee<sup>1</sup> (BERAC) identifies the need for technologies and tools to integrate and analyze data being generated through BER-funded research and at BER's EMSL<sup>2</sup> and JGI<sup>3</sup> user facilities, as well as data being hosted at other BER-supported community resources such as ESS-DIVE<sup>4</sup> and KBase<sup>5</sup>. In addition, to support BER's interest in advancing systems-level understanding in the earth and environmental sciences, the 2018 CESD Strategic Plan<sup>6</sup> identifies scientific grand challenges in biogeochemistry and hydrology/water cycle, both of which rely on analyses that requires integrating a wide variety of physical and chemical process data with biological process data. That plan also identifies data-model integration as a key challenge. While data on physical, chemical and biological processes are being generated by many different types of advanced instruments, including new bioimaging capabilities being developed with BER support<sup>7</sup>, and projects supported by the joint EMSL/JGI FICUS program<sup>8</sup>, progress has been slow in capturing the data from all of these different capabilities and projects to make them collectively available to the scientific community. Efforts such as MyEMSL<sup>9</sup> now enable users to access data generated by multiple EMSL instruments, but technologies and tools to integrate EMSL-generated data with data generated from other user facilities (e.g., JGI) or hosted by other

community resources (e.g., KBase, and ESS-DIVE) are not readily available, and there is a need for improved tools to analyze those combined data sets. There is considerable need to better integrate data from microbial, plant and fungal research efforts with physical and chemical data from the local environment surrounding these types of cells or communities, and in particular, to define the structure and function of the interface between the cell membrane/surface and the local physical and chemical environment. This need is articulated in part of the BERAC Grand Challenges report<sup>10</sup> and several other recent reports<sup>11-13</sup>.

Questions – Contact: Paul Bayer, [Paul.Bayer@science.doe.gov](mailto:Paul.Bayer@science.doe.gov)

## Office of Basic Energy Sciences (BES)

### d. **Application Area 4: Capabilities for Management, Mining and Knowledge Extraction from Chemical Databases**

The Chemical Sciences, Geosciences, and Biosciences (CSGB) Division supports experimental, theoretical, and computational research to provide fundamental understanding of chemical transformations and energy flow in systems relevant to DOE missions. This knowledge serves as a basis for the development of new processes for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use. Crosscutting problems within CSGB, in need for knowledge extraction tools include Ultrafast Chemistry, Chemistry at Complex Interfaces, Charge Transport and Reactivity, Reaction Pathways in Diverse Environments and Chemistry in Aqueous Environments. In these and other areas, the DOE-BES science community has identified priority research directions and published them in a series of Basic Research Needs workshop reports – refer to those mentioned in Application Area 4 ref. 3. Measurement and computation-based inquiries in these areas create large complex unstructured collections of data that require formalized turn-key computational tools for interrogating different aspects of these data sets for differing aspects of chemical sciences. Often it is the case that the questions BES scientists ask were not fully anticipated when the databases were created so the interest is in the creation of knowledge extraction methods that are agile enough to respond to such varying needs. Another common problem that CSGB scientists deal with is the lack of knowledge in critical regions of multidimensional property spaces – such as in regions far from equilibrium where dynamics is fast and new theories or experiments are needed. As a prelude to new hypotheses or theories, CSGB physico-chemical researcher find measurable qualifiers –scaling relationships—that reduce the complexity of heterogeneous multidimensional databases that contain kinetics and thermodynamics of chemical syntheses and reactions, reaction selectivity, phase transformations, transport in complex fluid mixtures, etc. Such qualifier identification is normally an iterative and demanding endeavor that needs more efficient methods. In order to measure progress along any of the areas mentioned above and to communicate with peers, CSGB scientists strive to first precisely define, and then characterize or compute benchmarks that qualify the degree of scientific advancement, for example the reach or limitations of new theories of chemical behavior under extreme conditions. Such knowledge must be derived from available databases, which are usually sparse, noisy, unstructured and uncertain.

Questions – Contact: Raul Miranda, [Raul.Miranda@science.doe.gov](mailto:Raul.Miranda@science.doe.gov) or Mark Pederson, [Mark.Pederson@science.doe.gov](mailto:Mark.Pederson@science.doe.gov)

**e. Application Area 5: Capabilities for Management, Mining and Knowledge Extraction from Materials Databases**

The Materials Sciences and Engineering (MSE) Division supports fundamental experimental, theoretical, and computational research to provide the knowledge base for the discovery and design of new materials with novel structures, functions, and properties. This knowledge serves as a basis for the development of new materials for the generation, storage, and use of energy and for mitigation of the environmental impacts of energy use. Crosscutting problems within MSE include the need for knowledge extraction tools for materials discovery, materials design, and functional materials for energy-relevant technologies. In these and other areas, the DOE-BES science community has identified priority research directions that are published in a series of Basic Research Needs workshop reports – for example, see the list below for Application Area 5. Measurement and computation-based inquiries create large, complex, unstructured collections of data that require formalized turn-key-ready computational tools for interrogating different aspects of these data sets for specific aspects of materials science. Often the questions MSE scientists ask were not fully anticipated when the databases were created, so the interest is for creation of knowledge extraction methods that are agile enough to respond to such varying needs. A common problem that MSE scientists deal with is the lack of knowledge in critical regions of multidimensional property spaces – such as in regions far from equilibrium where dynamics is fast and new theories or experiments are needed. As a prelude to new hypotheses or theories, MSE scientists must find measurable qualifiers or physical descriptors that reduce the complexity of multidimensional databases and enable inverse design concepts for new materials functionality and emerging behavior. Such qualifier identification is normally an iterative and demanding endeavor for which tools to accelerate the process are desired. Finally, in order to measure progress along any of the areas mentioned above and to communicate with peers, MSE scientists strive to first precisely define, and then characterize or compute benchmarks. These benchmarks qualify the degree of scientific advancement, for example, the reach or limitations and uncertainty quantification of new theories for materials behavior. Usually, these must rely on sparse, noisy, uncertified and unstructured data – novel approaches and capabilities to accommodate these challenges are desired. Another opportunity is development of capabilities with real-time visualization and manipulation of molecular dynamics or continuum simulations.

Questions – Contact: Matthias Graf, [Matthias.Graf@science.doe.gov](mailto:Matthias.Graf@science.doe.gov) or James Davenport, [James.Davenport@science.doe.gov](mailto:James.Davenport@science.doe.gov)

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**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 related facilities, 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 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](#).

**2. ADVANCED DIGITAL NETWORK OPERATIONS SUPPORT SERVICES**

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$1,500,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Advances in access link technologies for commercial networks are increasing consumer network link speeds to meet the growing demands of network based applications. 100+ Mbps links are now common in many parts of the U.S. and Gigabit/sec links are now being deployed in multiple locations throughout the country. While these developments offer physical connectivity at high speeds, translating these link speeds into routine application performance remains a significant challenge. Key among these challenges is providing individuals,

small businesses, and service providers with the tools and services that can accurately and easily report performance problems to both consumers and the Internet Service Provider's (ISP) operations staff.

This topic solicits proposals that address three major activities needed to improve network operations and application performance. The first is to develop better data collection tools and services. The second is to develop better analysis and debugging tools for network operations staff. The third is to develop better analysis and reporting tools for users.

**a. Data Collection Tools and Services**

Network operations staff and individual users currently collect data from a wide variety of network devices (i.e., hosts, routers, switches, middleboxes). Common types of data collection methods include (1) active measurements of throughput, delay, and jitter along specific network paths; and (2) passive collection of log data from devices and higher level services or network level flow data. The majority of tools and services deployed today rely on the network paths being static or changing slowly over time to build up valid time series data sets to show trends and behaviors.

Grant applications are sought to create new data collection tools and services that work in more dynamic and adaptive settings. Examples include, but are not limited to:

- Measuring the throughput of each link in a bonded network path
- Measuring the delay between a client and all servers located behind a load balancer middleware box
- Measuring the jitter between a client and all servers acting as members of an anycast group.

Active or passive tools and services are both valid approaches that may be explored. Tools that build upon or augment the perfSONAR suite of measurement tools are strongly encouraged. Proposals must describe how data will be made available for use by analysis tools while maintaining privacy protections for individuals. Proposals to develop analysis tools or services that use this data will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Richard Carlson, [richard.carlson@science.doe.gov](mailto:richard.carlson@science.doe.gov)

**b. Analysis and Debugging Tools or Services for Network Operators**

Network operations staff have access to a wide variety of data from the network itself. This includes, but is not limited to, SNMP based network interface counter data, NetFlow/SFlow aggregate based flow data, perfSONAR based delay, loss, and throughput data, and packet trace data. Routers and switches may also export exception or error messages back to a log host to inform operations staffs of significant changes or faults. Finally, advanced data collection services will generate new forms of data that provide details of the status and performance of the network. Making sense of all this data is a daunting challenge that requires advanced analysis tools and services.

Grant applications are sought to improve the usability and scalability of network analysis tools and services. Analysis or Debugging tools may operate in real-time, accepting data from links operating at 10 Gbps or greater speeds or they may provide post-hoc analysis capabilities from stored data archives. Tools may correlate data from multiple input sources or they may deeply analyze a single input data stream. Tools should use widely available data formats and visualization systems to display results. Proposals to develop new data collections tools or complete Network Management Systems will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Richard Carlson, [richard.carlson@science.doe.gov](mailto:richard.carlson@science.doe.gov)

**c. User Focused Analysis or Reporting Tools and Services**

Network users currently have few tools to help them determine if applications are performing properly. It is well known that performance problems at any level of the stack (i.e., path level congestion, host level mis-configuration, device limitations) impact performance and that the indicator is simply the application runs slower than expected. Network users also lack higher level services that can assist them in reporting when and where these performance problems exist (i.e., carrier backbone, provider access link, home WiFi LAN, inside the server or client host).

Grant applications are sought to develop data analysis, or reporting tools and services that can be used by individuals or small businesses to understand and report perceived performance problems. Reporting tools should present data to the user in a format that can be understood by novice users. Additionally tools should also contain both raw and analyzed data that can be forwarded to a network operations staff with enough detail to allow them to fix a problem. Proposals to develop new data collections tools or analysis tools for use by network operations staff will be considered nonresponsive to this subtopic and will not undergo merit review.

Questions – Contact: Richard Carlson, [richard.carlson@science.doe.gov](mailto:richard.carlson@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: Richard Carlson, [richard.carlson@science.doe.gov](mailto:richard.carlson@science.doe.gov)

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**3. INCREASING ADOPTION OF HPC IN ENERGY AND ENVIRONMENTAL CLEANUP TECHNOLOGIES**

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$1,500,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Over the past decades, The Department of Energy’s (DOE) supercomputing program has played an increasingly important role in the scientific discovery process by allowing scientists to create more accurate models of complex systems, simulate problems once thought to be impossible, and analyze the increasing amount of data generated by experiments. Computational Science has become the third pillar of science, along with theory and experimentation. Despite the great potential of modeling and simulation to increase understanding of a variety of important challenges, High Performance Computing (HPC) has been underutilized in some energy technologies such as fossil and geothermal as well as in environmental cleanup technologies.

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

This topic is specifically focused on bringing HPC solutions and capabilities to the energy and environmental cleanup market sectors.

Grant applications are sought in the following subtopics:

**a. Turnkey HPC Solutions for Energy and Environmental Cleanup**

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

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

HPC applications that address challenges in subsurface science, technology and engineering as well as environmental cleanup technologies. Issues to be addressed include, but are not limited to: Developing turn-key HPC application solutions, porting HPC software to platforms that have a more reasonable cost vs. current high end systems (this could also include porting to high performance workstations (CPU/GPU) which would provide justification for the procurement of HPC assets, small scale clusters, hybrid platforms or to a "cloud" type environment or service), HPC software or hardware as a service (hosted locally or in the "cloud"), near real time modeling and simulation tools, etc.

Questions – Contact: Ceren Susut, [Ceren.Susut-Bennett@science.doe.gov](mailto:Ceren.Susut-Bennett@science.doe.gov)

**b. Hardening of R&D Code or Software Tools for Use in the Energy and Environmental Research Sectors**

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

tools that require a lower level of expertise to utilize. This may include design, implementation and usability testing of Graphical User Interfaces (GUIs) or web interfaces, simplification of user input, decreasing complexity of a code by stripping out components not required by the energy and/or environmental cleanup sectors, user support tools/services, or other ways that make the code more widely useable to the energy and environmental cleanup sectors. In addition applicants may choose to strip out code components, harden them and join them with already mature code tools and/or suites of tools to increase the overall toolset and scalability of commercial software for use by the energy and environmental research sectors.

Questions – Contact: Laura Biven, [Laura.Biven@science.doe.gov](mailto:Laura.Biven@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: Ceren Susut, [Ceren.Susut-Bennett@science.doe.gov](mailto:Ceren.Susut-Bennett@science.doe.gov)

**Note:** In addition to local, cluster, or cloud computing resources, applicants may consider using DOE’s Open Science (DOE-SC) Computing facilities, the National Energy Research Scientific Computing Center (NERSC), the Argonne Leadership Computing Facility (ALCF), or the Oak Ridge Leadership Computing Facility (OLCF). Applicants wishing to run at the NERSC (<http://www.nersc.gov>) facility should send email to [consult@nersc.gov](mailto:consult@nersc.gov) and inquire about the Education/Startup allocation program. Descriptions of the allocation programs available at the ALCF can be found at <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](mailto: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 Jack Wells at [wellsjc@ornl.gov](mailto:wellsjc@ornl.gov). Proprietary work may be done at the ALCF and OLCF facilities using a cost recovery model.

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3. U.S. Department of Energy, 2015, Scientific Discovery through Advanced Computing Program(SciDAC), <http://www.scidac.gov> (June 2018)

**References Subtopic b:**

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#### 4. HPC CYBERSECURITY

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$1,500,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Large scale distributed and computationally intensive platforms, systems, centers, infrastructure, facilities or applications 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 critical 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.

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, large scale distributed applications, 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. Currently, there exist cybersecurity tools and products that provide security to networks, databases, hosts, clouds, or mobile devices; and some of these existing tools and products could potentially be enhanced or transitioned to help secure HPC, facilities, infrastructure, or large scale distributed systems. Any proposal idea must address solutions for state-of-the-art HPC systems clearly.

Applications 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-, and/or wireless-based solutions; internet; internet-of-things; data centers; basic research; natural language processing; computing clusters; human factors; visualization; social media; web applications; social networks; cryptanalysis; or encryption, will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Robinson Pino, [robinson.pino@science.doe.gov](mailto: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](mailto: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.energy.gov/~media/ascr/pdf/programdocuments/docs/ASCR\\_Cybersecurity\\_20\\_Research\\_Pathways\\_and\\_Ideas\\_Workshop.pdf](https://science.energy.gov/~media/ascr/pdf/programdocuments/docs/ASCR_Cybersecurity_20_Research_Pathways_and_Ideas_Workshop.pdf) (June 2018)
2. U.S. Department of Energy, 2015, ASCR Cybersecurity for Scientific Computing Integrity, DOE Workshop Report, [http://science.energy.gov/~media/ascr/pdf/programdocuments/docs/ASCR\\_Cybersecurity\\_For\\_Scientific\\_Computing\\_Integrity\\_Report\\_2015.pdf](http://science.energy.gov/~media/ascr/pdf/programdocuments/docs/ASCR_Cybersecurity_For_Scientific_Computing_Integrity_Report_2015.pdf) (June 2018)
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4. Malin, A.B., and Van Heule, G.K., 2013, Continuous Monitoring and Cyber Security for High Performance Computing, Los Alamos National Laboratory, Report LA-UR-13-21921 <http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-13-21921> (June 2018)

**5. COLLABORATIVE DEVELOPMENT PROJECTS**

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$1,500,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The ASCR program office is actively engaged in the development of next generation leadership class supercomputers. This topic solicits proposals that require a collaborative team of small businesses combining their different areas of expertise to develop more complex and operational subsystems or hardware/software modules for potential integration into future emerging supercomputers. A collaborative team approach, with up to 5 small businesses forming a multi-disciplinary team, may apply for funding under this topic.

**a. Photonic – Universal Accelerator Interconnect**

Over the past decade the use of Graphics Processing Units (GPUs) has evolved from a device to drive computer displays to a high performance accelerator for supercomputers. GPUs and other types of accelerators (e.g., Field-Programmable Gate Arrays (FPGA), Tensor Processing Unit (TPU), Application-Specific Integrated Circuit (ASIC), and other devices) are expected to play a significant role in future computer architectures. Currently each accelerator may use a different, and possibly unique, interconnect mechanism to connect the accelerator to the CPU/Memory subsystem. DOE is requesting proposals to develop a universal accelerator interconnect (UAI) to enhance overall system performance while allowing multiple types of accelerators to be integrated into future supercomputers.

The photonic UAI must deliver >1 TByte/s of bandwidth to the CPU/Memory/Accelerator at bandwidth densities of >800Gb/s per optical I/O channel. Accelerator chips may be located up to 100 meters distant from the CPU/memory. Any chip (e.g., CPU core, Memory module, or accelerator) must be able to communicate directly with any other chip. Components of the UAI should include:

- Server class CPU chip

- High Performance Memory subsystem
- Ten or more Accelerator chips (ASIC, FPGA, GPU, TPU, or other accelerator chip) using at least two different accelerator types.
- WDM optical transceivers matched to the I/O rates
- Reconfigurable optical interconnect fabric
- Low loss Optical connectors and/or integrated Micro Optical Bench assemblies
- Integration with the server class CPU chip, accelerator chips and memory can be 2.5D integration (in-package) or full 3D integration. The proposer should clarify their integration strategy both from the standpoint of cost and performance implications.

It is expected that a collaborative team of small businesses will work together to design and build this UAI device. Each business may include one or more academic or lab partners as subcontractors. Each business must submit a common Letter of intent and a collaborative full proposal. The full proposal must contain an identical narrative section and a common statement describing how any Intellectual Property (IP) issues will be addressed by the collaboration. Each proposal must have business specific budget & budget justification forms, biographical data for the PI and senior personnel involved in the project, and commercialization plan. The cover sheet for each submission must clearly show all businesses involved in the collaboration.

Questions – Contact: Richard Carlson, [Richard.Carlson@Science.doe.gov](mailto:Richard.Carlson@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: Richard Carlson, [richard.carlson@science.doe.gov](mailto:richard.carlson@science.doe.gov)

#### **References:**

1. Che, S., Li, J., Sheaffer, J. W., Skadron, K., & Lach, J., 2008, Accelerating compute-intensive applications with GPUs and FPGAs, In Application Specific Processors, Symposium on (pp. 101-107), [http://www.cs.virginia.edu/~skadron/Papers/che\\_sasp08.pdf](http://www.cs.virginia.edu/~skadron/Papers/che_sasp08.pdf) (June 2018)
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6. The Optical Society, 2018, OSA Industry Development Associates [http://www.osa.org/en-us/corporate\\_gateway/](http://www.osa.org/en-us/corporate_gateway/) (June 2018)
7. The American Institute for Manufacturing Integrated Photonics, <http://www.aimphotonics.com/> (June 2018)

## 6. EMERGING INFORMATION TECHNOLOGIES FOR SCIENTIFIC FACILITIES AND HPC ENVIRONMENTS

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$1,500,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The main objective of this topic is to leverage emerging information technologies to design and develop cutting-edge commercializable products that can improve productivity in scientific facilities and high-performance computing (HPC) environments. The focus will be on three major technical areas: a) quantum network technologies and b) FPGA-Based Edge Computing. It is anticipated that technologies developed will primarily address technical issues in the scientific environment.

### a. Quantum Networks Technologies

The focus of this subtopic system is on system level quantum network subsystems (components and devices) targeting Quantum Local Area Network (Q-LAN) and Quantum Wide Area Network (Q-WAN) infrastructures in the open science environment. The goal is to leverage advances in the interdisciplinary field of quantum optics, quantum mechanics, photonics, and optical communications to develop innovative quantum hardware and software subsystems based on proven theoretical foundations, with an ultimate aim to support the generation, encoding, detection, and transmission of quantum information over wide area transparent optical telecommunication infrastructures. Grant applicants interested in submitting to this subtopic should focus on the following specific technologies that include, but are not limited to:

- Quantum processors and memory;
- All-optical buffers and switches/routers for switching photonic information without OEO conversions to enable the control of internal quantum states;
- Quantum Mux/Demux for multiple users' quantum communications on a single hop quantum network Link;
- Early prototypes of quantum repeaters that extend the distances between trusted communication nodes;
- Quantum information generating sources (Single-photon sources and entangled photons)
- Single-photon detectors;
- Quantum key distribution (QKD) network devices and protocol stacks;
- Devices and subsystems for frequency conversion of single photons;
- Quantum-photonic interconnects.

Grant applications should focus only on those quantum network devices that are based on proven theoretical foundations. When necessary, appropriate references to the literature relevant to the theoretical foundation of the proposed technologies should be cited. Applications that are focused on low-level devices such as quantum Nano devices, silicon-based quantum gates, and quantum computing

devices that are not directly relevant to quantum networks will be considered nonresponsive. Additionally, grant applications must ensure that all proposed systems support DOE's science mission.

Questions – Contact: Thomas Ndousse-Fetter, [Thomas.Ndousse-Fetter@science.doe.gov](mailto:Thomas.Ndousse-Fetter@science.doe.gov)

**b. High-Performance FPGA-Based Edge Computing**

The impact of Moore's law coupled to the rise to low-power edge computing systems, Internet of Things (IoT) technologies, and smart systems is increasingly driving the demand for reconfigurable computing subsystems based on Field-Programmable Gate Array (FPGAs) and related technologies such as Systems on Chip (SoC) and Advanced RISC Machines (ARMs). These systems are typically deployed in the proximity of data generating sources for real computations or strategically placed where computations for real-time control of scientific instruments are critical. The focus of this subtopic is on FPGA-based computing subsystems for streaming analytics, smart controllers, and high-performance edge-based systems that can be deployed as turnkey or low-power embedded subsystems for time-sensitive applications. While these subsystems have broad applicability for industrial control, automobile and aerospace industries – to name but a few, the interest in this sub-topic is on those High-Performance FPGA-based edge computing systems that have direct applicability in scientific environments (i.e., HPC, instruments, observatories, and high-performance networks, etc.). Proposed systems must be based on commercially available FPGA platforms. Other computing approaches of interest include FPGA-based IoT sub-systems and low-power computing approaches that integrate GPUs, ARMs, SoC-IP, and CPUs into a single heterogeneous low-power edge computing systems.

Applications that focus on FPGA for software acceleration with no edge computing framework, Application Specific Integrated Circuits (ASICs) with unproven FPGA framework, and systems using non-standard FPGA or custom FPGA platforms will be considered nonresponsive.

Questions – Contact: Thomas Ndousse-Fetter, [Thomas.Ndousse-Fetter@science.doe.gov](mailto:Thomas.Ndousse-Fetter@science.doe.gov)

**c. Other**

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

Questions – Contact: Richard Carlson, [richard.carlson@science.doe.gov](mailto:richard.carlson@science.doe.gov)

**References: Subtopic a:**

1. Gasin, N., Threw, R., 2008, Quantum Communication, Arxiv, <https://arxiv.org/pdf/quant-ph/0703255.pdf> (June 2018)
2. Dur, W., Lamprecht, R., Heusler, S., 2017, Towards a quantum network, European Journal of Physics, <http://iopscience.iop.org/article/10.1088/1361-6404/aa6df7/pdf> (June 2018)
3. Wang, J., Bonneau, D., Villa, M., Silverstone, J.W., Santagati, R., Miki, S., Yamashita, T., Fujiwara, M., Sasaki, M., Terai, H., Tanner, M.G., Natarajan, C.M., Hadfield, R.H., O'Brien, J., Thompson, M.G., 2015, Quantum Photonic Interconnect, Arxiv, <https://arxiv.org/pdf/1508.03214.pdf> (June 2018)
4. Behera, B.K, Reza, T., Gupta, A., Panigrahi, P.K., 2018, Designing Quantum Router in IBM Quantum Computer, Arxiv, <https://arxiv.org/pdf/1803.06530.pdf> (June 2018)

5. Azuma, K., Tamaki, K., Lo, H.K., 2013, All-photonic quantum repeaters, Arxiv, <https://arxiv.org/pdf/1309.7207.pdf> (June 2018)
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**References: Subtopic b:**

1. Gomes, T., 2015, Towards an FPGA-based edge device for the Internet of Things, 2015 IEEE 20th Conference on Emerging Technologies & Factory Automation (ETFA). [https://www.researchgate.net/publication/305992267\\_Towards\\_an\\_FPGA-based\\_edge\\_device\\_for\\_the\\_Internet\\_of\\_Things](https://www.researchgate.net/publication/305992267_Towards_an_FPGA-based_edge_device_for_the_Internet_of_Things)
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3. Le, X. S., 2017, Software/FPGA Co-design for Edge-computing : Promoting Object-oriented Design, Université de Bretagne occidentale, p. 132. [https://tel.archives-ouvertes.fr/tel-01661568/file/These-2017-SICMA-Informatique-LE\\_Xuan\\_Sang.pdf](https://tel.archives-ouvertes.fr/tel-01661568/file/These-2017-SICMA-Informatique-LE_Xuan_Sang.pdf)
4. Jiang, S., He, D., Yang, C., Xu, C., Luo, G., Chen, Y., Liu, Y., and Jiang, J., 2018, Accelerating Mobile Applications at the Network Edge with Software-Programmable FPGAs, p. 8. <http://user.informatik.uni-goettingen.de/~ychen/papers/EdgeFPGA-INFOCOM18.pdf>

**7. TECHNOLOGIES FOR EXTREME-SCALE COMPUTING**

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$1,500,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Extreme-scale computing that is 50 to 100 times faster than the fastest systems of today is planned to be available in the 2021-23 timeframe. Computing at this scale will enable significant advances in many scientific domains, such as discovery of new materials, accurate prediction of severe weather events, reducing pollution, investigating new treatments for cancer, and enabling faster and more accurate engineering designs. Furthermore, the architectural makeup of these systems will form the basis for the next generation of widely deployed systems in data centers in the commercial and academic sectors, such as petaflop racks, teraflop servers, etc. Significant challenges exist to achieving the required unprecedented computing speeds, particularly in areas of expressing and managing billion-way concurrency, reducing overall power consumption of the system, complexity of node, memory, and storage architectures, and resiliency and reliability of the system.

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

**a. Algorithms for Scientific Applications**

Development of new algorithms to accelerate scientific simulation as well as data-intensive applications that improve time to solution, quality of solution, and minimize resource consumption on extreme-scale systems. Algorithms must be scalable to large-scale parallel systems or clusters with hundreds or thousands of nodes, each node comprising any combination of the following: manycore CPUs, GPUs,

FPGAs, or other accelerators. Application development areas in scope include: Chemistry and Materials, Energy, Earth and Space Sciences, Data Analytics and Optimization, and Co-design projects aimed at developing crosscutting capabilities.

Questions – Contact: Richard Carlson, [Richard.Carlson@Science.doe.gov](mailto:Richard.Carlson@Science.doe.gov)

**b. Software Technologies**

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

Questions – Contact: Richard Carlson, [Richard.Carlson@Science.doe.gov](mailto:Richard.Carlson@Science.doe.gov)

**c. Other**

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

Questions – Contact: Richard Carlson, [Richard.Carlson@Science.doe.gov](mailto:Richard.Carlson@Science.doe.gov)

If time is needed on the high-performance computing systems at the ASCR computing facilities (NERSC, ALCF, and OLCF) for code development and/or testing, please include a section describing development and/or runtime needs for the code being developed and a statement requesting an appropriate amount of time on one or more of the ASCR computing facilities to accomplish the project goals.

**References**

1. U.S. Department of Energy, Exascale Computing Project Website, <https://exascaleproject.org/> (June 2018)
2. Wallace, T., 2018, U.S. Should Regain Lead In Supercomputing, Albuquerque Journal, <https://www.abqjournal.com/1164689/us-should-regain-lead-in-supercomputing.html> (June 2018)
3. Sarrao, J., 2018, Exascale Computing Project: Status and Next Steps, Exascale Computing Project, [https://science.energy.gov/~media/ascr/ascac/pdf/meetings/201804/ECP\\_Update\\_ASCAC\\_20180417.pdf](https://science.energy.gov/~media/ascr/ascac/pdf/meetings/201804/ECP_Update_ASCAC_20180417.pdf) (June 2018)
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5. Larzelere, A.R., 2018, Wire Momentum Builds for US Exascale, HPC Wire, <https://www.hpcwire.com/2018/01/09/momentum-builds-us-exascale/> (June 2018)
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**PROGRAM AREA OVERVIEW: OFFICE OF BASIC ENERGY SCIENCES**

The Office of Basic Energy Sciences (BES) supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security. The results of BES-supported research are routinely published in the open literature.

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

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

For additional information regarding the Office of Basic Energy Sciences priorities, [click here](#).

**8. CYLINDRICAL WAVEGUIDE WITH CORRUGATIONS FOR MICROWAVE GENERATION AND AMPLIFICATION**

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Grant applications are sought to develop cylindrical copper waveguide with corrugations for application in microwave technology for generation and amplification of THz frequency electromagnetic wave, in electron accelerators for beam manipulation, and for novel wakefield accelerators that take advantage from a cylindrical geometry for superimposing the waveguide with the external focusing.

Grant applications are sought in the following subtopics:

**a. Development of Corrugated Cylindrical Waveguides**

Grant applications are sought to develop cylindrical copper waveguides with corrugation with applications in (i) microwave technology for generation and amplification of THz frequency electromagnetic waves acting as a slow-wave structure, (ii) electron accelerators for a beam manipulation and diagnostics using self-induced axial and transverse wakefields, and (iii) for novel wakefield accelerators that take advantage from a cylindrical geometry for superimposing the waveguide with the external focusing. The probable parameters are (i) the waveguide unit length is 50 cm or longer, (ii) the ID is 2 mm or less, and (iii) the straightness of the waveguide is 10  $\mu\text{m}$  or better. The period and the full depth of the preferred rectangular shaped corrugations is highly related to the operating frequency and are thought to be in the range of 50 – 150  $\mu\text{m}$  for the corrugation full depth and 150 – 300  $\mu\text{m}$  for the corrugation period.

Questions – Contact: Eliane Lessner, [eliane.lessner@science.doe.gov](mailto: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](mailto:eliane.lessner@science.doe.gov)

**References:**

1. Paoloni, C., Di Carlo, A., Brunetti, F., Mineo, M., Ulisse, G., Durand, A., and Gohier, A., 2012, “A European Project on Vacuum Tube Amplifiers for THz Amplification,” Proceedings of UCMMT2012, p. 5. <http://orbit.dtu.dk/files/12287704/UCMMT2012.pdf>
2. Mineo, M., and Paoloni, C., 2010, Corrugated Rectangular Waveguide Tunable Backward Wave Oscillator for Terahertz Applications, IEEE Transactions On Electron Devices, Vol.57, Issue 6, pp.1481-1484. <https://ieeexplore.ieee.org/document/5447683/>
3. Nanni, E. A., Huang, W. R., Hong, K.-H., Ravi, K., Fallahi, A., Moriena, G., Miller, R. J., and Kärtner, F., 2015, Terahertz-driven Linear Electron Acceleration, Nature Communications, Issue 6, 8486, p. 8. <https://www.nature.com/articles/ncomms9486.pdf>
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**9. NON-DESTRUCTIVE ELECTRON BEAM INSTRUMENTATION FOR HIGH REPETITION RATES**

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic seeks new approaches to non-destructive instrumentation and least-invasive techniques for the characterization of low-emittance and high-rate electron beams as drivers for X-ray Free Electron Laser (XFEL) light sources. Careful understanding of the dynamics and evolution of the accelerated beam transverse and longitudinal phase space is required for optimization of the X-ray output. Non-destructive approaches will

allow almost real-time data acquisition and analysis without spoiling the downstream XFEL performance. Any proposed methods must limit intercepted beam losses to comply with safety systems operation, such as the machine protection system and beam containment system, and not initiate machine trips by violating radiation production thresholds. Additional restrictions apply to the linac and cryomodule beamlines, such as limiting induced quenching of the cavities and the particulate-free ultra-high vacuum environment. The principle investigator or the proposing company must have significant prior experience in similar development and adequate facilities for the proposed task.

Any proposed instrumentation and methods must be consistent for integration with and control by a modern computer-based interface such as EPICS, MATLAB, Python, or similar. The analyzed machine data should be available for online and real-time state modeling, magnet and accelerator feedback control systems, and the emerging application of machine learning and artificial intelligence for XFEL optimization and to minimize the configuration setup time.

Grant applications are sought in the following subtopics:

**a. Development of Novel Non-Destructive Electron Beam Instrumentation and Least-Invasive Techniques for High-Repetition Rates and High-Powered Beams**

Proposals are sought for development of novel non-destructive methods and least-invasive techniques to characterize low-emittance electron beams at high rates and beam powers with the following parameters: a) repetition rate: 0.1 – 1 MHz; b) bunch charge: 10 – 300 pC; c) average current: 1 – 300  $\mu$ A; and d) max beam power:  $\sim$ 1 MW.

Specific beam measurements of interest are (but not limited to) are:

- 1) transverse spatial profile monitoring to obtain 2-D charge distributions (or sets of 1-D projections)
- 2) transverse beam emittance: projected (single bunch or ensemble average) and slice emittance
- 3) longitudinal phase space distribution (or sets of 1-D projections)
- 4) peak current and bunch length (absolute measurements or relative quantities used for feedback)
- 5) bunch time of arrival and timing jitter/stability measurements and control methods

Methods which sense the passing electric and magnetic fields of the electron bunches such as those based on radiofrequency detection, electro-optical sampling, and photoconductive materials and devices are encouraged. Least-invasive methods include techniques that produce minimal emittance growth due to scattering and almost no additional beam losses. Such approaches for minimally-scattering methods using gas jets, liquid targets, or novel thin solids that can quickly scan through the beam will be considered.

The proposal must include careful discussion and description of the extent to which the diagnostic is “non-destructive” or “least-invasive” and to clearly identify potential failure modes and the associated risk to the beam and to the machine. Maximum operating rates and beam powers limitations should be discussed. Non-destructive methods are advantageous over invasive techniques and are useful at all repetition rates in the range specified above. However, all devices must be able to passively allow high-rate (1 MHz) beams to be transported, for instance, by including impedance-matching structures to avoid wakefield-induced emittance growth.

The applicant should identify cases where coherent (coherent synchrotron, edge, diffraction radiation, etc.) or collective (e.g. space charge) effects can limit performance and propose ways to mitigate these limitations.

Questions – Contact: Eliane Lessner, [eliane.lessner@science.doe.gov](mailto:eliane.lessner@science.doe.gov)

**b. Development of a Beam Halo Monitor**

Proposals are sought for development of instrumentation and techniques to characterize beam halo at various stages of the bunch formation and beam acceleration process. Halo is a broad term meant to include any electrons which end up outside of the phase space of the main beam core. These electrons can arise from field emission in gun and accelerating cavities (dark current) and be emitted independently in time and space from the photoelectric emission at the cathode due to the drive laser. Halo particles may instead be generated by stray light on the cathode or by space charge forces at low energy.

Regardless of the source, the halo electrons typically have very different properties than the main beam and are often lost in acceleration and transport, either purposefully at collimator locations and otherwise unintentionally all along the machine lattice. These losses are tolerable at low rates, but represent significant operational challenges at high rates and therefore must be eliminated or minimized.

This subtopic specifically addresses the need for beam halo characterization. Proposed methods may be interceptive to beam halo at any rate, provided the average steady-state intercepted beam power is low (on the order of several watts). Such methods would only intercept the halo and allow the main beam to safely pass without scattering. Examples include “holey” scintillator screens and multi-scintillator arrays.

Other methods may intercept the entire electron bunch at reduced rate with similar average power limits imposed by machine safety systems. Such approaches require large dynamic range acquisition to cover at least 5 orders of magnitude of intensity with reasonable (10 ~ 50 micron) spatial resolution limits. This resolution limit includes the combination of all deleterious effects like scintillator thickness, optical blooming, imaging optics point spread function, sensor pixilation, etc.

A completely non-contacting or least-invasive method is preferred such as using shaped gas jets or synchrotron radiation monitoring. The ability to have time-resolved measurements (or time-gated integration) and to distinguish dark current from photo-current is highly desired. Proposals combining these approaches will be given high priority.

Questions – Contact: Eliane Lessner, [eliane.lessner@science.doe.gov](mailto:eliane.lessner@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: Eliane Lessner, [eliane.lessner@science.doe.gov](mailto:eliane.lessner@science.doe.gov)

**References:**

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## 10. COMPACT, COOPERATION LENGTH PHASE SHIFTER MAGNETS FOR X-RAY FELS

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic seeks the development of compact phase shifter magnet design for X-ray free electron lasers to manipulate and control their spectral properties. Small phase shifters capable of controlling the relative phase of electron oscillations and the electromagnetic field within one wavelength are a standard element of X-ray free electron lasers. Several theoretical and experimental studies have shown that by introducing within the undulator several more powerful phase shifters, capable of delaying the electron respect to the radiation field by one to ten or more cooperation length, it is possible to reduce the X-ray pulse line width, and/or creating spectral combs consisting of a series of very short, atto-second duration, spikes separated by femtoseconds. This form of line width reduction is particularly useful to complement other methods, like HGHG, Echo and self-seeding, in spectral regions where they are not applicable, and for very high repetition rate linacs.

Grant applications are sought in the following subtopics:

### a. Compact Cooperation Length Phase Shifter Magnets for X-Ray Free Electron Lasers

Until now the use of the large phase shifter has been mostly limited to R&D work because of their rather large size and the amount of space they require in an undulator beam line. However developments in the areas of high field superconducting magnets, cryogenic magnets, permanent magnets, and other design improvements might help remove these limitations. Grants are sought that develop a design study followed by a prototype development of compact phase shifters capable of delaying the electron beam by several cooperation length, without introducing any harmful effect on the electron beam properties. The

successful product can bring substantial improvements in X-rays performance, and benefit the exploration of atomic and molecular science.

Questions – Contact: Eliane Lessner, [eliane.lessner@science.doe.gov](mailto: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](mailto:eliane.lessner@science.doe.gov)

**References:**

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**11. SUPERCONDUCTING UNDULATOR WITH FAST SWITCHING VARIABLY POLARIZED RADIATION**

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Superconducting undulator (SCU) technology has progressed significantly in the last several years. The SCUs generate higher magnetic field for the same period length and magnetic gap compared with permanent magnet undulators. As a result, these devices noticeably outperform permanent magnet-based undulators in terms of delivering higher x-ray brightness, particularly for undulators with periods larger than 15 mm. Also, superconducting undulator technology offers a possibility of building both planar and helical undulators. Two planar SCUs and one helical SCU are successfully operating at the two of the Scientific User Facilities. This topic seeks the development of a superconducting undulator prototype that generates either linear or helical configurations of magnetic field on the axis of the undulator, and is capable of fast switching between them.

Grant applications are sought in the following subtopics:

**a. Development of a Superconducting Undulator Capable of Generating Fast Switching Variably Polarized Radiation**

Grant applications are sought to design and build an undulator prototype that is capable of fast switching between linear and helical configurations of the magnetic field generated on the axis of the undulator. Changes in field configurations should ideally be executed with the frequency not less than 1 Hz, thus allowing to vary undulator radiation polarization with a rate not achievable with permanent magnet undulators.

The successful development of SCUs with variable fast switching radiation polarization will represent a breakthrough in the field of insertion devices and will deliver a unique tool for materials science and chemistry research to light source users.

Questions – Contact: Eliane Lessner, [eliane.lessner@science.doe.gov](mailto: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](mailto:eliane.lessner@science.doe.gov)

**References:**

1. Polarization control of an X-ray free electron laser with a diamond phase retarder, M.Suzuki, Y.Inubushi, M.Yabashi and T.Ishikawa, Journal of Synchrotron radiation, 21, 466-472, 2014.
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**12. HIGH-ACCURACY ANGLE GENERATOR FOR ANGULAR CALIBRATIONS TO SUPPORT OPTICAL METROLOGY LABORATORIES AND LIGHT SOURCE FACILITIES**

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic seeks the development of High-Accuracy Angle Generator for Angular Calibrations to support optical metrology laboratories and x-ray mirror metrology. Currently, one of the limiting factors in the quality of x-ray science that can be performed at synchrotron Radiation (SR) or Free Electron Laser (FEL) light sources is the characterization and metrology of super polished x-ray mirrors used to focus the x-rays. With the advent of FELs and next generation, diffraction limited SR, requirements for the surface figure of these mirrors will become more critical. Currently, metrology labs use a slope-measuring scanning method to measure the surface form of the mirrors. Such techniques use an autocollimator, a Shack Hartman sensor, or a laser beam to measure the local slope (angle) of the mirror. The main source of error, keeping practitioners from reaching the accuracy required for current and next generation mirrors, is the calibration of the autocollimator or other slope measuring device [1-3]. All DOE BES light source facilities rely on calibrations performed with a precision rotary system at the national metrology institute of Germany (the PTB) for high-accuracy autocollimators. No such device exists in the United States. This means several months of waiting and all metrological traceability going through a single device.

Grant applications are sought in the following subtopics:

**a. High-Accuracy Angle Generator for Angular Calibrations**

To overcome the above-mentioned limitations, we solicit proposals to develop a high-accuracy angle generation device capable of performing the precision angular calibrations on demand for all DOE BES light

source facilities. At a minimum, these calibrations require an automated plane angle generator with positioning uncertainty less than 50 nrad (0.01 arcsec) over a range of about 20 mrad (4000 arcsec). In addition, such a system would need to have the ability to perform calibrations at short working distance ( $\leq 100$  mm, shortest working distance possible at PTB is 250 mm) and have the capacity to use a variety of artifacts as the reflector during calibrations (e.g. x ray mirrors of size 300 mm x 50 mm x 50 mm, mirror coated or uncoated glass, etc.). Applicants are encouraged to demonstrate applicability through collaboration with light source facilities. Priority will be given to those grant applications that include collaborations with all scientific user light source facilities.

Questions – Contact: Peter Lee, [peter.lee@science.doe.gov](mailto:peter.lee@science.doe.gov)

**b. Other**

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

Questions – Contact: Peter Lee, [peter.lee@science.doe.gov](mailto:peter.lee@science.doe.gov)

**References:**

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**13. TRANSPARENT X-RAY BEAM IMAGING SYSTEM**

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic seeks the development of advanced, transparent x-ray beam imaging systems. Advanced light source facilities have shortened the allocation of user time for each experiment to improve efficiency. Many beamlines dynamically change the beam parameters – flux, size, shape and energy – of the beam to meet user needs, often through the use of dynamic focusing elements such as toroidal mirrors. In such cases, the beam optimization procedure is often time consuming and complex, requiring several iterations before the desired beam parameters are obtained. There is a need for beam monitoring devices with fast feedback, calibrated flux response and wide dynamic range, which are capable of imaging the x-ray beam in real time for efficient beam optimization.

Grant applications are sought in the following subtopics:

**a. Direct, Minimally Invasive Imaging of X-Ray Beams**

Grant applications are sought for development of a monitoring device that offers the fast feedback, flux response, and dynamic range as specified above. The requirement for the device would have a pixel size of <50  $\mu\text{m}$ , be transparent (90% +) for monochromatic beams >5keV, have a calibrated ability to measure incident flux from 107 photons/s to 1016 photons/sec per pixel with no more than 5% error, and be able to produce images at >10 Hz. The device should incorporate real time digital data acquisition and feedback controls to drive dynamic focusing optics in order to achieve the desired beam shape and position. In addition, the device should take less beam path than a standard ion chamber (~10 cm) and be addressable from modern synchrotron controls systems so as to be an integral part of a beam delivery system.

Questions – Contact: Peter Lee, [peter.lee@science.doe.gov](mailto:peter.lee@science.doe.gov)

**b. Other**

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

Questions – Contact: Peter Lee, [peter.lee@science.doe.gov](mailto:peter.lee@science.doe.gov)

**References:**

1. Zhou, T., Ding, W., Gaowei, M., De Geronimo, G., Bohon, J., Smedley, J., and Muller, E., 2015, Pixelated Transmission-Mode Diamond X-ray Detector, Journal of Synchrotron Radiation, Vol. 22, Issue 6, p. 1396-1402. <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4629867/>

**14. X-RAY DETECTOR TECHNOLOGY FOR LIGHT SOURCE FACILITIES**

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

This topic seeks the development of high-energy x-ray (>30 keV) micron-scale pixel detectors. Diffraction-limited synchrotron light sources will increase the coherent flux up to a few orders of magnitude, and reduce the horizontal beam divergence, which in turn will increase the brilliance. This will pose severe requirements for detectors used in applications making use of coherence (e.g., coherent diffraction imaging, ptychography) or those which benefit from the higher brilliance (e.g., X-ray photon correlation spectroscopy). These techniques provide unique structural information at the micro- and nano-scale, which accelerates the pace for the discovery of novel materials that can impact every aspect of our daily lives, including the generation, transmission and use of energy. High-energy x-ray microscopy and Bragg coherent diffraction imaging are being developed to tackle these challenges. However, these techniques are severely limited when applied at the high X-ray energies (>30 keV) due to the limitation of the suitable detectors. In particular, these techniques require detectors with micron-scale spatial resolution while efficient at the high X-ray energies. At these high energies, the only currently available option is based on optical scintillation microscopes, which have poor detection efficiencies. The poor efficiency not only limits the broad applications of these techniques to model material systems but also limits the extent of time-resolved experiments.

Grant applications are sought in the following subtopics:

**a. High-Energy Micron-Scale Pixel Detectors**

Grant applications are sought to develop detectors which directly detect X-rays instead of converting X-rays to optical photons, to address the above described issues. Reaching micron-scale spatial resolution is particularly challenging for high-energy X-ray photons. Silicon is a near-perfect sensor material for photon energies up to 15 keV, but its limited stopping power for higher-energy photons results in greatly reduced quantum efficiencies above 25 keV. Possible solutions for high-energy photons may include: (1) stacking silicon-based pixels array detectors; (2) high-Z semiconductors pixels detectors with high quantum detection efficiency. Possible solutions to reach micron-scale spatial resolution may include: (1) sub-pixel position resolution with position interpolation using hybrid pixel array detectors; (2) intrinsic micron-scale spatial resolution using monolithic active pixel array detectors.

Questions – Contact: Peter Lee, [peter.lee@science.doe.gov](mailto:peter.lee@science.doe.gov)

**b. Other**

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

Questions – Contact: Peter Lee, [peter.lee@science.doe.gov](mailto:peter.lee@science.doe.gov)

**References:**

1. Ulvestad, A., Singer, A., Clark, J. N., Cho, H. M., Kim, J. W., Harder, R., Maser, J., Meng, Y. S., and Shpyrko, O. G., 2015, "Topological Defect Dynamics in Operando Battery Nanoparticles", *Science Magazine*, Vol. 348, Issue 6241, p. 1344–1347. <http://smeng.ucsd.edu/wp-content/uploads/Topological-defect-dynamics-in-operando-battery-nanoparticles.pdf>
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**15. MULTI-DIMENSIONAL ELECTRON MICROSCOPY**

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The Department of Energy seeks to advance multimodal electron microscopy technologies that facilitate fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels. The Department is particularly interested in forefront advances in electron

microscopy to extend imaging and analysis techniques to multidimensional data display and analysis. Time-dependent phenomena at atomic through microscale dimensions are important and tools are needed to increase understanding phenomena for use in present and future energy applications. Advances are needed in four research subtopic areas to develop the next generation multimodal and multidimensional electron microscopy tools and techniques. All subtopics are related to acquiring, visualizing and analyzing the output from very high frame rate direct electron detectors that generate data sets approaching 1 terabyte. Low temperature and environmental specimen holders are also needed for multimodal in-situ TEM measurements. Grant applications that address solutions for detectors having lower than 100,000 frames per second do not fall within the topic and will not be considered.

Grant applications are sought in the following subtopics:

**a. Multi-Modal Visualization Software for Electron Microscopy**

Modern electron microscopy is increasingly multi-modal, with multiple imaging modalities used on a single specimen, and spectroscopic methods that yield multi-element maps. Visualizing such datasets is extremely difficult, often requiring substantial human effort to select color schemes and display parameters that highlight experimentally-relevant features without inducing artifacts that mislead experimenters. Improved visualization software is crucially required, which would automatically select an imaging scheme that optimally displays a particular dataset. Such software would ideally consider both the distribution of values in the dataset, as well as spatial organization of the multi-modal signals within the imaging space, to yield a clear and valid representation of the data. Powerful tools for exploring such datasets using machine-guidance would enable more rapid validation and analysis.

Grant applications are sought to develop a set of coordinated software tools that would take multi-model 2D and 3D microscopy/imaging datasets (in particular the data formats used on modern electron microscopes) and yield visualizations of the data that allow the multiple measured data channels to be simultaneously visualization. The software tools should use advanced methods--tuned to the scientific problem space--to select automatically visualization parameters (colormaps, brightness/contrast, thresholding, etc.) that allow multiple channels of data to be visualized simultaneously. The auto-selected values should balance between human recognition, and fidelity to the underlying dataset; tools must be provided to allow the user to adjust visualization parameters to suit specific needs. The ability to visualize both 2D images and 3D datasets (showing either individual slices or a volumetric reconstruction) is required.

Questions – Contact: George Maracas, [george.maracas@science.doe.gov](mailto:george.maracas@science.doe.gov)

**b. Live-Processing of Terabyte-sized Electron Microscopy Data**

The development of large data rate direct electron detectors is enabling new modes of electron microscopy (EM) for both high resolution imaging and diffraction analysis of materials. Direct electron detectors currently produce >100 GB data sets per measurement and will soon reach into the Terabyte regime. Such rapid advancement in the size of data sets is vastly outpacing the capabilities of current data analysis techniques available in the electron microscopy community. The prevalence of such imaging data sets is expected to increase as a proliferation of new detectors is expected in the near-term.

Tools are sought to closely integrate high-performance computing with EM instrumentation to provide live feedback (bright/dark field images) to assure the acquired data sets are valid during precious EM beam time. In addition, these tools should enable advanced imaging techniques (electron counting,

ptychography, 3D tomography, etc.) that currently cannot be applied to large Terabyte datasets to provide actionable feedback during the experiment. These tools should consist of High Performance Computing (HPC) pipelines for data analysis, data management and data visualization, especially for non-experts in big data computation. The tools should implement highly parallelized algorithms to convert the raw one-Terabyte-sized data sets into interpretable scientific images with live (or at least minimal) turnaround time.

Grant applications are sought for tools that simultaneously address the following three topics:

**Data Management:** Converting raw data in a raw stream format from a direct electron detector into an organized HDF5 (or other open source format) file capable of advanced processing and long-term storage. The data will also contain the metadata describing the data acquisition properties and the experimental parameters.

**Data Analysis:** Development of a customizable, parallelized pipeline optimized for DOE's HPC resources that will read direct electron detector data and process it for rapid display and further analysis by an end user. Multiple instances of the pipeline should be able to work on the same data to provide different processed results simultaneously. The pipeline should allow for custom algorithms to be implemented by researchers.

**Data Visualization:** A framework will be developed for feedback of very large data sets (during an experiment and after) stored on the HPC to the user's local machine. This is to facilitate live data exploration as well as final data processing. All processing for data analysis and visualization will occur on the HPC with minimal requirements for a user's local machine.

Questions – Contact: George Maracas, [george.maracas@science.doe.gov](mailto:george.maracas@science.doe.gov)

### c. Electron Source Development

Major instrumentation needs for enabling breakthrough scientific opportunities call for the development of multi-dimensional atomic resolution electron microscopy to advance condensed matter physics, materials science and quantum information science (see the 2014 Report of the Basic Energy Sciences workshop on “Future of Electron Scattering and Diffraction”, the 2017 Report on “Basic Research Needs for Innovation and Discovery of Transformative Experimental Tools”, and the 2017 Report on “Opportunities for Basic Research for Next-Generation Quantum Systems”, <https://science.energy.gov/bes/community-resources/reports/>). A main challenge is the energy resolution of electron energy loss spectroscopy in scanning transmission electron microscopy, where research needs justify the goal to advance energy resolution to 1 meV in EELS. Moreover, needs for beam monochromaticity are critical for new imaging applications that are now under development, such as microscopy techniques using the quantum wave nature of the electrons [1-4]. Energy spread in electron beams starts at the emission process. For example field emission from tungsten tips, as in cold field emission electron guns (cold-FEG), usually leads to energy spread of several hundred meV. The development of monochromators has improved the energy resolution of EELS to the range of 10 meV [5]. However, the filtering of the energies by the monochromator reduces the beam current, which increases data acquisition time for adequate signal-to-noise. The needs for beams that combine exceptionally small energy spread and sufficient intensity justify the development of new electron emitters that provide better monochromaticity right at the emission process. Examples of electron emission strategies that have been shown to improve monochromaticity in comparison with cold-FEGs include emission from states in semiconductor structures (observed energy spread  $\sim 100$  meV) [6], emission from superconducting states

(observed energy spread  $\sim 25$  meV) [7], and other strategies may exist. Grant applications are sought for the development of electron guns that enable generation of electron beams with superior energy spread and intensity compared to monochromated cold-FEG sources.

Questions – Contact: George Maracas, [george.maracas@science.doe.gov](mailto:george.maracas@science.doe.gov)

#### **d. In-Situ TEM Holder Development**

##### **i) Specimen holders for in situ electron microscopy study of air-sensitive materials**

Study of degradation mechanisms in battery materials using electron microscopy is now possible thanks to the commercially available side entry electrochemistry holders. These holders are typically used in combination with a liquid cell that consist of electron-transparent windows and recent studies have already started to shed light on mechanisms such as solid electrolyte interphase (SEI) formation, electrolyte decomposition and delithiation mechanisms. More recently, scientists in the field of energy storage have expressed strong interest in using solid-state systems with the help of polymer- or garnet-based solid electrolytes that could potentially allow the use of metallic anodes such as lithium and provide substantially high capacities in batteries compared to the state-of-the-art ones. In situ electron microscopy study of such systems that involve air-sensitive materials would require holders that are not only capable of performing electrochemical cycling during observation under the microscope but also avoiding exposure to air before insertion of specimen into the microscope.

Proposals are invited for designing a TEM holder that would allow air-free loading and transfer of specimens into the microscope while also being capable of performing in situ experiments such as heating, biasing and electrochemical measurements. Such a system is expected to be useful in fundamental studies of mechanisms relevant to areas of research such as batteries, fuel cells, corrosion, catalysis and corrosion.

##### **ii) Specimen holders for in situ electron microscopy at cryogenic temperatures**

Electrical measurements at cryogenic conditions are important for measuring the functional properties of quantum materials. TEM sample holder solutions are needed for simultaneously cooling samples to cryogenic temperatures while performing electrical and optical measurements.

Questions – Contact: George Maracas, [george.maracas@science.doe.gov](mailto:george.maracas@science.doe.gov)

#### **e. Advanced Solutions for High Frame-Rate Electron Microscopy**

##### **i) Computational methods for high-frame rate microscopy**

Advances in dynamic control of TEM data acquisition are enabling new and better ways to collect and analyze data. Camera multiplexing and compressive sensing offer kHz image acquisition rates and enable customized control over the timing of experimental sequences. These techniques also offer users the potential to utilize novel computational methods for data analysis and reconstruction that are not viable with standard video frame rate camera technologies.

There is a need to develop computational methods and data analysis workflows that take advantage of the kHz framerates offered by camera multiplexing and compressive sensing technologies. Compressively sensed TEM data has the potential to be directly transformed into application specific basis formats that

lend themselves to machine learning and big data analysis. Proposals are sought to develop computational techniques and software environments that leverage the data throughput and pre-compression advantages of camera multiplexing and compressive sensing hardware.

#### ii) High-throughput data collection

The utility of TEMs is often limited by low data throughput, especially for big multidimensional datasets. Improvements in camera frame rate and automation are driving a shift toward applications of big data and machine learning computational techniques in electron microscopy. Even so, throughput remains limited by camera readout times in many cases. Developing camera multiplexing and compressive sensing to capture multiple measurements from a single camera readout to drastically improve the throughput of TEM data acquisition across application spaces and camera technologies is needed.

Combined with advanced data reconstruction methodologies this technology makes detailed multidimensional studies of materials and molecules more efficient and accessible, turning standard electron microscopes into drivers of modern R&D processes powered by big data.

Application areas:

- STEM diffraction
- In situ TEM
- Materials design and discovery

#### iii) Rapid multi-exposure imaging

By taking control of the exposure for each camera sub-frame at sub-microsecond timescales, camera multiplexing enables dynamic processes to be captured beyond the limitations of camera exposure and readout timings. Since many material processes exhibit nonlinear kinetics it is desirable to tune in situ microscopy experiments to across multiple time scales. In a laser sintering experiment for example, multiplexing enables the capture of initial microsecond melting dynamics followed by millisecond scale solidification and grain growth. Developing software techniques for combining these time scales is key to carrying out a wide variety of large scale materials design studies across materials science domains.

Application areas:

- Dynamic in-situ measurements of advanced battery / electrode materials
- Radiation dose control in biological samples
- Materials design for additive manufacturing / laser sintering
- Tomography

Questions – Contact: George Maracas, [george.maracas@science.doe.gov](mailto:george.maracas@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: George Maracas, [george.maracas@science.doe.gov](mailto:george.maracas@science.doe.gov)

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**16. PHYSICS-BASED ARTIFICIAL INTELLIGENCE FOR SCANNING PROBE-GUIDED ATOMIC FABRICATION OF NANOSTRUCTURES**

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The ability to control matter at the level of single atoms holds great promise for future breakthroughs in materials and chemistry, including the pursuit of quantum information device manufacturing. Scanning

tunneling microscopes (STM) have been a primary tool for manipulating matter on atomic and molecular levels for over 25 years. However, the cost and throughput of the existing approaches remains such that developing research grade few-qubit devices remain the only viable target application. Some specific obstacles are the assessment of probe/image quality, inference of information/conclusions about atomic structures and their functionalities, and the STM action, all of which rely largely on the educated guess of a human operator, with a limited capacity for performing these tasks ‘on-the-fly’ These limitations in rapid data analysis and control have precluded practical implementation of atom-by-atom manufacturing of quantum devices via STM. Therefore, we seek proposals that advance the atom up fabrication process with STM by implementing a physics-based Artificial Intelligence system for real time image processing and atomic manipulation. Grant applications that use existing commercial software and software that only analyzes and displays stored data (i.e. not during real-time data acquisition) do not fall within the topic and will not be considered.

Grant applications are sought in the following subtopics:

**a. Real Time Image Analytics for Scanning Tunneling Microscopy**

There is a need for an Artificial Intelligence (AI) framework capable of extracting complete information about materials structural and electronic parameters from STM images in real time. This includes, but is not limited to, the information on lattice symmetry, precise position of lattice atoms and defects/impurities, and local electronic and magnetic properties. The needed frameworks must go beyond “off-the-shelf” AI models for image analysis (e.g., ResNet, Inception) by fully respecting the physics of a problem, that is, they must be able to enforce physical constraints both in time and space, including thermodynamic stability and transition probabilities of various atomic and defect configurations. In order to avoid a “black box problem”, a procedure for choosing hyperparameters in the prospective AI frameworks must be guided (to the degree that is possible) by the physics of a problem at hand. The method should be capable of working with data of varying noise levels and different image resolution.

Successful development of a proposed AI framework will be a critical step towards creating a fully-autonomous (“self-driving”) microscope that makes decisions based on the knowledge of physics that it was “taught.” Grant applications are sought to develop an AI framework that will enable real time image analysis of scanning tunneling microscopy data from “physics-based” constraints.

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**b. Reinforcement Learning for In-Situ Probe Preparation**

The reproducibility of STM-based atomic manipulation strongly depends on the structure of the tip apex, which is hard to control, and which can easily change during a scan. Currently, the preparation and/or “healing” of the STM tip during an experiment relies largely on the educated guess of a human operator and is characterized by a very low reproducibility. Hence, there is a need for developing an algorithm that can perform ‘on-the-fly’ learning that leads to an optimal ‘control policy’ for STM tip preparation for each specific type of experiment (details of tip-surface interactions are different for different surfaces). It is possible that such a learning process may resemble a process of a computer learning how to play a video game or a chess game. Grant applications are sought that can perform “on-the-fly learning” for optimally controlling STM tips during an experiment.

For Phase II: In order to have a true economic impact, it will be necessary to build the cause-and-effect libraries for probe-induced transformations for different groups of defects/impurities on multiple samples that will be used for the automated atomic manufacturing on a larger scale. Then one can use theoretical

calculations to predict new interesting (for basic and applied sciences) nanostructures, which are chemically and thermodynamically stable, and test if it is possible to realize them in experimental STM setup using the constructed libraries. This will also allow rigorous testing of many-body quantum theories in controllable systems (in a way reproducible among different groups), especially those phenomena that are difficult to simulate with cold atoms.

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**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](mailto:george.maracas@science.doe.gov)

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## 17. INSTRUMENTATION AND TOOLS FOR MATERIALS RESEARCH USING NEUTRON SCATTERING

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

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

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

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

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

Grant applications are sought in the following subtopics:

### a. Advanced Sample Environments

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

- Development of faster cooling furnace and cryostat: DOE's high flux sources enable faster data collection, but the existing furnaces and cryostats used for heating and cooling the samples significantly limit the efficient utilization of the valuable neutron beam time for experiments. An advancement in the technology and design of neutron scattering compatible cryostats and furnaces (with or without sample changer options) that can speed up the cooling and heating is needed to substantially decrease the down time for various types of high-throughput experiments.
- Development of steady state high field magnets: The steady-state high-field magnet systems currently available at US neutron scattering facilities are limited to a maximum field of 16 tesla, which prohibits the structure and dynamics studies of ultra-high magnetic field states of both quantum matter and in-situ materials processed at high magnetic fields [5-7]. To address this gap, development is needed for high field magnets, based on technologies employing composite conductors made of high temperature superconductor materials, suitable for neutron scattering applications.
- Development of 3D printed collimators for sample environment: 3D printed radial collimators made of neutron friendly materials with embedded or alloyed neutron absorbing elements are expected to revolutionize neutron scattering measurements with significant improvement in signal-to-noise. There is a need to develop materials and processes for 3D printing of radial collimators that incorporate neutron absorbing elements such as B, Gd and Cd which can be combined with metals such as Al. These will enable building custom built collimators that couple with a variety of sample environments used for neutron scattering to improve signal-to-noise. Development is needed for materials containing neutron absorbing elements that can be used for building 3D printed collimators for various sample environment in the neutron scattering beam lines. [8,9]

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#### **b. Advanced Detectors**

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

- High Spatial Resolution Detectors for Single Crystal Diffractometers: Novel detector technologies having resolutions from 300 $\mu$ m to 600 $\mu$ m FWHM with superior gamma rejection of  $< 1e-06$  are needed to enable efficient measurement of small single crystals for diffraction and diffuse scattering measurements. Also, of interest are technologies that have curved detector surfaces allowing near  $4\pi$  solid angle coverage with minimum dead area and reduced parallax. It is expected that these detectors have efficiencies  $\geq 60\%$  for 1 $\text{\AA}$  neutrons with minimal dead time.
- Large Area Time of Flight Detectors for Imaging Science: High rate  $> 20\text{MHz}$  time of flight (TOF) detectors are needed for novel science applications in neutron imaging. Current technologies based on charge coupled device (CCD) or complementary metal oxide semiconductor (CMOS) cannot efficiently keep up with the high data rates as they collect images by frames. The goal is to replace frame-based systems for use at spallation neutron sources which simultaneously encode position and wavelength information to enable image enhancement. Large area detectors (15cmx15cm) with spatial resolutions of 100 $\mu$ m or better are of highest interest. It is expected that these detectors have efficiencies  $\geq 60\%$  for 2 $\text{\AA}$  neutrons.
- High Data Rate Detectors for Neutron Reflectometers: The availability of detectors having resolutions of 1-2mm FWHM and very high rate capability (20 MHz) remains a challenge for neutron reflectometers where a large active area (15cmx15cm) and excellent gamma rejection  $< 1e-6$  are required. Current detector technologies fall short of the count rate requirements

measured at neutron sources by two orders of magnitude. It is expected that these detectors have efficiencies  $\geq 60\%$  for  $2\text{\AA}$  neutrons.

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**c. Advanced Choppers**

Short-pulse neutron sources provide the brightest neutron beams and future sources will push this even further, particularly at longer wavelengths. Current Fermi choppers allow the use of only single wavelength neutrons for measurements at pulsed neutron sources. Novel developments are needed in the design of Fermi choppers by incorporating neutron reflecting mirrors. Such a device, known as Magic Chopper [10], will enable the use of a wide range of wavelengths available at pulsed neutron sources and maximize the scientific output.

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**d. Other**

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

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

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## 18. SOFTWARE INFRASTRUCTURE FOR WEB-ENABLED CHEMICAL- AND MATERIALS-PHYSICS SIMULATIONS

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The Office of Basic Energy Sciences (BES), within the DOE's Office of Science, seeks to advance the standards for predictive computational modeling in chemical physics and materials science and to support delivery of exascale-ready software by 2021.

Grant applications are sought in the following subtopics:

### a. Webware and Depot for Chemical- and Materials-Physics Simulations and Data

The Department of Energy seeks to speed up discovery and delivery of new molecular and material systems for clean energy by enabling prediction of functionalities and processes of such systems prior to synthesis. Such computational predictive capabilities are also of importance to atomic and molecular physics, chemistry and chemical biology, coherent control of chemical reactions, materials sciences, magnetic- and electric-field phenomena, optics, and laser engineering. Recent advances in theory, algorithms, and hardware in materials and chemical sciences are yet to be widely available to the majority of scientifically and technically capable communities in the United States, especially those in the commercial sector and especially for the exascale. This topic seeks to reverse this situation and contribute to one goal of the Materials Genome Initiative which includes enhancing the rate of breakthroughs in complex materials chemistry and materials design. Creation of national web-enabled infrastructure for predictive theory and modeling is needed to facilitate the coordination and sharing of information and data, scalable codes, and for their implementation on, or transfer to new architectures, especially for exascale computing. In addition, a web-based infrastructure is needed to impose universal standards for data inputs and outputs in the multitude of codes and methodologies or to capitalize upon semantic strategies for bypassing the need for universal standards altogether. Industrial needs that are dependent on rapid insertion of capabilities developed by basic energy scientists include:

- Commercially viable transitioning and/or sustainably availing of validated computational approaches that span vast differences in time and length scales.

- Commercially viable transitioning and/or sustainably availing of robust and sustainable computational infrastructure, including software and applications for chemical- and materials-physics modeling and simulation.
- Commercially viable exascale-ready computational software for chemical- and materials-physics modeling and simulation.
- Commercially viable computational software for multiscale modeling, integrating atomic first-principles theory with mesoscale molecular dynamics, phase-field or continuum simulations.

Resulting infrastructure should provide economically feasible means that allow networks consisting of specialized computational chemical and computational materials science simulation groups to be linked with researchers in academia, industry, and government.

Grant applications are sought to develop and improve web-based tools for access to predictive theory and modeling.

Questions – Contact: Mark Pederson, [mark.pederson@science.doe.gov](mailto:mark.pederson@science.doe.gov), or Matthias Graf [matthias.graf@science.doe.gov](mailto:matthias.graf@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: Mark Pederson, [mark.pederson@science.doe.gov](mailto:mark.pederson@science.doe.gov), or Matthias Graf [matthias.graf@science.doe.gov](mailto:matthias.graf@science.doe.gov).

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## 19. MEMBRANES FOR ELECTROCHEMICAL APPLICATIONS

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Membranes encompass a wide range of ceramic, polymeric, and composite materials that enable separation technologies to recover, isolate, and purify products in many industrial processes with reasonable energy efficiency. Accordingly, the Department of Energy supports the development of high-risk, innovative membranes which possess greater thermal and chemical stability, greater reliability, improved fouling and corrosion resistance, and higher selectivity leading to better performance in a broad range of industrial applications, including electrochemical energy conversion and storage. Higher ion selectivity is critical for many electrochemical applications where the membrane must play the key role in separating the transport of ions and electrons between electrodes, with ions passing selectively through the electrolyte and membrane and the electrons passing externally through a circuit.

Membranes that act as ionically-conductive, electrically-insulating separators are found in virtually every electrochemical energy storage and conversion device including Li-ion rechargeable batteries, proton-exchange membrane fuel cells, redox flow batteries, solar fuel generators, and electrolyzers. Understanding the detailed mechanism for ion transport in membrane materials and the physical and electrochemical basis for ion selectivity will enable new materials with superior, longer life performance in electrochemical applications. 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. An opportunity exists to develop novel, multifunctional membranes with highly selective ionic conductivity that enable new chemistries, new 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 applications such as Li-ion intercalation batteries do not fall within this topic and will not be considered.

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

Grant applications are sought in the following subtopics:

### a. Innovative Approaches to Ion-Selective Membranes for Advanced Electrical Energy Storage

Membranes providing physical separation between the electrodes of a lithium-ion rechargeable battery are usually highly optimized polymeric materials or composite materials that prevent physical contact between the electrodes, allow transport of the Li working ion between electrodes, and accommodate a liquid electrolyte in its porous structure.<sup>1</sup> These 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, accurate assessment of the potential for new battery chemistries and architectures is often complicated when borrowing membrane

separators developed for Li-ion intercalation batteries. Thus, there exists a need for advanced ion-selective membranes to enable new energy storage chemistries and architectures using liquid electrolytes. For example, membranes which block the shuttling of polysulfide anions while providing stable Li ion conduction are needed to decouple the effects of sulfur redistribution in a sulfur cathode and shuttling anions to the lithium metal anode. Similarly, development of ion-selective membranes that are highly ion-selective, resist swelling, and are mechanically robust could greatly accelerate the development of non-aqueous flow batteries for grid storage applications. In general, ion-selective membranes developed through this subtopic should have properties and characteristics required for advancing electrochemical energy storage beyond Li-ion batteries, which may include the following:

- Membranes with high ion-selectivity derived by physical, chemical, or combined means to prevent unwanted crossover in redox flow battery architectures
- Membranes with controlled porosity coupled to a designed tortuosity to optimize ionic conductivity with minimal cell impedance
- Membranes designed for use with novel liquid electrolytes including ionic liquids, deep eutectics, or highly concentrated salt-in-solvent (either aqueous or non-aqueous)
- Membranes with a ion transference number approaching unity for non-Li working ions
- Membranes with a reversible shutdown mechanism
- Membranes that prevent the shuttling of polysulfide anions in Li-S storage systems
- Membranes that adapt at metal electrode interfaces (e.g., Li or Mg metal) to form beneficial interphases and/or control the chemistry and structural dynamics at the interface
- Membranes with resistance to fouling, swelling, and other degradation mechanisms in non-aqueous redox flow batteries

The goal of any proposed work under this subtopic should be to produce a fundamental scientific understanding of the mechanism for selective ion transport in advanced membranes for energy storage beyond Li-ion. Advances in multimodal characterizations and in modeling and simulation may be appropriate where necessary to extend this fundamental understanding across length and time scales. Process-structure-property relationships should be developed where possible to guide future development activities for new promising families of membrane materials. Demonstrations of the relevance of the underlying scientific 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](mailto:Craig.Henderson@science.doe.gov)

#### **b. 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<sup>2</sup>, 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 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](mailto:Christopher.Fecko@science.doe.gov)

**c. Other**

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

Questions – Contact: Craig Henderson, [Craig.Henderson@science.doe.gov](mailto:Craig.Henderson@science.doe.gov), or Chris Fecko, [Christopher.Fecko@science.doe.gov](mailto:Christopher.Fecko@science.doe.gov)

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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>

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**20. HIGH PERFORMANCE MATERIALS FOR NUCLEAR APPLICATION**

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

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

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

Please note: following award, all DOE SBIR/STTR grant projects requiring high performance computing support are eligible to apply to use the DOE National Energy Research Scientific Computing Center (NERSC)

resources. NERSC is the primary scientific computing facility for the DOE. If you think you will need to use the computing capabilities of NERSC during your Phase I or Phase II project, you may be eligible for this free resource. Learn more about NERSC and how to apply for NERSC resources following the award of a Phase I or Phase II project at <http://www.nersc.gov/users/accounts/allocations/request-form/>.

Grant applications are sought in the following subtopics:

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

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

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

Questions – Contact: Sue Lesica, [sue.lesica@nuclear.energy.gov](mailto:sue.lesica@nuclear.energy.gov)

**b. Ceramic Composites**

Grant applications are sought to develop improved design and fabrication methods targeted at reducing cost and/or allowing joining of nuclear-grade SiC-SiC composites that can be used in the Generation IV gas-cooled and liquid fluoride salt-cooled reactors at temperatures up to 850°C. Additional consideration will be given to proposals for SiC-SiC materials and forms that are also compatible for use as fuel cladding.

Questions – Contact: Sue Lesica, [sue.lesica@nuclear.energy.gov](mailto:sue.lesica@nuclear.energy.gov)

**c. In-Situ Mitigation and Repair of Materials Degradation**

Grant applications are sought to develop technologies for the in situ mitigation and repair of materials degradation in Light Water Reactor systems and components, in order to extend the service life of current light water reactors. Approaches of interest include new techniques for the repair of materials degradation in metals, concrete, and cables; and methods that can mitigate irradiation and aging effects in existing reactors and components.

Questions – Contact: Sue Lesica, [sue.lesica@nuclear.energy.gov](mailto:sue.lesica@nuclear.energy.gov)

**d. Molten Salt and Material Interactions**

Grant applications are sought to (1) develop technologies for in situ characterization of interfacial interactions between molten salt and materials; (2) fundamental understanding of phenomena governing interfacial behavior of materials in molten salt reactor environments; and (3) computational models for predicting thermochemical and transport properties in complex of molten salts.

Questions – Contact: Stephen Kung, [Stephen.Kung@nuclear.energy.gov](mailto:Stephen.Kung@nuclear.energy.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 description above.

Questions – Contact: Sue Lesica, [sue.lesica@nuclear.energy.gov](mailto:sue.lesica@nuclear.energy.gov)

**References:**

1. U.S. Department of Energy, 2010, Nuclear Energy Research and Development Roadmap, Report to Congress, p. 60. [http://energy.gov/sites/prod/files/NuclearEnergy\\_Roadmap\\_Final.pdf](http://energy.gov/sites/prod/files/NuclearEnergy_Roadmap_Final.pdf)
2. U.S. Department of Energy, Office of Nuclear Energy, Science and Technology, Fuel Cycle Research and Development Program. <http://www.energy.gov/ne/nuclear-reactor-technologies/fuel-cycle-technologies>
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5. U.S. Department of Energy, Office of Nuclear Energy, Light Water Reactor Sustainability (LWRS) Program. <http://www.energy.gov/ne/nuclear-reactor-technologies/light-water-reactor-sustainability-lwrs-program>

**21. IMPROVEMENT OF SUBSURFACE SIGNALS VIA ADVANCED COMPUTATIONAL METHODS**

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Subsurface sources constitute the Nation’s primary source of energy (providing more than 80 percent of total U.S. energy needs today), and they are also critical to the Nation’s secure energy future. Next generation advances in subsurface technologies will enable access to more than 100 gigawatt-electric (GWe) of clean, renewable geothermal energy, as well as safer development of domestic natural gas supplies. The subsurface provides hundreds of years of safe storage capacity for carbon dioxide (CO<sub>2</sub>) and opportunities for environmentally responsible management/disposal of hazardous materials and other energy waste streams. The subsurface can also serve as a reservoir for energy storage for power produced from intermittent generation sources, such as wind and solar. Increasing domestic hydrocarbon resource recovery enhances

national security and fuels economic growth. Thus, understanding and effectively harnessing subsurface resources while mitigating impacts of their development and use are critical pieces of the Nation's energy strategy moving forward.

The Department of Energy's (DOE) Office of Basic Energy Sciences (BES) teams with the Geothermal Technologies Office (GTO) and Office of Fossil Energy (FE), to advance the state of the art in subsurface signals indicative of how stress, geologic features, fluids, and natural resources are distributed within the subsurface. Of particular interest is the development of advanced computational methods to describe and predict parameters including but not limited to temperature, fluid flow, mechanical stress, and chemical interactions within heterogeneous, time-dependent geologic systems. Such computational methods may include software or algorithm development, data science/data-driven analysis, machine learning methods, quantum information science and quantum sensing, application of blockchain technology, etc.

Responsive applications to this topic could include (but are not limited to) advances in:  
Imaging subsurface stress, incorporating rheological properties of rocks and effects of mechanical discontinuities to improve our understanding of the initial and evolving state of stress;  
Measuring geochemical characteristics and processes to include imaging subsurface fluid flow;  
Modeling how mechanical and geochemical perturbations to subsurface rock systems are coupled through fluid and mineral interactions; and  
Understanding how heterogeneous time-dependent geologic systems can improve models of hydraulic fracturing and its environmental impacts.

Grant applications are sought to research, develop, and deploy new computational methods and algorithms that improve the quality and/or utility of subsurface signals in the following subtopics:

**a. Geothermal Subtopic**

Applications of interest under this subtopic should focus on the challenges related to improving subsurface signal specific to geothermal energy development in conditions with elevated temperatures (> 200°C) and crystalline lithology.

Specifically of interest are advanced computational methods that improve the understanding of how fractures within geothermal reservoirs evolve over time, both naturally and under the influence of operations such as well stimulation, maintenance, or flexible operating conditions. This can include improving the accuracy of seismic velocity models, improving parsing/identification of relevant seismic wave single components linked to fracture evolution, prediction of induced seismicity and other operational reservoir parameters, or analysis of existing data sets within the Geothermal Data Repository (GDR) at <https://gdr.openei.org/>.

Questions – Contact: William Vandermeer, [william.vandermeer@ee.doe.gov](mailto:william.vandermeer@ee.doe.gov)

**b. Oil and Gas Subtopic**

Applications for this subtopic should focus on advanced computational methods for analyzing subsurface signals that improve current capabilities to advance hydraulic fracture diagnostics for unconventional oil and gas wells, manipulating physiochemical fluid-rock interactions, manipulating flow paths to enhance/restrict fluid flow, characterizing fracture dynamics/geomechanics and fluid flow, novel stimulation technologies, and managing produced water. Uncertainty estimates should be determined

through modeling of various reservoir scenarios, rather than running a model only for the “most likely” case.

Questions – Contact: Olayinka Ogunsola, [olayinka.ogunsola@hq.doe.gov](mailto:olayinka.ogunsola@hq.doe.gov), or William Fincham, [William.fincham@netl.doe.gov](mailto:William.fincham@netl.doe.gov)

**c. Carbon Storage Subtopic**

Applications for this subtopic should focus on advanced computational methods for analyzing subsurface signals that improve current capabilities to characterize complex CO<sub>2</sub> storage reservoirs and cap rocks and to detect and/or forecast potential environmental hazards from fluid leakage and induced seismicity. This can include, but is not limited to, improved methods for measuring or understanding state of stress and its evolution during and after injection operations; detecting the presence of fracture and faults in the near or far field; enhancing 4-D image resolution of pressure and fluid migration; and diagnosing and monitoring wellbore integrity and leakage.

Questions – Contact: Darin Damiani, [darin.damiani@hq.doe.gov](mailto:darin.damiani@hq.doe.gov)

**d. Other**

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

Questions – Contact: James Rustad, [James.Rustad@science.doe.gov](mailto:James.Rustad@science.doe.gov)

**References:**

1. U.S. Department of Energy Office of Science, 2015, Controlling Subsurface Fractures and Fluid Flow, DOE Roundtable report, p. 24.  
<https://www.energy.gov/sites/prod/files/2016/01/f28/BES%20Report%20Controlling%20Subsurface%20Fractures%20and%20Fluid%20Flow.pdf>

**22. ADVANCED FOSSIL ENERGY TECHNOLOGY RESEARCH**

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

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

The only areas considered in this opportunity announcement include research and technology issues and opportunities in shale gas conversion to liquid fuels and chemicals, advanced non-cryogenic air separation technology, catalytic utilization of carbon dioxide, and numerical model development for supercritical CO<sub>2</sub> oxy-combustion. In addition, refer to the FE related collaborative topic: Improvement of Subsurface Signals via

Advanced Computational Methods. This topic serves as a bridge between basic science and the fabrication and testing of new technologies. Small scale applications, such as residential, commercial and transportation will not be considered. Applications determined to be outside the mission or not mutually beneficial to the Fossil Energy and Basic Energy Sciences programs will not be considered.

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

Grant applications are sought in the following subtopics:

**a. Shale Gas Conversion to Liquid Fuels and Chemicals**

With the discovery of vast quantities of natural gas available in various shale gas formations in the U.S. comes the opportunity to convert this gas, traditionally used directly as fuel, into more value added products. Traditionally, petroleum has been used to make ethylene, propylene and other building blocks used in the production of a wide range of other chemicals. We need to develop innovative processes that can readily make these chemical intermediates from natural gas.

The methane fraction can be converted into intermediates such as ethylene via oxidative coupling or reforming to synthesis gas for further processing via compact Fischer-Tropsch, whereas the ethane/propane fraction can be converted into ethylene via conventional steam pyrolysis. Since methane is rather inert and requires high temperatures to activate strong chemical bonds, practical and cost-effective conversion technologies are needed. Attempts to develop catalysts and catalytic processes that use oxygen to make ethylene, methanol, and other intermediates have had little success as oxygen is too reactive and tends to over-oxidize methane to common carbon dioxide. Recent advances with novel sulfide catalysts have more effectively converted methane to ethylene, a key intermediate for making chemicals, polymers, fuels and, ultimately products such as films, surfactants, detergents, antifreeze, textiles and others.

Proposals are sought to develop novel and advanced concepts for conversion of shale gas to chemicals based on advanced catalysts. Processes must have high selectivity and yield compared to existing state of the art. Proposals must be novel and innovative and show clear economic advantages over the existing state of the art. Microwave and plasma based processes will not be considered in this year's subtopic. Proposals that can utilize the ethane/propane/butane fraction are strongly encouraged.

Questions – Contact: Doug Archer, [douglas.archer@hq.doe.gov](mailto:douglas.archer@hq.doe.gov)

**b. Advanced Non-Cryogenic Air Separation Technology**

Gasification plants can run more efficiently and be configured to more economically capture CO<sub>2</sub> if the oxidant is oxygen rather than air. The combustion of fossil fuels in nearly pure oxygen, rather than air, can simplify CO<sub>2</sub> capture in fossil fuel power plants. When pure or enriched oxygen stream is used in a power plant, the volume of flue gas can be reduced by 75% compared with air-fired combustion [1]. The lower off-gas volume can not only reduce the removal cost of pollutants but also NO<sub>x</sub> production due to nearly zero N<sub>2</sub>. However, producing oxygen is expensive. For example, on-site oxygen production for coal

gasification conventionally uses cryogenic air separation technology. The cryogenic air separation unit (ASU) in a conventional IGCC plant typically accounts for 12 to 15 percent of the overall capital cost of the plant, and requires a large parasitic power load primarily to operate gas compressors [2]. These high costs are the impetus for development of advanced air separation technology to produce commercial-scale quantities of oxygen at significantly lower cost than the conventional cryogenic systems currently used. Grant applications are sought for research and development of air separation that can show significant capital cost reduction compared with a commercial/conventional cryogenic ASU, in application of smaller, modular systems, of which size is in the range of 1 to 5 MW (megawatt) of total power capacity. Areas of interest are not limited but exclude high temperature ion transport membrane technology (ion-electron mixed conducting membrane), high temperature ion transport membrane technology (oxygen ion conducting membrane) using electricity and oxygen sorbents of perovskites. The applicant must provide how their proposed technology would reduce capital cost and improve performance. Phase I effort should demonstrate the feasibility of the concept in a lab-scale testing.

Questions – Contact: Jai-woh Kim, [jai-woh.kim@hq.doe.gov](mailto:jai-woh.kim@hq.doe.gov)

**c. Catalytic Utilization of Carbon Dioxide**

There is a growing need to utilize carbon dioxide to make products such as fuels, high value chemicals, building products, and polymers that are environmentally sustainable. There are nearly two million metric tonnes of CO<sub>2</sub> from our industrial sector either in high or moderate concentrations that could be utilized instead of emitted to the atmosphere. Most utilization pathways for these materials require catalysis using either heterogeneous or homogeneous catalysis. The challenges with conventional catalytic materials is the high cost such as palladium based catalysts. In contrast, lower cost materials such as Cu-based catalysts are known for both CO<sub>2</sub> hydrogenation to methanol/water and the reverse reaction, methanol reforming, but require high temperature (> 200 °C) and/or high pressure (> 50 bar) for both forward and reverse reactions. Novel methods of manufacturing low cost catalyst materials that increase surface area to increase yields, conversion efficiency, reduce energy demand (temperature, pressure, electricity, or even photo) are necessary to reduce the capital and energy costs for conversion (lower temperature and pressure). Catalysts can be rationally designed by studying the mechanism on a molecular level and thus the overall catalytic activity can be improved to reduce the energy requirement.

Proposals are sought to convert CO<sub>2</sub> to high value chemicals at low temperature with homogeneous or heterogeneous catalysis in an economically viable process. Process intensification schemes using catalysts which can be incorporated into the power plant process (direct in line with flue gas or integrated as part of the air pollution control system) as either a heterogeneous or homogeneous catalyst are also of interest to reduce the cost of adding an additional process to the power plant system.

Questions – contact John Litynski. [John.litynski@hq.doe.gov](mailto:John.litynski@hq.doe.gov)

**d. Numerical Model Development for Supercritical CO<sub>2</sub> Oxy-Combustion**

Supercritical CO<sub>2</sub> (SCO<sub>2</sub>) power cycles utilize CO<sub>2</sub> as the working fluid in the turbomachinery and represent a promising technology to attain higher efficiencies and smaller builds. The cycles are operated at high pressures in the supercritical regime such that the CO<sub>2</sub> does not undergo phase change and high fluid densities are attained to make the cycle more efficient.

In a direct-fired SCO<sub>2</sub> cycle (e.g., Allam cycle), fossil fuels such as natural gas or coal-derived syngas combust with O<sub>2</sub> at high pressure and in a highly CO<sub>2</sub> diluted environment. The resulting steam/CO<sub>2</sub> is then

used to drive the turbine. Typical conditions are around 300 bar pressure, 700 °C preheat temperature and 1100 °C combustion temperature. Optimal performance of these systems requires the optimization of a number of design parameters including among others: a) Injector design to minimize amount of CO as well as NOX and SOX from any contaminants present in the fuel, b) adequate mixing to generate uniform temperature profile in the combustor exhaust which drives the turbine, and c) design of CO<sub>2</sub> flow split to minimize heat transfer to the combustor wall and control the wall surface temperature. Resolving these design issues will be facilitated by the development of numerical models under this effort as part of high-fidelity simulations to provide design support. However, the lack of experimental data in this regime makes it difficult to validate numerical models and therefore proposals must also include a test program to generate validation data for the numerical models developed as part of this effort. Some of the specific areas to be addressed in this effort as part of a large numerical model framework for design support include the following:

- Real fluid effects: Under supercritical conditions, real fluid effects become prominent, particularly for mixtures of CO<sub>2</sub> with water and other contaminants. For SCO<sub>2</sub> oxy-combustion, previous numerical studies have reported that even in the hot reaction zone a deviation from ideal gas behavior is exhibited. The characterization of the relevant thermodynamic and transport properties for mixtures under these operating conditions is essential for combustor analyses. The development of analytical equations of state models validated against test data in this regime are sought.
- Chemical kinetics effects induced by impurities: Depending on the level of purity attainable from the air separation unit (ASU), inert contaminants such as N<sub>2</sub> and Ar may be introduced in the oxidizer stream. Similarly, various impurities are present in natural gas as well as syngas from high-sulfur coal. As a result, SCO<sub>2</sub> oxy-combustion may lead to the generation of meaningful amounts of acid gases such as NO<sub>x</sub> and SO<sub>x</sub>, which in turn may impact the underlying chemical kinetics. Moreover, for the safe storage of the captured CO<sub>2</sub>, it is important to quantify and minimize the presence of NO<sub>x</sub> and SO<sub>x</sub> in the CO<sub>2</sub> stream. Development of reduced kinetic models with adequate fidelity as part of CFD frameworks are desired. The reduced kinetic models would ideally be validated against fundamental test data with impurities to ensure accuracy.

Grant applications are sought which develop and validate modeling approaches for real fluids and chemical kinetic interactions with impurities suitable for direct-fired SCO<sub>2</sub> power cycles. Plans to obtain fundamental validation data for verifying model accuracy in this regime must be addressed. Development of comprehensive CFD-based analysis frameworks and demonstrations of the improved predictive capabilities for design support are also desirable.

Questions – contact Bhima Sastri, [bhima.sastri@hq.doe.gov](mailto:bhima.sastri@hq.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 description above.

Questions – Contact: Doug Archer, [douglas.archer@hq.doe.gov](mailto:douglas.archer@hq.doe.gov)

**References: Subtopic a:**

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### 23. TECHNOLOGY TRANSFER OPPORTUNITIES: BASIC ENERGY SCIENCES

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Applicants to TECHNOLOGY TRANSFER OPPORTUNITIES (TTO) should review the section describing these opportunities on page 7 of this document prior to submitting applications.

Grant applications are sought in the following subtopics:

**a. SUBTOPIC REMOVED**

**b. Technology Transfer Opportunity: Metal-Organic Frameworks for the Separation of O<sub>2</sub> from Air**

Sandia National Laboratories researchers have developed a novel method to synthesize open pored metal organic frameworks (MOFs) nanoporous materials which exhibit high selectivity for O<sub>2</sub>, enabling the separation of O<sub>2</sub> from N<sub>2</sub> and other air components for O<sub>2</sub> purification. Oxyfuel combustion is a promising technology with the potential to replace contemporary combustion sources with increased energy savings yet requires high purity oxygen derived from air separation processes. Contemporary O<sub>2</sub> purification techniques such as cryogenic air separation produce high quality O<sub>2</sub> (with purity approaching 99%), but are accompanied with energy-intensive and expensive facilities. Alternative O<sub>2</sub> purification techniques, such as Pressure Swing Absorption (PSA) exist, but utilize adsorbents such as zeolites which are costly and inefficient. Sandia's MOFs demonstrate highly selective O<sub>2</sub> separation from air mixtures while demonstrating better sorbent purity, sorption, and fewer structural defects than zeolites. Owing to the open-pore framework which gives access to the metal center (comprised of Sc and Fe) in the MOF structure, Sandia's MOFs demonstrate improved O<sub>2</sub> sorption via enhanced O<sub>2</sub>-framework interactions. In conjunction with PSA techniques, Sandia's MOFs have the ability to produce dramatic process efficiency improvements competitive with cryogenic air separation technique at reduced costs.

**Licensing Information:**

Sandia National Laboratories

Contact: Robert Westervelt ([rtweste@sandia.gov](mailto:rtweste@sandia.gov), (505) 284-6752)

SNL Technology ID: SD 12911

Patent Status: US Patent Application 15/269,745

Website: <https://ip.sandia.gov/technology.do/techID=164>

Questions – Contact: Raul Miranda, [Raul.Miranda@science.doe.gov](mailto:Raul.Miranda@science.doe.gov)

## PROGRAM AREA OVERVIEW: OFFICE OF BIOLOGICAL AND ENVIRONMENTAL RESEARCH

The mission of the Biological and Environmental Research (BER) program is to support transformative science and scientific user facilities to achieve a predictive understanding of complex biological, earth, and environmental systems for energy and infrastructure security and resilience. The program seeks to understand the biological, biogeochemical, and physical principles needed to fundamentally understand and be able to predict processes occurring at the molecular and genomics-controlled smallest scales to environmental and ecological processes at the scale of planet Earth. Starting with the genetic information encoded in organisms' genomes, BER research seeks to discover the principles that guide the translation of the genetic code into the functional proteins and metabolic and regulatory networks underlying the systems biology of plants and microbes as they respond to and modify their environments. Gaining a predictive understanding of biological processes will enable design and reengineering of microbes and plants for improved energy resilience and sustainability, including improved biofuels and bioproducts, improved carbon storage capabilities, and controlled biological transformation of materials such as nutrients and contaminants in the environment. BER research also advances the fundamental understanding of dynamic, physical, and biogeochemical processes required to systematically develop Earth System models that integrate across the atmosphere, land masses, oceans, sea ice, 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 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, and the terrestrial ecology; 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 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 integrated experimental and computational resources researchers need to understand the physical, biogeochemical, chemical, and biological processes that underlie DOE’s energy and environmental mission. The data activity encompasses observations collected by dedicated field experiments, routine and long term observations accumulated by user facilities, and model generated information derived from earth models of variable complexity and sophistication.

For additional information regarding the Office of Biological and Environmental Research priorities, [click here](#).

## **24. TECHNOLOGIES FOR CHARACTERIZING AND MONITORING COMPLEX SUBSURFACE SYSTEMS INCLUDING THE RHIZOSPHERE**

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$1,500,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The focus of this topic is on the development of improved technologies for characterizing and monitoring complex subsurface systems, extending from the soil surface, through the rhizosphere and vadose zone down to the bedrock. The ability to characterize and monitor the distribution and transport of water, nutrients and contaminants through and across these subsurface compartments, and to understand their interactions with plants and microbes, is of vital importance for better understanding subsurface system structure and functioning and for advancing DOE’s energy and environmental missions.

The focus of Subtopic a. is on the rhizosphere which serves as the substrate for natural and managed terrestrial vegetative systems. A holistic consideration of plant-microbe-mineral interactions within a larger environmental context is required to better understand and optimally manage vegetative systems including biofuel crops. An important motivation for this subtopic is to support innovative sensing technologies that will enable the development and optimization of next generation plant feedstocks for biofuel and bioproduct production. The focus of Subtopic b. is on the development of fieldable technologies for capturing the in situ hydrobiogeochemical structure and functioning of complex subsurface systems within the context of watershed and terrestrial ecosystems extending from the bedrock to the vegetative canopy. Important applications also include the characterization and monitoring of contaminated soils and groundwater at DOE legacy waste sites that pose significant cleanup challenges as well as interactions with surface water bodies (groundwater-surface water interaction).

Grant applications are sought in the following subtopics:

### **a. Technologies for Characterizing the Rhizosphere: Plant-Microbe-Mineral Interactions**

The rhizosphere, the soil region immediately surrounding plant roots, is a nexus of biological and mineral processes. New or improved technologies are sought for characterizing the rhizosphere at the molecular through tissue/microbial community scale to inform the development of sustainable biofuel feedstocks. Knowing the complex interdependencies of plant-microbe-mineral systems is critical to understanding and developing sustainable biofuel production practices. Great potential for improving crop sustainability lies in the design of optimally mutualistic plant-microbe interactions. This requires deep insight into plant-microbe-mineral interactions of rhizosphere ecosystems important for sustainable bioenergy crop production.

Through the SBIR/STTR programs, DOE BER seeks to support the development of new technologies or extensions of existing technologies to characterize the dynamics or dynamical elements of rhizosphere interactions that can advance the understanding and characterization of such interactions. Technologies are sought to characterize the system at and across scales including molecular, cellular and plant tissue or “community” scale. The “community” of interest is considered to include microbial and plant biotic components and their interactions, as well as their interactions with abiotic components.

Examples of eligible technologies include but are not limited to sensor systems, imaging methods and other analytical tools and may be field deployable or laboratory/facility-based. Biotechnological and biodesign approaches are excluded except where used to specifically enhance the potential to characterize a system. Development of accessories that enhance the utility of existing tools for characterizing rhizosphere or its components are also encouraged.

Areas of interest include but are not limited to characterization of molecular- to tissue/community-scale processes of:

- interactions among rhizosphere components (e.g. algae-bacteria, fungi-bacteria, bacteria-phage or biotic-abiotic, etc.) that have been demonstrated to be critical to a rhizosphere ecosystem. The specific interaction network proposed for study must have already been discovered.
- root exudate composition and its interactions with microbial symbionts
- rhizosphere soil biochemical processes

Questions – Contact: Amy Swain, [Amy.Swain@science.doe.gov](mailto:Amy.Swain@science.doe.gov)

**b. Real-Time, In Situ Measurements of Hydrobiogeochemical Processes in Complex Subsurface Systems**

Reactive transport models are increasingly used to model hydrobiogeochemical processes in complex subsurface systems (soils, rhizosphere, sediments, aquifers and the vadose zone) for many different applications and across a wide range of temporal and spatial scales (e.g., pore to core to plot to watershed). With increasing computational capability it is possible to simulate the coupled interactions of complex subsurface systems with high fidelity. The predictive value of these advanced models is limited, however, by the availability and accuracy of the data that are used to populate the models and represent the system structure and intrinsic properties. Furthermore, robust testing of these increasingly complex models requires high frequency and high fidelity measurements of the hydrobiogeochemical structure and functioning of subsurface systems over the relevant spatial and temporal scales. Key measurements that are currently difficult to obtain in real time include the compositions and/or oxidation states of constituents in sediment gases, pore water, surface water, and sediments.

Sensitive, accurate, and real-time monitoring of hydrobiogeochemical processes are needed in subsurface environments, including soils, the rhizosphere, sediments, the vadose-zone and groundwaters. In particular, highly selective, sensitive, and rugged in situ devices that can measure concentrations of solutes and gasses are needed for low-cost field deployment in remote locations, in order to enhance our ability to monitor processes at finer levels of resolution and over broader areas. Therefore, grant applications are sought to develop improved approaches for the autonomous and continuous sensing of key elements such as carbon, nitrogen, sulfur and phosphorus in situ; improved methods to measure and monitor dissolved oxygen, vertically resolved soil moisture distributions, and groundwater age.

The ability to distinguish between the relevant oxidation states of redox sensitive elements such as iron, manganese, nitrogen, sulfur and other inorganics is of particular concern. Innovative approaches for monitoring multi-component biogeochemical signatures of subsurface systems is also of interest, as is the development of robust field instruments for multi-isotope and quasi-real time analyses of suites of isotope systems of relevance to hydrologic and biogeochemical studies (e.g.  $2\text{H}$ ,  $18\text{O}$ ,  $\text{CH}_4$ ,  $\text{CO}_2$ , nitrogen compounds, etc.).

Grant applications 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 (i.e., free of anticipated physical/chemical/biological interferences). Approaches that leave significant doubt regarding sensor functionality in realistic multi-component samples and realistic field conditions will not be considered.

Grant applications are also sought to develop integrated sensing systems for autonomous or unattended applications of the above measurement needs. The integrated system should include all of the components necessary for a complete sensor package (such as micro-machined pumps, valves, micro-sensors, solar power cells, etc.) for field applications in the subsurface. Approaches of interest include: (1) automated sample collection and monitoring of subsurface biogeochemistry; (2) fiber optic, solid-state, chemical, or silicon micro-machined sensors; (3) biosensors (devices employing biological molecules or systems in the sensing elements) that can be used in the field – biosensor systems may incorporate, but are not limited to, whole cell biosensors (i.e., chemiluminescent or bioluminescent systems), enzyme or immunology-linked detection systems (e.g., enzyme-linked immunosensors incorporating colorimetric or fluorescent portable detectors), lipid characterization systems, or DNA/RNA probe technology with amplification and hybridization; and (4) smart environmental sensing networks (or smart cyber physical systems) to characterize and capture "hot spots and hot moments" using wireless or wired sensing nodes.

Grant applications submitted to this topic 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. Claims of relevance to field sites or locations under investigation by DOE, or of commercial potential for proposed technologies, must be supported by endorsements from relevant site managers, market analyses, or the identification of commercial spin-offs. Grant applications that propose incremental improvements to existing technologies are not of interest and will be declined. Collaboration with government laboratories or universities, either during or after the SBIR/STTR project, may speed the development and field evaluation of the measurement or monitoring technology. BER funding to the National Laboratories is primarily through Scientific Focus Areas (SFAs). The [Subsurface Biogeochemical Research \(SBR\)](#) supported SFAs, and the field sites where they conduct their research, are described at the following website: <http://doesbr.org/research/sfa/index.shtml>. The [Terrestrial Ecosystem Science \(TES\)](#) program also supports several interdisciplinary field research projects focused on carbon and nutrient cycling: <http://tes.science.energy.gov/>. These field research sites may also be appropriate venues for testing and evaluation of novel measurement and monitoring technologies. Proposed plans to conduct testing at these DOE supported research sites should be accompanied by a letter of support from the project PI.

Grant applications must describe, in the technical approach or work plan, the purpose and specific benefits of any proposed teaming arrangements.

Questions – Contact: David Lesmes, [david.lesmes@science.doe.gov](mailto:david.lesmes@science.doe.gov) or Paul Bayer, [paul.bayer@science.doe.gov](mailto:paul.bayer@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: David Lesmes, [david.lesmes@science.doe.gov](mailto:david.lesmes@science.doe.gov) or Paul Bayer, [paul.bayer@science.doe.gov](mailto:paul.bayer@science.doe.gov)

**References: Subtopic a:**

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2. U.S Department of Energy, Office of Biological and Environmental Research, 2015, Biological Systems Science Division, Strategic Plan, p. 18. <http://genomicscience.energy.gov/pubs/BSSDStrategicPlan.pdf> (June 2018)

**References: Subtopic b:**

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6. U.S. Department of Energy, Office of Biological and Environmental Research, 2014, Building Virtual Ecosystems: Computational Challenges for Mechanistic Modeling of Terrestrial Ecosystems, Workshop Report, p. 48, DOE/SC-0171. <http://science.energy.gov/~media/ber/pdf/workshop%20reports/VirtualEcosystems.pdf> (June 2018)

## 25. ATMOSPHERIC MEASUREMENT TECHNOLOGY

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$1,500,000
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 Climate and Environmental Sciences Division (CESD) 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). CESD scientific grand challenges include the integrated water cycle, biogeochemistry, high latitudes, and drivers and responses in the earth system (Reference 1).

Addressing these scientific grand challenges requires data from field campaigns and long-term observations to quantify local atmospheric processes including aerosol formation, chemical evolution, and optical properties; initiation and microphysical properties of cloud droplets, ice crystals, and precipitation; details of atmospheric turbulence and water vapor; and feedbacks involving the terrestrial-aerosol-cloud-precipitation system. These data are necessary both for fundamental process understanding and for evaluation of numerical models that are used to assess the predicted impacts to global and regional systems. Clouds and aerosols continue to contribute the largest uncertainty to estimates and interpretations of the Earth's changing energy budget (Reference 2).

This topic is specifically focused on developing technologies for robust field-deployable measurements of aerosol, cloud, turbulence, precipitation, or water vapor properties suitable for deployment at field sites (such as the Atmospheric Radiation Measurement [ARM; [www.arm.gov](http://www.arm.gov)], AmeriFlux [<http://ameriflux.lbl.gov/>], or Next Generation Ecosystem Experiment (NGEE; <https://ngee-arctic.ornl.gov/>] sites) or on small unmanned aerial or tethered balloon platforms (<https://www.arm.gov/capabilities/observatories/aaf/uas>). While existing technologies can measure the specific atmospheric properties of interest under ideal conditions, technological innovations and improvements are required to develop instrumentation that is more robust and automated for long-term operation at remote field sites that has higher accuracy or resolution than existing instrumentation, or that has lower weight and power requirements for deployment at remote field sites or on small aerial platforms.

Grant applications submitted to this topic 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 should (1) specifically describe how the proposed work is a technical advance over existing commercial instrumentation and how it will improve either the robustness, automation, accuracy, resolution, or weight/power requirements compared to existing 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). Grant applications proposing 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.

Grant applications are sought in the following subtopics:

**a. Field-Deployable Aerosol Absorption Measurements**

The role of atmospheric aerosols in the earth's radiation balance as well as influencing cloud processes is complex, and the quantitative impacts of aerosols on the atmosphere have many uncertainties. Through their ability to absorb and scatter radiation (direct effect) and alter cloud properties (indirect effect), aerosols influence the global radiation budget and thermodynamic balance of the planet. One particular class of aerosols, light-absorbing aerosols, contribute disproportionately and substantially to this net uncertainty in aerosol forcing despite their small relative abundances compared to non-absorbing aerosol types. Optically absorbing aerosols (AA) both reduce the amount of sunlight reaching the surface and heat their surroundings. By doing so, they modify the vertical distribution of heat in the atmosphere and affect atmospheric thermodynamics and stability, possibly hastening cloud drop evaporation, and thereby affecting cloud amount, formation, dissipation and, ultimately, precipitation. Deposition of AA on snow and ice reduces surface albedo leading to accelerated melt. Classes of AA include mineral dust, combustion soot, and organic matter containing optically active chromophores. The importance of absorbing aerosols is due to their atmospheric impacts and the difficulty of obtaining artifact-free measurements of this fraction of the atmospheric aerosol burden (Reference 3).

Therefore, grant applications are sought to develop new measurement technology, or to improve instruments using current measurement principles for direct, in-situ measurement of optical absorption of suspended aerosols in field conditions. Note that inferring absorption from the measurement of scattering and total extinction is not considered a direct measurement of absorption for this solicitation. Applications must meet three primary requirements: 1) the technique used must measure the optical absorption of ambient aerosol suspended in air, not deposited on a filter or substrate. 2) The instrument must be capable of independent measurements using multiple wavelength(s), to quantify spectral dependence of absorption. Desired wavelengths should span the visible or near ultraviolet region. Wavelengths that nominally match existing optical scattering instruments (450, 550, or 700 nm) are especially useful. 3) The instrument must operate autonomously and include a co-developed field calibration methodology. Either ground-based or aircraft-deployable instruments are of interest for this topic.

The following technical specifications are strongly desired:

- A sensitivity goal of  $1 \text{ Mm}^{-1}$  ( $2\sigma$  at 10-s averaging) with a response time of 5 s,
- Single or multiple wavelengths from UV – NIR: 350-1064 nm, compatible with existing extinction and absorption measurements using existing techniques,
- Capable of field calibrations. Explain how instrument is to be calibrated,
- Flow rate less than  $\sim 2$  LPM due to drying constraints,
- Capability of measurement over a modest range of humidity so that exploration of aerosol response to relative humidity is not precluded,
- Robust, automated operation, and
- If proposing an instrument for aircraft deployment, size, weight, power and environmental conditions must be described.

If this set of technical specifications cannot be met, the approach proposed must include a discussion of tradeoffs.

Questions – Contact: Rick Petty, [Rick.Petty@science.doe.gov](mailto:Rick.Petty@science.doe.gov)

**b. Ground-Based Atmospheric Water Vapor and Liquid Water Measurements**

One of the scientific grand challenges of the Climate and Environmental Sciences Division (CESD) is to advance understanding of the integrated water cycle (Reference 1). The amount and vertical distribution of water in the atmosphere is a key element of the integrated water cycle and is important for understanding atmospheric processes important to weather and climate including cloud formation, atmospheric circulations, and radiative transfer processes. The distribution of water in the atmosphere is highly temporally and spatially variable; therefore long-term continuous observations of atmospheric water are needed for process studies (Reference 4).

While technologies for ground-based remote sensing measurements of atmospheric water vapor and liquid water currently exist (including passive microwave [Reference 5], differential absorption lidar [Reference 6], Raman lidar, and infrared interferometer methods [Reference 8]), measurements with improved robustness, accuracy, sensitivity, temporal or vertical resolution, and ability to operate under a wider range of conditions are desired to address integrated water cycle questions. Additionally, commercialization of technologies that currently only exist as research instruments will enable wider deployment of instruments at field sites around the globe. A review of current remote sensing technologies for thermodynamic profiling of the lower atmosphere is provided in Reference 4.

Grant applications are sought to develop new remote sensing measurement technologies or improve existing remote sensing technologies for: 1) simultaneous ground-based measurements of atmospheric total water vapor path & liquid water path, 2) simultaneous ground-based vertical profiles of tropospheric atmospheric water vapor and temperature as a function of height, or 3) ground-based vertical profiles of liquid water content as a function of height. Instruments must be able to operate continuously and autonomously in field conditions and include a field calibration methodology.

Applicants are encouraged to consult Reference 4 on desired technical specifications for water vapor measurements and Reference 5 for current status of ARM microwave radiometer network.

Specific technology innovations could include:

- New technologies not currently available in commercial instrumentation such as differential absorption radar techniques (Reference 8);
- Improved calibration techniques, calibration stability, and/or accuracy of measurements and therefore of derived water vapor and/or liquid water content values;
- Improved vertical resolution of atmospheric water vapor and/or liquid water content profiles;
- Improved sensitivity to low water vapor path and/or low liquid water path conditions; and/or
- Improved technologies for measurements of water vapor and liquid water under precipitating conditions and water vapor within clouds.

Questions – Contact: Sally McFarlane, [Sally.McFarlane@science.doe.gov](mailto:Sally.McFarlane@science.doe.gov)

**c. Other**

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

Questions – Contact: Rick Petty, [Rick.Petty@science.doe.gov](mailto:Rick.Petty@science.doe.gov)

**References:**

1. U.S. Department of Energy, 2018, Climate and Environmental Sciences Division, Strategic Plan, DOE/SC-0192, [https://science.energy.gov/~media/ber/pdf/workshop%20reports/2018\\_CESD\\_Strategic\\_Plan.pdf](https://science.energy.gov/~media/ber/pdf/workshop%20reports/2018_CESD_Strategic_Plan.pdf) (June 2018)
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3. U.S. Department of Energy, 2016, Climate and Environmental Sciences Division, Absorbing Aerosols Workshop Report, DOE/SC-0185, <http://science.energy.gov/~media/ber/pdf/workshop%20reports/CESD-AbsorbingAerosol2016.pdf> (June 2018)
4. Wulfmeyer, V., R. M. Hardesty, D. D. Turner, A. Behrendt, M. P. Cadeddu, P. DiGirolamo, P. Schlüssel, J. Van Baelen, and F. Zus, 2015, A review of the remote sensing of lower tropospheric thermodynamic profiles and its indispensable role for the understanding and the simulation of water and energy cycles, AGU 100 Advancing Earth and Space Science Rev. Geophys.,53,819–895, <https://doi.org/10.1002/2014RG000476> (June 2018)
5. Cadeddu, M. P., Liljegren, J. C., and Turner, D. D., 2013, The Atmospheric radiation measurement (ARM) program network of microwave radiometers: instrumentation, data, and retrievals, Atmospheric Measurement Tech., 6, 2359-2372, <https://doi.org/10.5194/amt-6-2359-2013> (June 2018)
6. Spuler, S. M., Repasky, K. S., Morley, B., Moen, D., Hayman, M., and Nehrir, A. R., 2015, Field-deployable diode-laser-based differential absorption lidar (DIAL) for profiling water vapor, Atmospheric Measurement Tech., 8, 1073-1087, <https://doi.org/10.5194/amt-8-1073-2015> (June 2018)
7. Turner, D. D. and Löhnert, U., 2014, Information Content and Uncertainties in Thermodynamic Profiles and Liquid Cloud Properties Retrieved from the Ground-Based Atmospheric Emitted Radiance Interferometer (AERI), American Meteorological Society 53, 752–771, <https://doi.org/10.1175/JAMC-D-13-0126.1> (June 2018)
8. Lebsock, M. D., K. Suzuki, L. F. Mill'án, and P. M. Kalmus, 2015, The feasibility of water vapor sounding of the cloudy boundary layer using a differential absorption radar technique, Atmospheric Measurement Tech., 8, 3631–3645, <https://www.atmos-meas-tech.net/8/3631/2015/> (June 2018)

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

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$1,500,000
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. BER supports a portfolio of resources to enable experiments for studying and understanding structural and functional processes of importance to BER Genomic Science program (GSP)–funded investigators and centers. The resource portfolio includes research technologies, methodologies, instruments and expertise at DOE synchrotron and neutron user facilities.

### a. Tools or Instruments for Structural Characterization of Biological Systems Ranging from Atomic to Cellular Scales

This subtopic solicits the development of robust tools that are needed to improve structural biology capabilities for researchers studying microbial or plant systems related to DOE interests. For this solicitation, structural biology targets range from the atomic to cellular scale. Technology areas for structural characterization include x-ray or neutron-based techniques as well as cryo-EM, NMR or other approaches for determining the 3D structures of macromolecules, macromolecular complexes, cells or cellular components. Examples of concepts responsive to this announcement include but are not restricted to tools or instruments for sample preparation, handling, positioning or detection for any of the above mentioned technology areas. The purpose is to encourage development and commercialization of tools that ease use, improve results or overcome obstacles associated with existing technologies. Except where needed for the proposed tool, algorithm development, software or informatics solutions are not included under this subtopic, but should 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](mailto: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](mailto:Amy.Swain@science.doe.gov)

### References:

1. U.S. Department of Energy, Office of Biological and Environmental Research, 2015, Biological Systems Science Division, Strategic Plan, p. 18. <http://genomicscience.energy.gov/pubs/BSSDStrategicPlan.pdf> (June 2018)
2. BER Structural Biology Resources at Synchrotron and Neutron Facilities, BER Structural Bio Portal, <http://www.BERStructuralbioportal.org> (June 2018)

## 27. BIOIMAGING TECHNOLOGIES FOR BIOLOGICAL SYSTEMS

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$1,500,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

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

### a. New Instrumentation and Bioimaging Devices for Non-destructive, Functional Metabolic Imaging of Plant and Microbial Systems

Applications are invited to develop new imaging instrumentation and imaging devices for in situ, non-destructive, functional imaging and quantitative measurement of key metabolic processes in living organisms such as within and among microbial cells and microbial communities in terrestrial environments, and/or multicellular plant tissues. The instrumentation and devices to be developed for imaging biological systems will have high likelihood to enable an understanding of the spatial/temporal relationships, physical connections, and chemical exchanges that facilitate the flow of information and materials across membranes and between intracellular partitions. The primary interest for this solicitation is for new innovative, bioimaging devices with small footprints, which are fully capable of operation independently of heavy equipment and large instruments (e.g. neutron and light sources, cryoelectron microscopes, high resolution mass spectrometers), and can be easily deployed in public and private sector to make them accessible to the larger scientific community.

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

Questions – Contact: Prem Srivastava, [Prem.Srivastava@science.doe.gov](mailto:Prem.Srivastava@science.doe.gov)

### b. Other

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

Questions – Contact: Prem Srivastava, [Prem.Srivastava@science.doe.gov](mailto:Prem.Srivastava@science.doe.gov)

### References:

1. U.S. Department of Energy, Office of Biological and Environmental Research, 2016, Mesoscale to Molecules: Bioimaging Science (Technology) Program 2016, Principle Investigator Meeting

Proceedings, p. 24. [https://science.energy.gov/~media/ber/pdf/community-resources/2016\\_Bioimaging\\_Technologies\\_PI\\_Meeting.pdf](https://science.energy.gov/~media/ber/pdf/community-resources/2016_Bioimaging_Technologies_PI_Meeting.pdf) (June 2018)

2. U.S. Department of Energy, Office of Biological and Environmental Research, 2015, New Bioimaging Technologies for Plant and Microbial Systems, Science.Energy.Gov p, 16. [https://science.energy.gov/~media/ber/pdf/community-resources/bioimaging\\_technologies.pdf](https://science.energy.gov/~media/ber/pdf/community-resources/bioimaging_technologies.pdf) (June 2018)
3. U.S. Department of Energy, Office of Biological and Environmental Research, 2014, Financial Assistance Funding Opportunity Announcement, Novel In Situ Imaging and Measurement Technologies For Biological Systems Science, p. 53. [http://science.energy.gov/~media/grants/pdf/foas/2014/SC\\_FOA\\_0001192.pdf](http://science.energy.gov/~media/grants/pdf/foas/2014/SC_FOA_0001192.pdf) (June 2018)

## 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 Nuclear Physics (NP) Program is to develop and support the scientists, techniques, and facilities that are needed for basic nuclear physics research and isotope development and production. 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. NP is constructing a future Facility for Rare Isotope Beams (FRIB) at Michigan State University. The NP community is also developing a proposed electron ion collider (EIC).

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

Our ability to continue making a scientific impact on the general community relies heavily on the availability of cutting edge technology and advances in detector instrumentation, electronics, software, accelerator design, and isotope production. 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](#).

## 28. NUCLEAR PHYSICS SOFTWARE AND DATA MANAGEMENT

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Large scale data storage and processing systems are needed to store, access, retrieve, distribute, and process data from nuclear physics experiments conducted at large facilities, such as Brookhaven National Laboratory's 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), currently under construction, will require considerable speed and flexibility in collecting data from its detectors. 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 data sets of size 1 to 10 Petabytes (PB). A single experiment can produce data sets of many 100s of Terabytes (TB) which are then distributed to institutions worldwide for analysis, and with the increasing data generation rates at RHIC and TJNAF, multi-PB datasets will soon be common. Research on the management of such large data sets, and on high speed, distributed data acquisition will be required to support these large scale nuclear physics experiments.

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

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

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

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

Grant applications are sought only in the following subtopics:

**a. Tools for Large Scale Distributed Data Storage**

A trend in nuclear physics is to maximize the availability 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 as local computing resources, university based clusters, major DOE funded computing resources, and commercial cloud offerings.

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

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, [Michelle.Shinn@science.doe.gov](mailto:Michelle.Shinn@science.doe.gov) or the NP SBIR/STTR Topic Associate for Software and Data Management: Frank E (Ted) Barnes, [Ted.Barnes@science.doe.gov](mailto:Ted.Barnes@science.doe.gov).

**b. Software-Driven Network Architectures for Data Acquisition**

The building blocks of an important subset of experimental data acquisition systems are flash digitizers and integrating digitizers of analog signals measuring time, pulse height, and electric charge of the particles entering the detectors. These digitizers convert detector signals into a digital form in real time. The total charge, the number of coincident elements, and other information are used to determine whether an interesting scattering event has occurred. In many current data acquisition systems, this information is hardwired in high-speed logic. The end result is a trigger signal used to start readout of the digitizers. If justified by the trigger, the digitizer data are assembled into a time-correlated event for later analysis, a process called event building. At present, the elements of these systems are typically connected by buses (e.g., VME, cPCI), custom interconnects, or serial connections (USB) with networks used for higher level aggregation.

Future experiments anticipate rates of tens to hundreds of thousands of events per second. Each event will contain hundreds to millions of bytes of data from the digitizers. The large latencies possible in highly buffered flash ADC architectures can be used to advantage in the design of a data acquisition architecture. This will have digitizers or digitizer systems connected by commercial network fabrics, moving data to general purpose processors for software “trigger” determination and event building. The hardware architecture is simplified, composed of digitizers, networks and fast general purpose processors. What used to be a largely hardwired logic system is now a software-driven system. The fundamental requirement for success of this system is that the data from each detector element be labeled with a precisely synchronized time and location before transmission on the network.

An interesting possibility regarding the next generation of data acquisition systems is that they may ultimately be composed of separate ADCs for each detector element, connected by commercial network or serial technology. This software-driven architecture must integrate efficiently with available network bandwidth and latencies. Desirable features of this architecture are (1) synchronize clock phase across all channels to nanosecond or sub-nanosecond precision, (2) synchronize time stamps across all channels to 10 ns precision or better, (3) possibly determine a global trigger from information transmitted by a subset of individual digitizer elements with minimal latency, and then notify the digitizer elements of a successful trigger, in order to apply a fast filter on the data before transmission; (4) collect event data from the individual elements to be assembled into events; and (5) develop software tools to monitor and validate the synchronization, triggering, and event building during normal operation. Time synchronization is critical to the success of this architecture, as is the concurrent validation of synchronization. This architecture and its implementation could form the basis of a standard for next-generation data acquisition in nuclear physics as it could be made available for integrating custom front end electronics, and could also be integrated with various ADC and TDC components to form complete commercial solutions. It should be inherently scalable, from small, test stands of a single computer with an appropriate network card, to large complex detector systems.

For NP experiments at these current and planned facilities there is an increasing need for real-time decision making processing such as error correction and recovery as well as real-time quality control. Data collection and device control would benefit greatly from scalable and versatile control systems. As the number of channels increases, current control systems based solely on EPICS cannot provide the truly distributed and scalable infrastructures needed. Advances are needed in the areas of integrating disparate systems at low software cost, as well as support for highly secured remote control rooms.

Applications are invited in the following areas; 1) the development of high performance streaming data acquisition and control systems, with: (a) protocols and data formats to maximize throughput, decrease latencies, facilitate event building, improve efficiency of data retrieval from permanent storage, and facilitate real time monitoring of the detector performance; (2) trigger decision systems that may be fully software based or have hardware assists (e.g. FPGA accelerators); (3) data flow systems that are capable of responding to trigger accepts by reading data from the digitizers and making it available to interested clients; (4) free running data flow systems into which time stamps are injected for later data correlation; (5) scalable event builders that accept data from the data flow system and produce events for online analysis and, if rate permits, logging; (6) protocols and middle-ware that can tie this system together and provide relatively high level interfaces to user software; and 7) soft core FPGA module(s) to implement the network protocol for 10g and 100g Ethernet and/or 40g and 100g Infiniband (and possible future generations), with sufficient buffering to support data aggregation using a commercial network switch.

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, [Michelle.Shinn@science.doe.gov](mailto:Michelle.Shinn@science.doe.gov) or the NP SBIR/STTR Topic Associate for Software and Data Management: Frank E (Ted) Barnes, [Ted.Barnes@science.doe.gov](mailto:Ted.Barnes@science.doe.gov).

### c. **Data Science / Distributed Computing Applications**

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 in an ad-hoc way by the experimentalists themselves. Recently, the data science community has developed tools and techniques for handling such tasks at scale in an efficient and more generic manner. These tools are generally open-source and can be deployed on inexpensive, distributed computing resources provided by commercial web services firms that are both inexpensive and scalable on demand. 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.

Adaption of these new technologies to the analysis of nuclear physics data requires the development of domain specific tools. Specifically, we seek applications for (1) the development of high-throughput, low-latency methods to parse and securely transfer binary experimental data to commercial cloud services (e.g., AWS, Google Cloud), (2) distributed data analysis for experimental physics applications implemented using data processing systems such as Apache Spark for local or cloud use, (3) the application of machine-learning techniques with standard libraries (Google TensorFlow, Theano, scikit-) to automate analysis tasks and provide intelligent diagnostics, and (4) the creation of lightweight packages, leveraging libraries in modern, widely-adopted analysis environments to facilitate common physics analysis methodologies. Applicants are expected to address a specific application domain in experimental nuclear physics data analysis. Proposals should address performance and plan to demonstrate feasibility with working prototypes.

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, [Michelle.Shinn@science.doe.gov](mailto:Michelle.Shinn@science.doe.gov) or the NP SBIR/STTR Topic Associate for Software and Data Management: Frank E (Ted) Barnes, [Ted.Barnes@science.doe.gov](mailto:Ted.Barnes@science.doe.gov).

### d. **Heterogeneous Concurrent Computing**

Computationally demanding theory calculations as well as detector simulations and data analysis tasks can be significantly accelerated through the use of general purpose Graphics Processing Units (GPUs). The ability to exploit these graphics accelerators has been significantly constrained by the effort required to port the software to the GPU environment. Much more capable cross compilation or source-to-source translation tools are needed that are able to convert conventional as well as very complicated templated 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. Existing analysis codes do not sufficiently reveal the concurrency necessary to exploit the high performance of the architectures in these systems (both GPU and Xeon Phi). 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 HPCs and LCFs for the applications and data-intensive workflows characteristic of experimental NP.

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, [Michelle.Shinn@science.doe.gov](mailto:Michelle.Shinn@science.doe.gov) or the NP SBIR/STTR Topic Associate for Software and Data Management: Frank E (Ted) Barnes, [Ted.Barnes@science.doe.gov](mailto:Ted.Barnes@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 general description at the beginning of this topic.

Questions – Contact: Michelle Shinn, [Michelle.Shinn@science.doe.gov](mailto:Michelle.Shinn@science.doe.gov) or the NP SBIR/STTR Topic Associate for Software and Data Management: Frank E (Ted) Barnes, [Ted.Barnes@science.doe.gov](mailto:Ted.Barnes@science.doe.gov)

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## 29. NUCLEAR PHYSICS ELECTRONICS DESIGN AND FABRICATION

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

The DOE Office of Nuclear Physics (NP) seeks new developments in detector instrumentation electronics with significantly improved energy, position, timing resolution, sensitivity, rate capability, stability, dynamic range, and background suppression. Of particular interest are innovative readout electronics for use with the nuclear physics (NP) detectors described in Topic 31 (Nuclear Instrumentation, Detection Systems and Techniques). An important criterion is the cost per channel of electronic devices and modules.

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

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

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

Grant applications are sought only in the following subtopics:

**a. Advances in Digital Processing Electronics**

Digital signal processing electronics are needed to replace analog signal processing, following low noise amplification and anti-aliasing filtering, in nuclear physics applications. Grant applications are sought to develop high speed digital processing electronics that, relative to current state of the art, improve the accuracy in determining the position of interaction points of particles or photons to smaller than the size of the detector segments. Emphasis should be on digital technologies with low power dissipation.

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, [Michelle.Shinn@science.doe.gov](mailto:Michelle.Shinn@science.doe.gov) or the NP SBIR/STTR Topic Associate(s) for Electronics and Circuits: Manouchehr Farkhondeh, [Manouchehr.Farkhondeh@science.doe.gov](mailto: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 detectors (e.g., silicon pixel and strip detectors

including drift versions, silicon photomultipliers (SiPMs), germanium detectors, and gas detectors) used in nuclear physics experiments. Areas of specific interest include (1) very low-noise amplifiers and filters, very high precision amplitude and timing measurement circuits, analog-to-digital and time-to-digital converters; (2) front-end ASICs for solid-state highly pixelated detectors; (3) integrated circuits for very high dynamic range; (4) integrated circuits for very high timing resolution, and (5) large front-end ASICs in the form of systems-on-chip (SoC) characterized by extensive programmability and functionality, digital signal processing capability, and standard digital interfaces and protocols for compatibility with commercial devices. Relative to the state of the art these circuits should be low-power, 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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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### c. Next Generation Pixel Sensors

Active Pixel Sensors (APS) in CMOS (complementary metal-oxide semiconductor) technology have largely replaced Charge Coupled Devices 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 contains 356 million (21x21x50  $\mu\text{m}$ ) APS pixels. Future proposed high luminosity colliders such as the Electron Ion Collider (EIC) plan to operate at luminosities in the range  $10^{33}$ – $10^{35}$   $\text{cm}^{-2} \text{s}^{-1}$  and will require radiation hard tracking devices placed at radii below 10 cm. Therefore, cost effective alternatives to the present generation high density APS devices will be required. An ambitious goal is to develop extremely thin  $\sim 0.1\%$  radiation length detector modules capable of high rate readout. In low energy nuclear physics applications, the bulk silicon substrate is high-resistivity and is depleted and used as the active volume. 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 also are 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; novel 2D- 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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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**d. Manufacturing and Advanced Interconnection Techniques**

Grant applications are sought to develop (1) manufacturing techniques for large, thin, multiple-layer printed circuit boards (PCBs) with plated-through holes, dimensions from 2m x 2m to 5m x 5m, and thicknesses from 100 to 200 microns (these PCBs would be used in cathode pad chambers, cathode strip chambers, time projection chamber cathode boards, etc.); and (2) techniques to add plated-through holes, in a reliable, robust way, to large rolls of metallized mylar or kapton (which would have applications in detectors such as time expansion chambers or large cathode strip chambers).

In addition, many next-generation detectors will have highly segmented electrode geometries covering areas up to several square meters. Conventional packaging and assembly technology cannot be used with these large areas. Grant applications are sought to develop (1) advanced microchip module interconnect technologies that address the issues of high-density area-array connections – including modularity, reliability, repair/rework, and electrical parasitics; (2) technology for aggregating and transporting the signals (analog and digital) generated by the front-end electronics, and for distributing and conditioning power and common signals (clock, reset, etc.); (3) low-cost methods for efficient cooling of on-detector electronics; and (4) low-cost and low-mass methods for grounding and shielding.

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

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

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**e. Other**

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

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### 30. NUCLEAR PHYSICS ACCELERATOR TECHNOLOGY

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
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 under construction at Michigan State University, and technologies relevant to the development of a future [Electron Ion Collider](#) (EIC), under consideration for the next major facility after the completion of FRIB. A major focus in all of the above areas is superconducting radio frequency (SRF) accelerators, superconducting magnets, and related technologies. Relevance to nuclear physics must be explicitly described, as discussed in more detail below.

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

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

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

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

Grant applications are sought only in the following subtopics:

**a. Materials and Components for Radio Frequency Devices**

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

- 1) peripheral components for both room temperature and superconducting structures, such as low particulate ultra-high vacuum seals, terminations, and high beam current, low-impedance bellows;
- 2) SRF cavity joining techniques that create vacuum seals without resorting to the use of bolted flanges in order to minimize particulates;
- 3) cleaning techniques for removal of  $> 0.01 \mu\text{m}$  particulates in diameter from superconducting cavities which can replace or compliment high-pressure water rinsing (e.g., methods for cleaning whole cryomodules, alternative techniques to dry ice and high pressure water cleaning);
- 4) alternative cavity fabrication techniques to produce seamless SRF cavities of various geometries (e.g., elliptical, quarter, half wave resonators and crab cavities) , including utilizing high strain rates using novel techniques including electrohydraulic forming to improve material formability as compared to standard deep drawing. The resulting SRF accelerating structures should achieve  $Q_0 > 1 \times 10^{10}$  at 2.0 K at an  $E_{acc} \sim 20 \text{ MV/m}$ , or equivalently,  $R_s < 5 \text{ n}\Omega$  and  $E_{peak} > 60 \text{ MV/m}$ , with correspondingly lower  $Q$ 's at higher temperatures such as 4.5 K;

- 5) adding high quality layers of copper or other high conductivity materials to the outside of SRF cavities for thermal and mechanical stabilization or conduction cooling without degradation of the superconducting properties of the cavity; and
- 6) metal forming techniques, including the use of bimetallic materials, with the potential for significant cost reductions by simplifying 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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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#### **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 field control of ion acceleration structures ( $0.1^\circ$  or less of phase and 0.1% amplitude RMS jitter) and electron acceleration structures ( $0.1^\circ$  of phase and 0.01% amplitude RMS jitter) in the presence of 10-100 Hz variations of the structures' resonant frequencies (0.1-1.5 GHz);
- 2) passive or active methods for damping microphonic modes of cavities installed in cryomodules or reducing coupling between such modes and external vibration sources;
- 3) development of tunable (with respect to the center frequency of up to  $10^{-4}$ ) superconducting RF cavities for acceleration and/or storage of relativistic heavy ions;
- 4) development of alternative efficient accelerating structures for low energy CW ion beams as an alternative to conventional radio frequency quadrupole structures, and
- 5) 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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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#### **c. Particle Beam Sources and Techniques**

Grant applications are sought to develop

- 1) methods and/or devices for improving emission capabilities of photocathode sources 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 which are capable to generate high-intensity, high-brightness, high charge state heavy ion beams, for example:  $\sim 12 \mu\text{A}$  of uranium beam at charge state  $q=40$  with an rms emittance of  $0.1\pi$  mm-mrad; and

- 3) novel methods for in situ high-density surface cleaning (scrubbing) of ultrahigh vacuum long (~ 100 m or longer) narrow tubes to reduce secondary electron yield and outgassing.

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

- 1) novel beam transport methodologies for transporting, merging, injecting, extracting and manipulating magnetized electron beams for hadron beam cooling with minimal emittance growth and degradation of magnetization; and
- 2) component studies and development for introducing an ion clearing gap in the pulse structure of the injector to alleviate the trapping of ions in high current ERLs. A typical profile would be 100 ns gaps at a 1 MHz repetition rate. This must be imposed on an injected beam current of more than 100 mA. Technologies that create such a time structure must do so without disturbing the beam quality of the pulses that are injected to the linac or creating substantial halo, which must remain  $< 10^{-5}$  of the beam current.

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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#### **d. Polarized Beam Sources and Polarimeters**

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

- 1) CW polarized electron sources and/or associated components delivering beams of ~50 mA for at least 24 hours, with longitudinal polarization greater than 90%; and a photocathode quantum efficiency  $> 10\%$  at ~780 nm. At lower ( $\leq 1$  mA) beam currents, the specifications for polarization and quantum efficiency are the same as listed above but should be capable of delivering high bunch charges  $> 5$  nC/bunch for EIC based storage rings. (Note: applications proposing the use of diamond amplifiers and variants will be considered nonresponsive.);
- 2) advanced software and hardware to facilitate the manipulation and optimized control of the spin of polarized beams; and
- 3) absolute polarimeters for spin polarized  $^3\text{He}$  beams with energies up to 160 GeV/nucleon

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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#### **e. Rare Isotope Beam Production Technology**

Grant applications are sought to develop

- 1) development of bearings that are radiation resistant, high vacuum compatible, and operate at temperatures of ~500° C and at rotational speeds of 5000 rpm for high-power target applications; and

- 2) Development of efficient time-of-flight separation techniques for high energy (>120 MeV/u) secondary beams.

(Additional needs for high-radiation applications can be found in subtopic e “Technology for High Radiation Environments” of Topic 31, 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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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#### **f. Accelerator Control and Diagnostics**

As accelerator facilities advance in their capabilities, it is important that diagnostics and controls keep pace. Grant applications are sought to develop advanced beam diagnostics for concepts and devices that provide high speed computer-compatible measurement, 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  $\mu$ A, with very high precision ( $<10^{-4}$ ) and short integration times;
- 2) non-destructive beam diagnostics for stored proton/ion beams, and/or for 100 mA class electron beams;
- 3) devices/systems that measure the emittance of intense (>100 kW) CW ion beams;
- 4) beam halo monitor systems for ion beams; and
- 5) electron cloud effect diagnostics and suppression.

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  $\sim 5\%$  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  $\mu$ s) 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 (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 such advanced methods as fast feedforward, neural networks or other expert systems, and advanced optimization techniques such as genetic algorithms and simulated annealing; 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 NP facilities.

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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

A full utilization of the discovery potential of a next-generation EIC will require a full-acceptance system that can provide detection of reaction products scattered at small angles with respect to the incident beams over a wide momentum range. Grant applications are sought for design, modeling and hardware development of the special magnets for such a detection system. Magnets of interest include

- 1) radiation-resistant large aperture ( $\geq 20$  cm) superconducting dipole ( $\geq 2$  T pole-tip field) with a field-exclusion region of about 3 cm in radius along the dipole bore;
- 2) cost-effective materials and manufacturing techniques for these magnets; and
- 3) high-efficiency cooling methods and cryogenic systems; power supplies and other related hardware for the magnets described above. More details are provided in the Report of the Community Review of EIC Accelerator R&D for the Office of Nuclear Physics. A link to the report is provided in the References.

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, [Michelle.Shinn@science.doe.gov](mailto: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.

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### 31. NUCLEAR PHYSICS INSTRUMENTATION, DETECTION SYSTEMS AND TECHNIQUES

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
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 will be needed for the 12 GeV Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF), at the future Facility for Rare Isotope Beams (FRIB) under construction at Michigan State University, at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Lab, at the Argonne Tandem Linac Accelerator System (ATLAS) at Argonne National Laboratory, and at a proposed future Electron-Ion Collider (EIC). Also of interest is technology related to future experiments in fundamental symmetries, such as neutrinoless double-beta decay (NLDBD) experiments and the measurement of the electric dipole moment of the neutron (nEDM). In the case of NLDBD experiments, extremely low background and low count rate particle detection are essential.

All grant applications must explicitly show relevance to the DOE NP Program. Grant applications must be informed by the state of the art in nuclear physics applications, commercially available products and emerging technologies. A proposal based on merely incremental improvements or little innovation will be considered

non-responsive unless context is supplied that convincingly shows its potential for significant impact or value to the DOE NP Program.

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

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

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

Grant applications are sought in the following subtopics:

**a. Advances in Detector and Spectrometer Technology**

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

- 1) Particle identification and counting detectors such as:
  - Low cost large area Multi-channel Plate (MCP) type detector with high spatial resolution, high rate capability, radiation tolerance, magnetic field tolerance, and timing resolution of < 10 ps for time-of-flight detectors. The accompanying readout system (i.e. electronics, application-specific integrated circuit, etc.) should be compatible with the above requirements;
  - Large area Multigap Resistive Plate Chamber (MRPC) detectors with very high rate capability, radiation and magnetic field tolerance and high timing resolution (<20-30 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;
  - Cherenkov detectors (Threshold, Ring-Imaging (RICH), Detection of Internally Reflected Cherenkov Light (DIRC), Aerogel-type) 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;
- 2) Machine learning techniques to enhance particle identification such as:
- Particle Flow algorithms to enhance hadron calorimetry;
  - Pattern recognition in Ring-Imaging and DIRC detectors;
  - Shower shape recognition to enhance electromagnetic calorimetry;

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, [Michelle.Shinn@science.doe.gov](mailto:Michelle.Shinn@science.doe.gov) or the NP SBIR/STTR Topic Associate(s) for Instrumentation, Detection Systems and Technique: Elizabeth Bartosz, [Elizabeth.Bartosz@science.doe.gov](mailto: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 high energy resolution for low-energy applications, high precision tracking of different types of particles, and fast triggering capabilities.

Grant applications are also sought to develop detector systems for rare isotope beams with focus on: Next generation, heavy ion focal plane detectors or detector systems for magnetic spectrometers and recoil separators with high time resolution ( $< 200\text{ps}$  FWHM), high energy loss resolution (1-2%), and high total energy resolution (1-2%), including associated readout electronic and data acquisition systems.

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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#### **c. Technology for Rare Decay and Rare Particle Detection**

Grant applications are sought for detectors and techniques to measure very weak or rare event signals. Such detector technologies and analysis techniques are required in searches for rare events such as NLDBD and searches for new nuclear isotopes produced at radioactive-beam and high intensity stable beam facilities. Rare decay and rare event detectors require large quantities of ultra-clean materials for shielding and targets.

Grant applications are sought to develop:

- 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, signal and high voltage interconnects, vacuum

feedthroughs, front-end amplifier FET assemblies and front-end ASICs; radiopurity goals are as low as 1 micro-Becquerel per kg);

- 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 detectors;
- Methods by which the background events in rare event searches, such as those induced by gamma rays or neutrons, can be tagged, reduced, or removed entirely;
- Particle 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 are eligible;
- Novel detector concepts (optical Parallel Plate Avalanche Counters (PPACs) for example) for charged particle tracking, capable of submillimeter position resolution (a few hundred micrometers), high counting rate capability (> 1 MHz), uniform energy-losses independent of the position, high dynamic range and low thickness (< a few mg/cm<sup>2</sup>); and
- New charged particle detectors for particle identification based energy loss measurement, with energy resolution (< a few % at 1 MeV), uniform response to a wide variety of heavy-ions (from <sup>1</sup>H to <sup>235</sup>U), and with high rate capability (> 1 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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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

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

Grant applications are sought to develop:

- New high density scintillating crystals with high light output and fast decay times;
- High light output plastic scintillating and wavelength-shifting fibers;
- Scintillators materials that can be used for n/gamma discrimination over large areas using timing and pulse shape information or other method; and
- Large area, high optical quality Cherenkov materials (e.g., Aerogel).

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. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

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**e. Technology for High Radiation Environments**

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

Improved models of radiation transport in beam production systems: The use of energetic and high-power heavy ion beams at future research facilities will create significant radiation fields. Radiation transport studies are needed to design and operate facilities efficiently and safely. Advances in radiation transport codes are in particular desired for) the inclusion of charge state distributions of initial and produced ions including distribution changes when passing through the material and magnetic fields.

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**f. Other**

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

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### 32. NUCLEAR PHYSICS ISOTOPE SCIENCE AND TECHNOLOGY

Maximum Phase I Award Amount: \$150,000	Maximum Phase II Award Amount: \$1,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Stable and radioactive isotopes are critical to serve the broad needs of modern society and conduct research in medicine, chemistry, physics, energy, environmental sciences, material sciences, and for a variety of applications in industry and national security. A primary goal of the Department of Energy’s Isotope Development and Production for Research and Applications Program (DOE IP) within the Office of Nuclear Physics (NP) is to support research and development of methods and technologies which make available isotopes that fall within the Isotope Program portfolio. The DOE IP produces isotopes that are in short supply in the U.S. for which insufficient domestic production capabilities exist. Exceptions include some special nuclear materials and molybdenum-99, for which the National Nuclear Security Administration has responsibility. The benefit of a research and development program includes an increased portfolio of isotope products, more cost-effective and efficient production/processing technologies, a more reliable supply of isotopes, and reduced dependence on foreign supplies.

All entities submitting proposals to the SBIR/STTR Isotope Science and Technology topic must recognize the moral and legal obligations to comply with export controls and policies that relate to the transfer of knowledge that has relevance to the production of special nuclear materials (SNM). All parties are responsible for U.S. Export Control Laws and Regulations, which include but may not be limited to regulations within the Department of Commerce, the Nuclear Regulatory Commission and the Department of Energy.

The subtopics below refer to innovations that will advance our nation’s capability to produce isotopes and increase isotope availability. Applicants are encouraged 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.

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

Grant applications are sought in the following subtopics:

**a. Novel or Improved Isotope Production Techniques**

Research should focus on the development of advanced, cost-effective, and efficient technologies for producing isotopes that are in short supply and are needed by the research or applied usage communities (e.g. nuclear medicine). Successful proposals should lead to breakthroughs that will facilitate an increased domestic supply of isotopes.

In the medical community, production of radionuclides capable of functioning as diagnostic/therapeutic (theranostic) pairs or single isotopes combining both traits (e.g.,  $^{64}\text{Cu}/^{67}\text{Cu}$ ,  $^{44}\text{Sc}/^{47}\text{Sc}$ , or  $^{186}\text{Re}$ ) are of particular interest, as are novel or in-demand radionuclides with radioactive emissions of high linear energy transfer (LET) such as alpha-particle emitters and Auger electron emitters (useful for their potential for high toxicity to diseased cells while sparing nearby healthy tissue from damage). The stable isotope  $^3\text{He}$  is used for cryogenics, homeland security, and medical applications. Proposals are sought for efforts leading to terrestrial production of  $^3\text{He}$ . Potential methodologies might include natural gas, reactors, or other means of production not listed. Additional guidance for research isotope priorities is provided in the Nuclear Science Advisory Committee Isotopes (NSACI) report published in 2015 ([http://science.energy.gov/~media/np/nsac/pdf/docs/2015/2015\\_NSACI\\_Report\\_to\\_NSAC\\_Final.pdf](http://science.energy.gov/~media/np/nsac/pdf/docs/2015/2015_NSACI_Report_to_NSAC_Final.pdf)).

The development of high quality, robust isotope production targets is required to utilize the higher-current and power-densities available from commercially available accelerators; of particular concern is improved methodologies for the design and fabrication of encapsulated salt and liquid metal targets, especially those composed of reactive materials. These targets could be subjected to proton beams with energies up to  $\sim 70$  MeV with intensities of between 100  $\mu\text{A}$  and 1 mA for extended periods of time. This includes breakthroughs in in-situ target diagnostics, novel self-healing materials with extreme radiation resistance for accelerator target material containment or encapsulation, advanced target fabrication approaches, and innovative approaches to model and predict target behavior undergoing irradiation in order to optimize yield and minimize target failures during isotope production. Improved thermal and mechanical modeling capabilities that include target material phase change and variable material density are also of interest to inform the design of targets exhibiting high tolerance to extreme radiation and thermal environments. Development of technologies advancing production and handling of irradiated target materials is encouraged. In addition, new approaches to in-hot cell target fabrication technologies to facilitate the recycling of enriched target materials used in production of high purity radioisotopes are also sought.

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 DOE IP application. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, [Michelle.Shinn@science.doe.gov](mailto:Michelle.Shinn@science.doe.gov) or the NP SBIR/STTR Topic Associate for Isotope Science and Technology: Ethan Balkin, [Ethan.Balkin@science.doe.gov](mailto:Ethan.Balkin@science.doe.gov).

**b. Improved Radiochemical Separation Methods for Preparing High-Purity Radioisotopes**

Separation from contaminants and bulk material and purification to customer specifications are critical processes in the production cycle of a radioisotope. Many production strategies and techniques presently used rely on old technologies and/or require a large, skilled workforce to operate specialized equipment, such as manipulators for remote handling in hot cell environments. Conventional methods may include liquid-liquid extraction, column chromatography, electrochemistry, distillation, or precipitation and are used to separate radioactive and non-radioactive trace metals from target materials, such as lanthanides, alkaline and alkaline earth metals, halogens, or organic materials. High-purity isotope products are essential for high-yield protein radiolabeling for radiopharmaceutical use, or to replace materials with undesirable radioactive emissions. Improved product specifications and reduced production costs can be achieved through improvements in separation methods. Of particular interest are developments that automate routine separation processes resulting in reduced operator labor hours and worker radiation dose, and the development of automation or robotics to handle and process large mass, highly radioactive, thick targets typically used in high energy and photo-transmutation accelerator-based production. Applications include radiation hardened semi-automated modules for separations or radiation hardened automated systems for elution, radiolabeling, purification, and dispensing. Such automated assemblies should be easily adaptable to different processes and different hot cell configurations, and should consider ease of compliance with current good manufacturing practices (cGMP) for clinically relevant radionuclides.

Proposals are also sought for innovative developments and advances in separation technologies to improve separation efficiencies, to minimize waste streams, and to develop advanced materials for high-purity radiochemical separations. In particular, breakthroughs are sought in lanthanide and actinide separations. Improvements are encouraged, in (1) the development of higher binding capacity and selectivity of resins and adsorbents for radioisotope separations to decrease void volume and to increase activity concentrations, (2) the scale-up of separation methods demonstrated on a small scale to large-capacity production levels, and (3) new resin and adsorbent materials with increased resistance to radiation. Proposals are also sought for novel processes that remove and capture residual tritium from U.S. Government (USG)-owned heavy water. After purification, the residual tritium levels in the heavy water must be below the EPA limit of 2  $\mu\text{Ci/Kg}$ .

With respect to radiochemistry, innovative methods are sought to: a) improve radiochemical separations of or approaches aimed at lower-cost production of high-purity alpha-emitting radionuclides such as  $^{211}\text{At}$ ,  $^{225}\text{Ra}$ ,  $^{225}\text{Ac}$ , and  $^{227}\text{Ac}$  from contaminant metals, including thorium, radium, lead, lanthanides, and/or bismuth; b) improve materials needed for generating  $^{212}\text{Pb}$  from  $^{224}\text{Ra}$ ,  $^{213}\text{Bi}$  from  $^{225}\text{Ac}$  and/or  $^{225}\text{Ra}$ , and  $^{44}\text{Ti}/^{44}\text{Sc}$ ; or c) the development and production of matched pair imaging radionuclides for the corresponding therapeutic alpha-particle emitters to accurately determine patient specific dosimetry and improve treatment efficacy and safety. The new technologies must be applicable in extreme radiation fields that are characteristic of chemical processing involving high levels of alpha- and/or beta-/gamma-emitting radionuclides. An example would be the development of compact mass separation technologies (to separate radioactive isotopes of the same element) that are applicable to in-hot cell environments.

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 DOE IP application. Applications not meeting this requirement will be considered nonresponsive and will not undergo merit review.

Questions – Contact: Michelle Shinn, [Michelle.Shinn@science.doe.gov](mailto:Michelle.Shinn@science.doe.gov) or the NP SBIR/STTR Topic Associate for Isotope Science and Technology: Ethan Balkin, [Ethan.Balkin@science.doe.gov](mailto:Ethan.Balkin@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.

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