U.S. Department of Energy

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

Topics

FY 2018

Phase I

Release 1

Version 4, October 16, 2017

Participating DOE Research Programs

- 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 17, 2017
Funding Opportunity Announcement Issued:	Monday, October 16, 2017
Letter of Intent Due Date:	Monday, October 30, 2017
Application Due Date:	Monday, December 4, 2017
Award Notification Date:	Monday, February 26, 2018*
Start of Grant Budget Period:	Monday, April 9, 2018

*** Date Subject to Change**

Table of Changes		
Version	**Date**	**Change**
Ver. 1	July 17, 2017	Original
Ver. 2	July 25, 2017	• Schedule Added • Topic 1, subtopic c: Additional Point of Contact • Topic 17, subtopic b: Modification to Title • Topic 22, subtopics b and c: Additional Point of Contact • Topic 23: Addition of subtopic d "Other" • Topic 24: Addition of subtopic b "Other"and Correction made to Reference 2 • Topic 25: Addition of subtopic b "Other"
Ver. 3	Sept. 27, 2017	Topic 26, subtopic d has been removed
Ver. 4	Oct. 16, 2017	• Schedule Dates Updated • Topic 23: Description Revised • Topic 23, subtopic a: Description Revised • Topic 23, subtopic b: Description Revised • Topic 23, subtopic c: Description Revised • Topic 23, References: Reference #1: Link Updated

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INTRODUCTION TO DOE SBIR/STTR TOPICS

This SBIR/STTR topics document is issued in advance of the FY 2018 DOE SBIR/STTR Phase I Release 1 Funding Opportunity Announcement scheduled to be issued in on August 14, 2017. 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 Technology Transfer Opportunity?
A Technology Transfer Opportunity (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.

With 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.

DOE GRANT APPLICATION PREPARATION SUPPORT – PHASE O ASSISTANCE PROGRAM

To increase the number of high-quality SBIR/STTR Phase I applications submitted to the DOE by women-owned and minority-owned small businesses, and small businesses from DOE's underrepresented states (see eligible state list below), the DOE provides a variety of application preparation and other related services, free of charge.

Phase 0 services are offered on a first-come, first-serve basis to eligible applicants. For more information on the DOE SBIR/STTR Phase 0 Assistance Program and to determine eligibility, please visit http://www.dawnbreaker.com/doephase0/.

The following states are underrepresented in the DOE SBIR/STTR programs: AK, DC, GA, HI, IA, ID, IN, KS, LA, ME, MN, MS, MT, NC, ND, NE, NY, OK, PA, PR, RI, SC, SD, WA, WI.

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. The topic below is a collaborative topic among multiple programs in the Office of Science.

1. BIGDATA TECHNOLOGIES FOR SCIENCE, ENGINEERING, AND MANUFACTURING

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

The offices of Advanced Scientific Computing Research, Biological and Environmental Research, Basic Energy Sciences, and Nuclear Physics in the Office of Science at the US Department of Energy (DOE) are soliciting grant applications in the broad technical area of "BigData" - technologies for managing and analyzing complex scientific and engineering data sets. The challenge of managing and analyzing increasingly BigData streams is impacting every sector of modern society from energy, defense, healthcare, and transportation to science and engineering. Unlike traditional structured data sets, today's BigData are characterized by multi-dimensional features that include large data volumes, variety, velocity and veracity. Despite the ubiquitous BigData challenge 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 streams. The focus of this topic is on the development of commercializable BigData technology products and services that reduce bottlenecks and increase efficiency in the management and analysis of complex data for the science, engineering, and manufacturing sectors.

Potential grant applicants should focus on the development of innovative BigData management 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. Additional information on BigData products and services of interest to participating Office of Science programs is described below.

Office of Advanced Scientific Computing Research

a) Complex-Data Management Technologies

Office of Biological and Environment Research

b) Advanced Data Analytic Technologies for Systems Biology and Bioenergy

c) Technologies for Managing and Analyzing Complex Data for Watershed and Terrestrial Ecosystems

Office of Basic Energy Sciences

d) HDF5 Extensions for Data Streaming

e) Visualization, Data Management, and Workflow Tools for Experimental Data

Office of Nuclear Physics (See the following the Nuclear Physics section of this solicitation)

- Software-Driven Network Architectures for Data Acquisition
- Large Scale Data Storage
- Data Science / Distributed Computing Applications

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 one or more attributes of BigData, namely, large data volume, variety, velocity and veracity. Priority will be given to grant applications with complex data sources drawn from the domain sciences of the DOE programs participating in this solicitation. An application can cover crosscutting issues but it must be submitted to a specific participating Office of Science program. Failure to do so will result in automatic declination of the application without review. Grant applications that focus exclusively on the following topics will be considered out of scope and will not be reviewed: a) data analytics algorithms that are not packaged as complete commercial products or services with the relevant BigData, b) improvements or extensions of data analytics and open software source stacks that do not lead to commercializable products or services, and c) other restrictions as specified in the detailed description of each sub-topic.

Office of Advanced Scientific Computing Research

a. BigData Management Technologies

This sub-topic focuses on complex data management technologies that go beyond traditional relational database management systems. The efficient and cost-effective technologies to collect, manage, and analyze distributed BigData is a challenge to many organizations including the scientific community. Database management technologies based on traditional relational and hierarchical database systems are proving to be inadequate to deal with BigData complexities (volume, variety, veracity, and velocity), especially when applied to BigData systems in science and engineering. While the primary focus is on the development of tools and services to support complex scientific and engineering data, all sources of complex data are in-scope for this sub-topic. The focus of this sub-topic is on the development of cost- and time-effective commercial grade technologies in the following categories:

1. BigData management software-enabling technologies – these include but are not limited to the development of software tools, algorithms, and turnkey solutions for complex data management such as NOSQL/graph databases to deal with unstructured data in new ways; visualization and data processing tools for unstructured multi-dimensional data, robust tools to test, validate, and remove defects in large unstructured data sets; tools to manage and analyze hybrid structured and unstructured data; BigData security and privacy solutions; BigData as a service system; high-speed data hardware/software data encryption and reduction systems; and online management and analysis of streaming and text data from instruments or embedded systems
2. BigData Network-aware middleware technologies – this includes high-speed network and middleware technologies that enable the collection, archiving, and movement of massive amounts of data within datacenters, data cloud systems, and over Wide Area Networks (WANS). These may include but are not limited to hardware subsystems such high-performance data servers and data transfer nodes, high-speed storage area network (SAN) technologies; network-optimized data cloud services such as virtual storage technologies; and other distributed BigData solutions. Grant applications must ensure the following: a) that proposed work is based on concrete BigData owned by the company or readily accessible, and b) that the proposed work goes beyond traditional data management system technologies.

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

Office of Biological and Environmental Research (BER)

b. 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", often summarized as the four Vs: volume, velocity, veracity, and variability. 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.

Applications are invited to develop innovative 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. This SBIR sub-topic seeks analytic solutions for biological BigData: including advanced data analytics, simulation, predictive modelling, multiscale algorithms, data visualization, visual data analytics and optimization, and data fusion to enable integrated analysis and comparison of data from multiple modalities. Of particular interest is the development of innovative and cost- and time-effective commercial technologies in the form of turnkey cloud services, and value added services to existing products. Areas of interest include (but are not limited to):

- Improved computational tools for management of petabytes of scientific, observational and experimental data sets, with real-time integration of new results with historical findings.
- Methods for management of complex analysis workflows, reproducible data analysis that support provenance, standardized data, storage and interfaces.
- Methods for data hosting, archiving, indexing and registration.
- Methods for automated feature detection, dimensionality reduction, and interpretation.
- Improved methods for data handling, data transport, data compression, data management, data processing, knowledge representation, machine learning, and mixed mechanistic and statistical simulation.
- New computational methods that can extract features to map onto mathematical models for further analysis and simulation, visualization and exploration.

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

Office of Biological and Environmental Research (BER)

c. 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 ecosystem 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. Another important challenge is the development of tools, approaches and workflows to facilitate the management and analysis of complex model simulation outputs and to facilitate data assimilation and uncertainty quantification.

This sub-topic focuses on the development of innovative technologies in the fields of complex data and advanced data analytics including predictive modelling, multiscale algorithms, machine learning, data interpretation and reduction, intelligent systems, and novel visualization methods to enable the integrated analysis and comparison of environmental system science data from multiple modalities. Examples of relevant methods and tools include (but are not limited to):

- The development of approaches and tools that enable flexible model-data integration workflows, including full provenance to support reproducibility.
- Tools and techniques to automate the QA/QC process for watershed and terrestrial ecosystem data typical of ESS projects.
- Tools and approaches that leverage the latest developments in open-source visualization tools (e.g., through SciDAC and Exascale projects) to demonstrate in situ data analysis and parallel visualization for watershed and terrestrial ecosystems typical of ESS applications.
- Design and develop modular components of a data system that can create integrated views of the heterogeneous and disparate data typically found in watershed and terrestrial ecosystem applications, and prepare it for visualization, exploration, and simulation.
- Design and develop approaches and tools to enable scientists to work effectively with data that is stored in federated distributed systems.
- For high-fidelity simulations, develop tools and approaches to facilitate: in situ data analysis, storage and access of full or partial data sets, post-processing including compression, indexing, distribution, and the application of machine learning techniques within and across data sets.

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

Office of Basic Energy Sciences

d. HDF5 Extensions for Data Streaming

HDF5 is becoming the de-facto standard for storing science data at light source facilities for user data analysis. HDF5, besides being compatible virtually with any modern photon science data analysis tool, provides an efficient means to organize images with awareness of exascale node layout, e.g. the high bandwidth memory (HBM) capacity, node topology and burst buffer layout.

In order to effectively adopt HDF5 as a primary data format, light source facilities will need to be able to read files while writing to them, with the ability to consolidate the output of multiple writers into consistent virtual datasets. These features have been introduced recently in HDF5, but they impose unwanted constraints:

1. The Single Writer/Multiple Readers feature, known as SWMR, doesn't support variable length datatypes.
2. The HDF5 virtual dataset does not work for irregular output patterns common with data acquisition. (First, one must specify the view ahead of time, and second, it must be a regular pattern. Dropped or missing shots are expected in data acquisition and contribute to the irregular pattern that needs a consistent view.)
3. Currently the virtual dataset view must be specified when the file is created. To deal with the irregular patterns in the previous point, the description of the virtual dataset must become mutable while running.

Removing these constraints is critical for being able to write HDF5 files directly from the data acquisition system. For example, some light sources are currently saving data in a custom data format, which does provide these streaming capabilities, and later on they translate these files into HDF5 to provide easy access to various users and analysis tools. This translation step is a bottleneck for large data throughputs and is unsustainable. While these capabilities are critical for light sources, we believe they will benefit all experimental facilities which adopt HDF5.

Grant applications grants are sought to:

- Add support for variable length datatypes in the HDF5 SWMR.
- Add support for irregular output patterns in the HDF5 virtual data set.
- Add support for mutable description of the HDF5 virtual dataset.

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

Office of Basic Energy Sciences

e. Visualization, Data Management, and Workflow Tools for Experimental Data

When users collect data at synchrotron and neutron beamlines at BES Scientific User Facilities they need immediate analysis feedback to ensure that a measurement is functioning properly; more detailed analysis is later needed for interpretation of the experimental results, which again is needed on a short timeframe. A wealth of software is employed for this, matching the wide range of experimental techniques, and where the algorithms used within may themselves be research topics, with frequent software customization and updates. Improvements in x-ray and neutron detection are accelerating rates that these instruments produce data; this combined with new sources, will create instruments that produce data rates circa a petabyte/day. Analysis of these data will require a migration to use of high performance computing resources.

Tools that will be able to assist computational scientists implement improved approaches to data analysis are sought. This includes (a) new approaches for graphical visualization of large and very high dimensionality data sets; (b) methodologies that allow existing software, typically written in Python, to be easily ported to run on petascale clusters; (c) data management and workflow tools that enable automation and data discovery and re-use; and (d) on-demand scheduling mechanisms that allow beamlines to obtain rapid access to HPC systems, with minimal impact on long-running tasks.

Questions – Contact: Eliane Lessner, Eliane.Lessner@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 TECHNOLOGIES AND MIDDLEWARE SERVICES

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

Advanced digital network technologies and middleware services play a significant role in the way DOE scientists communicate with peers and collect/process data. Optical networks operating at rates of more than 100 Gbps support the transfer of petabytes of data per day. These networks also peer with commercial networks allowing scientists remote access to instruments and facilities while also allowing citizens access to

the data and knowledge that has been produced. Improvements in the tools and services used to manage and operate this infrastructure are needed to meet the needs of both network operators and users.

Advances in access link technologies for commercial networks are driving consumer network speeds. 100+ Mbps links are now common in many parts of the U.S. and Gigabit/sec links are now being advertised. While these developments offer physical connectivity at high rates, translating these rates into routine application performance remains a significant challenge. Key among these challenges is providing individuals and small businesses tools and services that can accurately and easily report performance problems to both the consumers and ISP operations staff.

This topic solicits proposals that address issues related to developing tools and services that generate, collection, and store network operations data in a manner suitable for network engineers or application users and the hardening of middleware tools and services that deal with analyzing this data.

a. Network Analysis Tools and Services

Network operations staff collect 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, IDS systems and other security appliances also generate data that impacts 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 tools may operate in real-time, accepting data from links operating at 100 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 are out-of-scope for this subtopic.

Questions – Contact: Richard Carlson, richard.carlson@science.doe.gov

b. Operations Focused Data Tools and Services

Network operations staff currently collect data from a wide variety of network devices (i.e., hosts, routers, switches, middleboxes). Common types of data 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 to develop analysis tools or services that use this data are out-of-scope for this subtopic.

Questions – Contact: Richard Carlson, richard.carlson@science.doe.gov

c. User Focused Data 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 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 assist in reporting when and where these performance problems exist (i.e., carrier backbone, provider access link, home Wi-Fi LAN, inside the server or client host).

Grant applications are sought to develop data collection, 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 and contains 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 tools for use by network operations staff are out-of-scope for this subtopic.

Questions – Contact: Richard Carlson, 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

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3. INCREASING ADOPTION OF HPC MODELING AND SIMULATION IN THE ADVANCED MANUFACTURING AND ENGINEERING INDUSTRIES

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 30 years, 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 engineering and manufacturing challenges, High Performance Computing (HPC) has been underutilized.

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 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 advanced manufacturing and engineering market sectors.

Grant applications are sought in the following subtopics:

a. Turnkey HPC Solutions for Manufacturing and Engineering

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 manufacturing and engineering 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 focus on HPC applications that could be utilized in the advanced manufacturing supply chain including Smart Manufacturing are encouraged as well as applications that address the need to have solutions that are easier to learn, test and integrate into the product development cycle by a more general user (one with computational experience, but not necessarily an expert). Of particular interest are also HPC applications that address engineering challenges related to the design, integration, and fabrication of new devices for Beyond Moore's Law computing technologies including quantum computing. 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

b. Hardening of R&D Code or Software Tools for Industry Use

The Office of Science Office of Advanced Scientific Computing (ASCR) has invested millions of dollars in the development of HPC software in the areas of modeling and simulation, solvers, and tools. 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, or other ASCR programs, and "shrink wrap" them into tools that require a lower level of expertise to utilize. This may include Graphical User Interface Designs (GUIs), simplification of user input, decreasing complexity of a code by stripping out components, user support tools/services, or other ways that make the code more widely useable. Applicants may also choose to harden the codes developed by other projects provided that the potential industrial uses support the DOE mission. 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.

Questions – Contact: Lucy Nowell, Lucy.Nowell@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

Note: In addition to local, cluster, or cloud computing resources, applicants may consider using one of the following DOE Open Science Computing facilities, the National Energy Research Scientific Computing Center, the Argonne Leadership Computing Facility, or the Oak Ridge Leadership Computing Facility.

- Applicants wishing to run at the National Energy Research Scientific Computing Center (http://www.nersc.gov) facility should send email to consult@nersc.gov and inquire about the Education/Startup allocation program.
- Descriptions of the allocation programs available at the Argonne Leadership Computing Facility can be found at http://www.alcf.anl.gov/user-guides/how-get-allocation . Questions concerning allocations this facility can be sent to David Martin dem@alcf.anl.gov. Proprietary work may be done at this facility using a cost recovery model.
- Descriptions of the allocation programs available at the Oak Ridge Leadership Computing Facility are available at http://www.olcf.ornl.gov/support/getting-started/. Questions concerning allocations on this facility can be sent to Jack Wells wellsjc@ornl.gov. Proprietary work may be done at this facility using a cost recovery model.

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3. U.S. Department of Energy, Scientific Discovery through Advanced Computing (SciDAC). http://www.scidac.gov

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. 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.

Out of scope proposals for this topic include proposals that do not address the range of desired products mentioned in this specific topic or are primarily focused on: Single node/host-, handheld-, mobile-, cloud-, cryptography-, statistical-, and/or wireless-based solutions; internet; internet-of-things; data centers; basic research; natural language processing; human factors; visualization; social media; web applications; social networks; cryptanalysis; or encryption.

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

b. Other

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

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

References:

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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 Office of Advanced Scientific Computing Research 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 expertise's to develop more complex and operational

subsystems or software modules for these emerging supercomputers. A collaborative team approach, with up to five small businesses forming this team, will receive funding under this topic.

a. Photonic-Storage Subsystem Input/Output (P-SSIO) Interface

Over the past decade, numerous studies have shown that to be affordable, future supercomputers will have electric power limit of approximately 20 MW. This limitation will place a significant constraint on the I/O and memory subsystems due to the high cost of moving bits between system ICs (CPU, Memory, Bus controller, etc.). Replacing the electrical components of the Peripheral Component Interconnect Express (PCIe) Physical layer (copper traces, connectors, switches, etc.) with photonic based components would greatly increase the I/O and peripheral device bandwidth capacity of the supercomputer without exceeding the expected power budget. This topic seeks a collaborative team of small businesses to design, fabricate, build, and test a photonic based PCIe physical layer Storage Subsystem I/O interface that meets the following specifications.

- 4-8 Server class PCIe version 4.0 x32 controller chips (CPU or dedicated controller)
- 16 – 32 Non-Volatile Memory Express (NVMe) based Storage Subsystems connected at 16 GT/s I/O rate each
- Simultaneous access from every PCIe controller to multiple NVMe storage devices (256 GB/s aggregate I/O rate with 4 PCIe controllers)
- WDM optical transceivers matched to the PCIe I/O v 4.0 transmission rates
- Reconfigurable optical interconnect fabric
- Low loss Optical connectors and/or integrated Micro Optical Bench assemblies

The photonic components of the P-SSIO must be capable of operating on 0.5 pJ/b of power (not counting the PCIe or NVMe Controller or Storage Device electrical power). Storage devices (SSD) may be located up to 20 meters distant from the PCIe controller.

It is expected that a collaborative team of businesses will work together to design and build this P-SSIO device. Each business may include one or more academic or lab partners as subcontractors. Each business must submit a proposal that contains an identical narrative section and a common statement describing how any Intellectual Property issues will be addressed by the collaboration. Each proposal must have business specific budget and budget justification forms, biographical data for the Principal Investigator and senior personnel involved in the project, and commercialization plan. The title page for each submission must clearly show all businesses involved in the collaboration.

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

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6. SMART DEVICES AND TECHNOLOGIES FOR SCIENCE, ENGINEERING, AND MANUFACTURING

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

There is an increasing awareness that advancing the quality of life on our planet requires technological innovations that optimizes dwindling resources and leads to self-sufficiency through a smarter use of natural and engineered products. Smart systems, powered by smart sensors are emerging as a key technical innovation with potentials to support modern infrastructures from power grids, communication systems, scientific facilities, transportation, and manufacturing. It is also clear that the Internet of Things (IoT) is emerging as a paradigm of pervasive presence of a variety of things/objects in the Internet space through wireless and wired hyper-connectivity. It is envisioned that these things/objects will be embedded with local intelligent capabilities to enable them to cooperate with other things/objects to solve common problems and provide new services. It is also expected that SMART sensors and IoT devices will generate large amounts of aggregate data. Handling this BigData in an intelligent manner will be an essential component of any SMART environment.

Employing advanced computing technologies such as machine learning, data analytics, low-power microprocessors, and cyber physical systems in novel ways will make smart sensors with embedded computational intelligence functional across a wide range of SMART environments and infrastructures.

a. Smart Sensor Nodes for Science, Engineering, and Manufacturing Infrastructures

The specific focus of this sub-topic is on commercialized smart systems or smart cyber physical systems (SCPS). These SCPS consist of a variety of components—an interwoven network of sensors, communications devices, intelligent control element, and computational elements for pattern recognition, prediction, and decision-making.

Grant applicants should focus on the broad technical area of commercializable smart sub-systems or SCPS with a well-defined smart engine, network interfaces, applicable physical systems, and target infrastructures. Potential examples include, but are not limited to the following:

- Wired or Wireless Sensor Nodes (W2SNs) capable of collecting data, perform data analytics, perform local actions, and communicating with other sensor nodes or a central control center via wireless and wired communication channels;
- Soft Sensor Nodes (SSN) which are similar to W2SN except that it is entirely a software package that collects information or data from several sources, performs data analytics, takes local actions, and communicates with other SSNs via traditional network channels. These systems could be used for monitoring in large networks, computer systems, and other complex information systems;
- Sensor Web which uses geospatial capabilities such open GPS to provide location-aware services through turnkey systems, web or cloud services, or mobile apps in portable devices;
- Smart Cyber Physical Systems Technologies which targets SSN and W2SN development. These include components such as sensor node operating system or other critical software stacks, wireless sensor network routers, and embedded processors for real-time computational intelligence needed for networks, fuzzy logic, and light-weight machine learning technologies.

The target infrastructures for the above technologies include, but are not limited to, transportation networks, smart grids, computing and communication systems, complex manufacturing systems, environmental monitoring, complex scientific instruments such as light sources, accelerators, and observatories.

The following technologies will be considered out-of-scope: Biosensors, Nona sensors, micro-electrical systems, ultrasonic sensors, and gas sensors. Low level components such as actuators and transducers are also out-of-scope.

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

b. Internet of Things (IoT) Technologies for Science, Engineering, and Manufacturing

It is envisioned that IoT things/objects will be embedded with local intelligent capabilities to enable them to cooperate with other things/objects to solve common problems and provide new services. A significant challenge, or opportunity, for IoT related technologies is in creating networked digital, real, and virtual things/objects that will enable intelligent capabilities to support the emerging smart infrastructures such as smart utility grids, smart cities, smart transport, smart manufacturing, and other smart systems.

The IoT object/thing developed under this sub-topic should be able to do the following: a) passive communication – communicate when queried through wireless, wired, or RFID; b) active communication – communicate through wireless, wired, or RFID channels when necessary; c) take local action - performance simple computation or analytics on its own collected data and act accordingly; and d) and make autonomous decision in accordance with established rules. Examples of things/objects could include but are not limited to smart sub-systems (also referred to as cyber-physical systems) at all scales (nano, micro, mini, macro) with embedded sensing capabilities for monitoring its environment, computing capabilities to execute machine learning algorithms, and communication capabilities to interact with other things/objects. These proposed smart Things/Objects could be retrofitted in existing systems or integrated into new systems from smart homes, through smart science instruments to smart cars.

Grant applicants interested in this topic should focus on commercializable smart connected products or IoT enabling technologies that span many industries, communication gateways and infrastructures, wireless/wired communication services, online data analytics, and end users applications drawn from science, engineering, manufacturing infrastructures of interest to DOE.

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

c. Other

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

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

References: Subtopic a:

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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.

7. OUTER-COUPLING SCHEMES AND CODE DEVELOPMENT FOR FREE-ELECTRON LASER OSCILLATORS

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, is responsible for current and future user facilities including synchrotron radiation, free electron lasers (FELs), and the Spallation Neutron Source (SNS). This topic is specifically focused on the development of schemes for higher out-coupling efficiency for an X-ray free electron laser oscillator (XFELO) and development of a 3-dimensional simulation code for an XFELO. Grant applications that are not beyond the state-of-the-art nor do not fall within the topic will not be considered.

Grant applications are sought in the following subtopics:

a. Schemes for Higher Out-Coupling Efficiency for an X-ray FEL Oscillator

Self-amplified spontaneous emission (SASE) x-rays pulses are transporting x-ray photon sciences into the femtosecond domain at high-gain, single-pass FELs. An FEL based on a multi-GeV, Continuous-Wave (CW) superconducting RF linac can drastically increase the average brightness and widen the scientific opportunities [1]. A superconducting linac can also enable an X-ray FEL oscillator [2] to be added to the facility, with a minor incremental cost but major scientific benefits, producing 10^{10} photons of fully coherent pulses with high-spectral purity. The average brightness of an XFELO with 1 MHz bunch

repetition rate will then be about 10^{26} in the standard units (photons /s /mm^2 /mr^2 /0.1 % BW). This is an order of magnitude higher than that of an SASE FEL from the same linac [3]. The XFELO will complement the SASE, providing opportunities for transformative sciences in inelastic X-ray scattering, x-ray nonlinear optics, X-ray photon correlation spectroscopy, nuclear resonance scattering, etc. [4]. The power density on the intra-cavity crystals in the above XFELO is about 15 kW/mm^2. It was shown experimentally that high-purity diamond crystals survive without structural damage under such power level [5].

In the XFELO schemes considered so far, one of the x-ray cavity crystals is thin so that 4% of the intra-cavity x-ray power is extracted. The out-coupling efficiency is therefore 4%.

Since theoretical estimates of the damage threshold are higher by another two-to-three orders of magnitude, an XFELO brightness even higher than 10^{26} should be feasible at the same repetition rate [6]. This is an important possibility since a higher brightness will open up a wider scientific vista. A straightforward approach is to raise bunch charge, hence the intra-cavity power. The question is whether this can be accomplished without resulting in electron beam degradation and without reaching the damage threshold on diamond crystals.

It might also be possible to device an out-coupling schemes other than transmission through a thin crystal that gives rise to a higher out-coupling efficiency. Higher out-coupling efficiency is attractive since a higher output can be obtained with the same intra-cavity power. There are at least two possible schemes for higher out-coupling efficiency--the electron out-coupling [7] and the use of an unstable cavity for high-power laser [8]. The former was demonstrated for an infrared FEL and the latter is well-known for high-power atomic/molecular lasers.

Proposals are sought to develop practical out-coupling schemes of an XFELO with an efficiency significantly higher than 4%, including but not limited to the two schemes mentioned above—the electron beam out-coupling and the unstable cavity configuration.

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

b. 3-D X-Ray FEL Oscillator Simulation Codes

High-gain X-ray FELs have been transforming the x-ray photon sciences by providing intense x-ray pulses of unprecedented brightness. Nevertheless, the range and breadth of experimental techniques would be vastly improved if the x-ray beams from the FEL were longitudinally coherent. Two of the most promising schemes for increasing the longitudinal coherence include self-seeding [1,2] and employing the FEL in an oscillator configuration (XFELO) [3], both of which employ certain x-ray optical elements along the FEL. Unfortunately, present FEL simulation codes are not equipped to simulate these optical elements in any real detail, so that the frequency response has to typically be added by an external code, while the angular response and any coupling of the longitudinal and transverse degrees of freedom are typically ignored entirely. This is a significant deficiency, since most recent advances in FEL performance have been supported by extensive simulation efforts that have helped guide further progress. We are looking for an advance that will bring x-ray modeling capabilities to FEL simulation.

Proposals are sought for developing a 3-D-XFELO simulation code that will seamlessly incorporate a wide range of x-ray optical elements, including the full frequency-angular response of Bragg crystals, zone plates, and compound refractive lenses, into a computationally parallel FEL simulation tool. Possible

solutions may leverage existing FEL and/or x-ray optics software or employ entirely new platform(s), but must enable fast, efficient simulations of both amplifier and oscillator FEL configurations.

Questions – Contact: Eliane Lessner, 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

References: Subtopic a:

1. U.S. Department of Energy, Raubenheimer, T., LCLS-II, 2016, *LCLS-II-HE FEL Facility Overview*, Workshop on Scientific Opportunities for Ultrafast Hard X-rays at High Rep. Rate, SLAC, p. 33. https://portal.slac.stanford.edu/sites/conf_public/lclsiihe2016/Documents/160926%20LCLS-II-HE%20Raubenheimer.pdf

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1. Amann, J., et al., 2012, Demonstration of Self-seeding in a Hard-x-ray Free-electron Laser, *Nature Photonics*, Vol. 6, pp. 693-698. http://www.nature.com/nphoton/journal/v6/n10/full/nphoton.2012.180.html

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3. Kim, K-J., Shvyd'ko, Y., and Reiche, S., 2008, A Proposal for an X-ray Free-electron Laser Oscillator with an Energy-recovery Linac, *Physical Review Letters*, Vol. 100, Issue 24, 244802. https://www.ncbi.nlm.nih.gov/pubmed/18643591

8. ADVANCED MAGNET DESIGN CODE FOR X-RAY AND NEUTRON FACILITIES

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, is responsible for current and future user facilities including synchrotron radiation, free electron lasers, and the Spallation Neutron Source (SNS). This topic seeks the development of advanced, highly-parallel magnet design codes to support understanding and development of these user facilities. Grant applications that are not beyond the state-of-the-art nor do not fall within the topic will not be considered.

Grant applications are sought in the following subtopics:

a. Massively Parallel 3-D Magnet Design Codes

Available codes for 3-D modeling and design of electromagnet and permanent magnet systems have reached a high degree of sophistication and predictive accuracy. However, these codes suffer from either a total lack of parallelism or else poor parallel performance in applications that are relevant to particle accelerators. The lack of efficient parallelism leads to long turn-around times, which significantly hampers the design process. An example for which this is relevant is high-strength combined-function magnets for next-generation storage ring light sources.

In addition, serial magnet design codes suffer from memory limitations that significantly reduce the ability to obtain adequate detail and completeness in the magnet model. A significant factor is that accelerator magnets are physically large compared to the volume within which the particle beam travels. This significant difference in scales leads to competing requirements for the mesh size, leading to compromises in the accuracy of the predicted fields seen by the beam. Examples of systems for which this is a significant problem include: (1) septum magnets, which have a small, low-field bore for the stored beam separated by a thin material barrier from a relatively large, high-field bore for the incoming beam; (2) advanced insertion devices such as helical superconducting undulators, which have intricate conductor geometry at the ends; typically, such devices are simulated in sections, which leads to reduced fidelity (3) sequences of several closely-spaced magnets, as present in advanced multi-bend achromat lattices for next-generation storage ring light sources.

These issues can be resolved by a software system that incorporates an efficient parallel magnet modeling capability. In addition to efficient, highly parallel computation of magnetic fields, such a system would need to include basic features such as importation of geometry from external sources (e.g., CAD systems), generation of the problem mesh, saturable materials, permanent magnet materials, current-carrying conductors, optimization, and visualization.

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

b. Other

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

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

References: Subtopic a:

1. Jaski, M., et al., 2015, Magnet Designs for the Multi-Bend Achromat Lattice at the Advanced Photon Source, Proceedings, 6th International Particle Accelerator Conference (IPAC15 2015), pp. 3260-3263 http://inspirehep.net/record/1418083?ln=en

9. DIFFRACTIVE OFF-AXIS 2-D NANOFOCUSING OPTICS FOR HARD X-RAY IMAGING

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

Hard x-ray nanofocusing optics is important to many nano-imaging techniques at modern synchrotron facilities, including hard x-ray fluorescence nanoprobe, nano-diffraction, as well as nano-tomography. Recent developments of Multilayer Laue lenses (MLLs) [1] hold the potential to provide high-efficiency nanofocusing at sub-10 nm spatial resolution in the hard x-ray regime. Application of this type of off-axis diffractive optics requires sophisticated instrumentation with many degrees of freedom and a dedicated ultra-stable beamline, making nano-imaging experiments difficult to implement. The recent advance in bonded MLLs - a pair of off-axis MLLs bonded together to form a single 2-D focusing optic, has significantly reduced the complexity in nanofocusing instrumentation, making it possible to potentially extend high-resolution imaging to many readily available fluorescence microprobe beamlines. To optimally use such optic requires effective matching of the phase space of an x-ray source to the optic, which represents a challenge for bending magnets and wiggler beamlines. Wolter capillary optics [2] hold the potential to allow efficient focusing with micrometer-range resolution. Recent advances in the development of monolithic, axially symmetric x-ray mirror optics allow implementation of these optical elements as pre-focusing optics to potentially deliver sufficient flux-density to the MLL nanofocusing optics even on bending magnet beamlines. Furthermore, similar approach can be used to combine state-of-the-art lab-based x-ray sources with pre-focusing/MLL optics and deliver nm-scale resolution fluorescence imaging for wide-range of applications. The increased availability of hard x-ray nanofocusing optics with pre-focusing capillary will reduce the stringent requirements on beamline characteristics, thus enabling the addition of nanoscale focusing techniques to many beamlines currently using x-ray micro-beam techniques in a cost-effective and simplistic manner. Such development would greatly enhance the impact of the new and the established facilities and many existing beamlines. Grant applications that are not beyond the state-of-the-art nor do not fall within the topic will not be considered.

Grant applications are sought in the following subtopics:

a. Development of Combined Capillary and Diffractive Off-Axis 2-D Nanofocusing Optics for Hard X-ray Imaging at Nanoscale

We solicit proposals to develop a prototype system that combines a pair of bonded, high efficiency, off-axis diffractive nanofocusing optics in the energy range of 10 – 20 keV together with a single-bounce capillary pre-focusing optic to provide nanometer-scale fluorescence imaging capability at bending magnet or wiggler beamlines. The principal investigator or the proposing company must have significant prior experience in similar developments and adequate facilities for the proposed task. Applications are encouraged for those qualified proposals with already demonstrated sub-50 nm 2D spatial resolution using bonded off-axis diffractive nanofocusing optics.

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

b. Other

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

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

References: Subtopic a:

1. Nazaretski, E., Lauer, K., Yan, H., Bouet, N., et al., 2015, Pushing the Limits: an Instrument for Hard X-ray Imaging Below 20 nm, *Journal of Synchrotron Radiation*, Vol. 22, Issue 2, pp. 336-341. http://europepmc.org/abstract/med/25723934

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10. ADVANCED TEMPERATURE AND ENVIRONMENTAL CONTROL FOR NEAR-FIELD OPTICAL MICROSCOPY AND NANOMETER-SCALE INFRARED SPECTROSCOPY

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 *in operando* optical nanoprobe 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 sample environment temperature and pressure control to extend imaging and analysis techniques that combine nanometer-scale through micron-scale spatial resolution, optical excitation and spectroscopic detection over a large wavelength range. Time-dependent phenomena at nanoscale dimensions are important and tools are needed to explore energy flow, dynamics and surface structure of nanoscale materials, nanostructures and assemblies of nanostructures for use in present and future energy applications. Grant applications that do not fall within the topic will not be considered.

Grant applications are sought in the following subtopics:

a. High Spatial Resolution Nanometer Scale Optical Spectroscopy

There is a strong need to develop commercial instrumentation for advanced sample environment and temperature control for scanning near-field optical microscopy (SNOM) and nanometer-scale infrared (IR) spectroscopy. To date all commercial scanning near field optical microscopes are benchtop units that have a very limited temperature range of -20 to 80^{o}C and little environmental control other than small purge enclosures. New developments are needed to accurately understand the dynamics and surface structure of a material *in operando* under chemical reaction conditions or in extreme environments. The development of an ultrahigh vacuum (UHV) system coupled with SNOM and nanoscale IR techniques would provide temperature control ranging from cryogenic temperatures to temperatures in excess of 700 ^{o}C and environmental control ranging from UHV (<1 x 10^{-7} Torr) to 1 atmosphere or above. By cooling to cryogenic temperatures it should be feasible to significantly improve the spatial resolution to the single digit nanometer scale, well below the current spatial resolution of 10-30 nm of the most advanced commercial systems.

Grant applications are sought that make significant advancements in SNOM nanoscale IR spectroscopy by providing high spatial resolution over a wide temperature range and pressures from UHV to greater than1 atm. The improved resolution, temperature and environmental control will yield information that is valuable to a variety of scientific fields of research.

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

References:

1. U.S. Department of Energy, BESAC Subcommittee, 2015, Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science, A Report from the Basic Energy Sciences Advisory Committee, p. 78. https://science.energy.gov/~/media/bes/besac/pdf/Reports/Challenges_at_the_Frontiers_of_Matter_and_Energy_rpt.pdf

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11. INSTRUMENTATION FOR ULTRAFAST 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 development of ultrafast electron diffraction and microscopes (UED and UEM) has been identified as an enabling instrumentation to capture irreversible dynamic processes and exotic hidden states in condensed matter physics, materials science and structural biology (see for example, the 2014 Report of the Basic Energy Sciences workshop on "Electron Scattering and Diffraction", and the 2017 Report of "Basic Research Needs for Innovation and Discovery of Transformative Experimental Tools", https://science.energy.gov/bes/community-resources/reports/). Utilizing MeV-range high-energy electrons for ultrafast electron microscopy offers opportunities in minimizing space charge to pack large number of electrons in a pulsed beam while taking advantages of the strong interaction of electrons with matter and being accessible to high-order reflections in reciprocal space. However, development of MeV-electron microscopes remains a challenge. Grant applications that are not beyond the state-of-the-art or do not fall within the topic will not be considered.

Grant applications are sought in the following subtopics:

a. Low-aberration Imaging Systems for Time-resolved Microscopy with Relativistic Electrons

This subtopic aims at the development of compact ultrafast electron microscopes to achieve single-shot real-space imaging with a spatial/temporal resolution of 10 nm/10 ps.

Grant applications are sought to develop novel concepts, design and tests of imaging systems with efficient correction or compensation of geometrical aberrations including chromatic and spherical aberrations. Electron-optical subsystems of interest include probe forming, imaging and magnifying lenses and related components that can yield small beam size (<50μm) with tunable illumination angles and high spatial resolution (<10nm). The concepts have to be illustrated based on accurate modeling of magnetic elements, and overall electron optics with field solvers, particle tracking and minimization of image distortion due to systematic effects and field errors. The modeling and simulation should yield a design suitable for a prototype UEM that targets performance of single-shot imaging with 10^{-19} m*s spatial-temporal resolution.

Questions – Contact: Jane Zhu, jane.zhu@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: Jane Zhu, jane.zhu@science.doe.gov

References:

1. U.S. Department of Energy, 2014, ***Future of Electron Scattering & Diffraction***, Report of the Basic Energy Sciences workshop on the Future of Electron Scattering and Diffraction, p. 70. https://science.energy.gov/~/media/bes/pdf/reports/files/Future_of_Electron_Scattering.pdf

12. 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 Optical Components

Develop novel or improved optical components for use in neutron scattering instruments [2-5]. Such components include neutron guides, neutron focusing and imaging optics, neutron lenses, 3-D apertures and collimators, and neutron polarization devices including neutron spin flippers, polarizers, nutators, and radiofrequency coils for spin manipulation. Emphasis should be placed on producing devices that operate across a broad neutron wavelength band to enable effective time-of-flight methods.

Questions – Contact: James Rhyne, james.rhyne@science.doe.gov or Thiyaga Thiyagarajan, P.Thiyagarajan@science.doe.gov

b. Advanced Sample Environments

Develop instrumentation and techniques for advanced sample environments [6,7,8] 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.

Questions – Contact: James Rhyne, james.rhyne@science.doe.gov or Thiyaga Thiyagarajan, P.Thiyagarajan@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. Proposals focused on detectors will not be a priority area for FY 2018.

Questions – Contact: James Rhyne, james.rhyne@science.doe.gov or Thiyaga Thiyagarajan, P.Thiyagarajan@science.doe.gov

References:

1. U.S. Department of Energy, Office of Science, 2015, User Facilities, Neutron Scattering Facilities. http://science.energy.gov/bes/suf/user-facilities/neutron-scattering-facilities/

2. United States National Nanotechnology Initiative, 2005, *X-rays and Neutrons: Essential Tools for Nanoscience Research Workshop Report*, Report of the National Nanotechnology Initiative Workshop, p. 122. http://www.nano.gov/node/68.

3. International Atomic energy Agency (IAEA), 2012, Proceedings of the Twentieth International Collaboration on Advanced Neutron Sources (ICANS-XX) http://www.icansxx.com.ar/proceedings.php

4. Anderson, I.S., McGreevy, R., Bilheux, H.Z., 2009, Neutron Imaging and Applications: A Reference for the Imaging Community, A Reference for the Imaging Community, *Neutron Scattering Applications and Techniques*, Springer. http://www.springerlink.com/content/978-0-387-78692-6

5. Majkrzak, C., & Wood, J.L., 1992, Neutron Optical Devices and Applications, Proceedings / SPIE- the International Society for Optical Engineering, Vol. 1738, p.492. ISBN: 0819409111. http://books.google.com/books/about/Neutron_optical_devices_and_applications.html?id=XdhRAAAAMAAJ

6. Klose, et al., 2004, Proceedings of the Fifth International Workshop on Polarized Neutrons in Condensed Matter Investigations, *Physica B: Condensed Matter*, Vol. 356, Issue 1-4, pp. 1-280. http://www.sciencedirect.com/science/journal/09214526/356/1-4

7. Crow, J., et al, 2003, Workshop Report, SENSE: Sample Environments for Neutron Scattering Experiments Workshop, Tallahassee, FL, September 24-26, p.35. https://neutrons.ornl.gov/sites/default/files/SENSE_report_1-14-04.pdf

8. Rix, J.E., et al., 2007, Automated Sample Exchange and Tracking System for Neutron Research at Cryogenic Temperatures, *The Review of Scientific Instruments*, Vol. 78, Issue 1, http://scitation.aip.org/content/aip/journal/rsi/78/1/10.1063/1.2426878

13. 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: William Corwin, william.corwin@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: William Corwin, william.corwin@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

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

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

References:

1. U.S. Department of Energy, 2010, Nuclear Energy Research and Development Roadmap, Report to Congress, p. 60. http://energy.gov/sites/prod/files/NuclearEnergy_Roadmap_Final.pdf

2. U.S. Department of Energy, Office of Nuclear Energy, Science and Technology, Fuel Cycle Research and Development Program. http://www.energy.gov/ne/nuclear-reactor-technologies/fuel-cycle-technologies

3. U.S. Department of Energy, Office of Nuclear Energy, Science and Technology, Generation IV Nuclear Energy Systems, Nuclear Reactor Technologies. http://www.energy.gov/ne/nuclear-reactor-technologies

4. Greene, S.R., et al., 2010, Pre-Conceptual Design of a Fluoride-Salt-Cooled Small Modular Advanced High Temperature Reactor (SmAHTR), Oak Ridge National Laboratory, Oak Ridge, TN. ORNL/TM-2010/199. http://info.ornl.gov/sites/publications/files/Pub26178.pdf

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

14. PERFORMANCE AND MANUFACTURING ADVANCEMENTS FOR LEDS AND OLEDS FOR SOLID-STATE LIGHTING

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

The purpose of this solid state lighting (SSL) topic is to support early-stage fundamental research that encourages innovative quantum material science development or manufacturing innovations that exhibit substantial promise to achieve SSL products that perform closer to their theoretically predicted maxima by meeting or exceeding the aggressive device performance goals established by DOE in its SSL Research and Development Plan (RDP) 2, 3. Light-emitting diodes (LEDs)—one of the earliest quantum material to have enjoyed unprecedented technological and manufacturing evolution over the past several decades—remains a high priority for fundamental research.

With SSL market penetration today less than it could be, there is considerable opportunity to expand this emerging market with even more significant cost reductions and product performance improvements over the next decade. It is expected that these improvements will be made possible with the advent of new advanced materials and manufacturing methods applicable to the emerging wide spectrum of SSL products and components. Small business and academic researchers in universities and elsewhere have already made many

key enabling advancements to this rapidly evolving, energy-efficient and disruptive technology and are expected to continue to produce important innovations. The following subtopic descriptions highlight a few opportunities that are of special interest to this community and to DOE's SSL Program, which is explained more fully at https://energy.gov/eere/ssl/solid-state-lighting.

Responsive proposals sought must succinctly address and reference one or more of the key materials challenges described cost of SSL products. Applications that primarily address other related photonic materials or devices that are not directly related to general illumination in buildings – such as automotive lighting, projection or displays – will not be accepted. Similarly, applications that do not represent a significant opportunity for a fundamental breakthrough in basic materials science, performance or cost, and that propose only incremental advancements to existing materials or products, will be discouraged. The key metric for judging responsiveness of all proposals will be the risk associated with achieving the significant improvement described, balanced with evaluation of commercialization potential using recognized and quantitative comparison to existing materials or components that may be found in published sources such as the DOE SSL RDP noted above. Proposals that include substantial technical risk are encouraged, provided they articulate a viable plan to retire such risk during the Phase I period of performance, with appropriate proof of principle demonstration. Projects that result in important intellectual property are especially valuable, as they may provide future revenue in the form of royalties or cross-licenses to the benefit of small business or the participating technology transfer office or National Laboratory.

Grant applications are sought in the following subtopics:

a. LEDs

The ability to manufacture high-quality LEDs used for general illumination products has advanced remarkably over the past decade. LEDs must satisfy an eager solid-state lighting (SSL) market for energy-efficient, high-color-quality general illumination products worldwide [1]. Practical and attractive SSL products are available today whose efficiency routinely exceeds 100 lumens per watt (LPW) at a life cycle cost significantly less than the legacy lighting products they replace. Even with the proven viability of modern III-Nitride alloys used to manufacture phosphor-converted LEDs (pcLEDs) and multiple LED color-mixed light engines, there remains ample opportunity to advance relevant semiconductor technology to further increase the value of LEDs in this important market. There are many contributing technologies, components, intermediate materials and process technologies that could productively enter the stream of LED SSL commerce as either a key component, constituent material or contributory intellectual property.

There are also opportunities to develop more fundamental, basic yet new and novel III-Nitride alloys and/or buffer materials or thermal and light management solutions at the quantum-well and device levels, which could produce significant performance or longevity of LEDs without complete replacement of the existing manufacturing infrastructure. Examples of this could include efficient long-wavelength emitters; high-temperature encapsulants as alternatives to existing silicone systems, which might possess better thermal properties or provide more-favorable light control; elimination of costly conventional substrates using self-assembly of microchips or dice; roll-to-roll processing, either within an existing tool or using an alternative epitaxial growth technique; and growth of conventional epitaxial material on appropriately engineered inexpensive substrates or growth on large-format wafers. It is also possible to integrate emerging theoretical, computational or in-situ characterization tools into the manufacture or synthesis of key materials. Accurate prediction of composition and, ultimately, performance could be used to efficiently guide the synthesis route during crystal growth in a MOCVD, for example, thereby increasing

yield and quality while reducing waste and cost [4]. At the device level, opportunities to leverage existing research to advance light management or outcoupling efficiency using techniques such as microelectromechanical systems (MEMs) or liquid crystals or electrowetting are possibilities. New techniques to reduce or shift the impact of the droop in green LED efficacy or other non-radiative loss mechanisms and advanced downconverter concepts, particularly at the molecular level, are also possible opportunities for eventual commercial success.

Questions – Contact: James R. Brodrick, james.brodrick@hq.doe.gov

b. OLEDs

The performance of organic light-emitting diodes (OLEDs) suitable for general illumination purposes remains far below their theoretically predicted efficiency, for a variety of reasons. These include fundamental challenges in device design and development of entirely new materials. Among the most significant shortcomings is the low extraction probability of the light produced inside the OLED stack. Very little of the efficiently generated light escapes the device, due to refractive index mismatches (causing waveguiding within the thin planar substrate, anode and stack layers) and coupling of the light to surface plasmon modes. Cost-effective light extraction remains a high research priority, and innovative and imaginative solutions that represent viable alternatives to the traditional methods used to accomplish light extraction from OLEDs are sought. Candidate solutions also might use novel light-shaping optics, novel extraction layers, alignment of emitting molecules, cavity resonance or even alternative structures or geometries of an OLED system. If proven effective and practical in Phase I, such a novel new structure, component or IP could positively impact the evolution of OLED lighting technology by overcoming this significant performance limitation. Demonstration of commercial potential would be the subject of Phase II.

Another fundamental challenge in the development of optoelectronic materials is the simultaneous achievement of high electrical conductivity and low optical absorption. All commercial OLEDs use indium tin oxide (ITO) in the transparent electrodes, despite its well-known deficiencies. Potential replacements for improved transparent anode or cathode performance include graphene, nanowires, thin metals, doped metal oxides and conducting polymers. If successful, such materials should find application in many other applications of flexible electronics, including photovoltaic cells. Finally, development of stable yet efficient blue emission luminophores continues to be a challenge for commercial production of high-quality, long-life white OLEDs. The high energy of excitons capable of emitting blue light increases the probability of many non-radiative decay mechanisms, and new ways to bypass these incompletely characterized loss mechanisms may be found in more basic materials science research. The design and synthesis of all materials in which these non-photonic losses are suppressed remains a major challenge. Novel, stable emitter systems – perhaps involving quantum dots, perovskites, thermally activated delayed fluorescent (TADF) or TADF-assisted ("hyperfluorescent") emitters – are required for future, more-efficient OLED products. Analysis of new emitting materials and stable, high-energy hosts by quantum modeling and diagnostic tests could form a valuable Phase I proposal, preparing the way for longer-term studies of stability in the Phase II stage.

Questions – Contact: James R. Brodrick, james.brodrick@hq.doe.gov

All applications relevant to these technical subtopic areas must identify which topic is most relevant and submit to it accordingly. In addition, Letters of intent (LOIs) will be used to screen applications for technical

relevance, in addition to the criteria explained in the FOA. Within the constraints of the LOI format, responsive LOIs and full applications to this topic must:

- Be consistent with and have performance metrics linked to the 2017 DOE SSL RDP whenever possible. [2]
- Clearly define the proposed application, the merit of the proposed innovation and the anticipated outcome, with a special emphasis on the commercialization potential of the overall effort, including Phase I and Phase II.
- Include quantitative projections for price and/or performance improvement that are tied to representative values included in the RDP plan or in comparison to existing products [2, 3].
- Demonstrate commercial viability with a quantifiable return on DOE investment, as described elsewhere in this FOA.
- Justify all performance improvement claims with thoughtful and sound theoretical predictions or experimental data.

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: James R. Brodrick, james.brodrick@hq.doe.gov

References:

1. U.S. Department of Energy, Energy Efficiency & Renewable Energy, 2017, Solid-State Lighting Program Overview Brochure, *DOE Solid-State Lighting Program*, Modest Investments, Extraordinary Impacts, p. 8. http://energy.gov/eere/ssl/downloads/solid-state-lighting-program-overview-brochure

2. U.S. Department of Energy, Energy Efficiency & Renewable Energy, 2016, Solid-State Lighting R & D Plan, Prepared for Lighting Research and Development Building Technologies Program at the Department of Energy. https://energy.gov/eere/ssl/technology-roadmaps

3. U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Office of Basis Energy Sciences, 2016, DOE Joint Solid-State Lighting Roundtables on Science Challenges, p. 20. https://energy.gov/eere/ssl/downloads/2016-led-roundtable-reports

4. U.S. Department of Energy, Office of Basic Energy Science, 2016, 2016 Basic Research Needs for Synthesis Science for Energy Relevant Technology Workshop, p. 17. https://science.energy.gov/~/media/bes/besac/pdf/201606/DeYoreo_BESAC_presentation.pdf

15. SOFTWARE INFRASTRUCTURE FOR WEB-ENABLED CHEMICAL-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, which is a key for research conducted by researchers in universities, laboratories and industry.

Grant applications are sought in the following subtopics:

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

The Department of Energy seeks to speed 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. 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. 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 modeling and simulation.

Resulting infrastructure should provide economically feasible means that allow networks consisting of specialized 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

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

References:

1. Executive Office of The President National Science and Technology Council, 2011, Materials Genome Initiative for Global Competitiveness, p. 18. https://www.mgi.gov/sites/default/files/documents/materials_genome_initiative-final.pdf

2. Galli, G., Dunning, T., U.S. Department of Energy, 2009, Scientific Grand Challenges, Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale, p. 117.

http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/BES_exascale_report.pdf

3. Crabtree, G., Glotzer, S., McCurdy, B., U.S. Department of Energy, 2010, Computational Materials Sciences and Chemistry: Accelerating Discovery and Innovation Through Simulation-Based Engineering and Science, Report of the Department of Energy Workshop, p. 32. http://science.energy.gov/~/media/bes/pdf/reports/files/Computational_Materials_Science_and_Chemistry_rpt.pdf

4. U.S. Department of Energy, 2011, A Workshop to Identify Research Needs and Impacts in Predictive Simulation of Internal Combustion Engines (PreSICE), Sponsored by the Office of Basic Energy Sciences, Office of Science and the Vehicle Technologies Program, Office of Energy Efficiency and Renewable Energy, U.S Department of Energy, p. 54. http://science.energy.gov/~/media/bes/pdf/reports/files/PreSICE_rpt.pdf

5. U.S Department of Energy, 2010, Basic Research Needs for Carbon Capture: Beyond 2020, Report based on SC/FE Workshop, p. 196. http://science.energy.gov/~/media/bes/pdf/reports/files/Basic_Research_Needs_for_Carbon_Capture_rpt.pdf

6. U.S. Department of Energy, Subcommittee on Theory and Computation of the Basic Energy Sciences Advisory Committee, 2005, Opportunities for Discovery: Theory and Computation in Basic Energy Sciences, Report based on BESAC Deliberations, p. 50. http://science.energy.gov/~/media/bes/besac/pdf/Theory-and-Computation_rpt.pdf

16. ENGINEERED SYSTEMS FOR INNOVATIVE WET AND GASEOUS WASTE VALORIZATION

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

Developing technologies designed to close waste loops and optimize resource utility is strategically important, and is viewed by the US Department of Energy as critical to maintaining and advancing sustainable economic growth in a resource constrained world. Viewing wastes, such as traditional wet organic wastes and even inorganic waste gases such as CO_2, as resources is a paradigm driving new innovations that will allow higher value fuels and products to be generated from underutilized renewable feedstocks. Beyond simply using waste feedstocks, new systems and strategies for wet and gaseous wastes need to be developed to improve the carbon conversion efficiency of wet wastes and to better manage carbon dioxide emissions. This solicitation therefore seeks proposals for engineered systems that move beyond traditional anaerobic digestion for wet waste conversion, or that couple unique catalytic and biological approaches to manage waste carbon.

Within the constraints detailed in each section, grant applications are sought for the following subtopics:

a. Beyond Biogas: Valorization of Wet Organic Waste Streams

Organic waste streams contain substantial amounts of chemical energy. Since these resource streams, including, but not limited to, food and beverage wastewaters, municipal wastewater, livestock manure slurries, the non-recyclable fraction of municipal solid waste, and other industrial food wastes are biogenic

in origin, energy produced from them can be considered renewable, as the U.S. Environmental Protection Agency has done in granting eligibility to fuels produced from these sources for cellulosic Renewable Identification Numbers[1]. While some of the available energy is currently being captured, a significant amount remains untapped[2-4].

The U.S. Department of Energy (DOE) is interested in processes to produce biofuels, bioproducts, and/or relevant precursors from these wet organic feedstocks. One particular focus is to extend the idea of Integrated Biorefineries (IBRs) to wet organic waste streams[5], in support of burgeoning industry interest in "energy-positive water resource recovery" facilities, which produce clean water, energy, and nutrients from municipal wastewaters[6, 7]. The DOE's recent report on Biofuels and Bioproducts from Wet and Gaseous Waste Streams[8] identified several possible technological pathways to achieve these aims; this portion of the solicitation seeks to build on that document. In particular, it targets alternatives to traditional anaerobic digestion that produce products with better value propositions than biogas, such as relevant intermediates to enable the production of jet and diesel blendstocks.

While some specifics vary, the following criteria will apply to all applications:

- Proposed systems must utilize wet organic waste streams as the primary feedstock to produce fuels, or fuel and product mixtures. Wet waste streams are defined in the Bioenergy Technologies Office Multi-Year Program Plan[9]. For purposes of this subtopic, biogas is specifically excluded as a feedstock or process intermediate. Note that anaerobic systems that generate and upgrade intermediates other than biogas, such as the carboxylate pathway, will be considered.
- By Phase II, and preferably within Phase I, proposed projects should employ actual (rather than model or synthetic) waste streams as feedstocks.
- Successful applications will propose to develop and run pilot systems by the end of Phase II, at a relevant scale (e.g., 100–1,000 L reactor volume).
- Proposals must include quantifiable phase I objectives, the attainment of which will be a key evaluation factor in the consideration of phase II applications
- Applications must address the energy efficiency of the system. Successful applications will minimize the ratio of required energy inputs to the energy potential of proposed outputs.
- Carbon efficiency is another important metric. Applications will be evaluated on their probability of maximizing the utilization of the biogenic carbon available in relevant resource streams.
- Projects that contribute to and/or leverage the development of fundamental scientific knowledge in areas, including, but not limited to, advanced separation strategies for volatile fatty acids, carboxylic acids or products derived therefrom from heterogeneous aqueous mixtures, improved understanding of product toxicity to heterogeneous microbial and archaeal communities, and advances in toolkit development in terms of proteomics, metabolomics, transcriptomics, and other related areas are of particular interest.
- End products should include at least either three carbon molecules, or at least two carbon molecules with one or more double bonds. Acetylene is specifically excluded.
- Proposals that utilize algae, even if grown on wastewater, and dry waste streams, such as corn stover, or the herbaceous and woody fractions of municipal solid waste, will be considered non-responsive.
- Feedstocks that could be processed to inputs for human or animal food or feed products, including waste glycerol from biodiesel processes, are specifically excluded.
- Transesterification of yellow grease to produce biodiesel is also specifically excluded. Brown grease, however, is an acceptable feedstock. Renewable diesel is strongly preferred over biodiesel as an end product.

- In all cases, the DOE is interested in projects that present the possibility of producing commercially relevant and economically competitive higher hydrocarbons from biogenic sources to displace petroleum. Examples include, but are by no means limited to, butanol, 1,4-butanediol, and medium-chain fatty acids, such as succinic, muconic, and lactic acids.
- Additionally, proposals that strive to complete the conversion of relevant feedstocks to jet or diesel blend stocks suitable for incorporation into existing refinery processes by the end of phase II are particularly encouraged.
- Hydrogen, ethanol, and methanol are not allowed as end products, but are acceptable as intermediates, if the proposal is clear how the intermediates will be incorporated into processes to produce biofuels or bioproduct precursors by the completion of phase II.
- Applications that propose to produce only biopower will be considered non-responsive.

Although all topical applications that conform to the above constraints will be considered, there is particular interest in systems that employ either arrested methanogenesis or hydrothermal liquefaction technologies. Some specific considerations for various systems are:

- Arrested methanogenesis (production of biofuels and bioproduct precursors via arrested methanogenesis)

One of the clearest participant messages from the 2014 Waste-to-Energy workshop was that anaerobic digestion that produces biogas might not be the most cost-effective pathway to liquid fuels[10]. In response to this input, the DOE seeks alternatives to the methanogenesis stage of anaerobic digestion. Production of biofuels and bioproduct precursors from volatile fatty acids is one promising option, and other possibilities will be entertained[11]. Applications should address specific mechanisms to constrain methanogenesis, measures to minimize inhibition of valuable product production, and strategies to convert the products of the earlier stages of anaerobic digestion into biofuels and bioproduct precursors[12-15]. Successful proposals will articulate strategies to address the challenges of intermediate and product separations, and success will be judged by cost-effective titers and yields of final products, not simply volatile fatty acids. Again, applications that propose to complete conversion of relevant feedstocks to jet or diesel blend stocks by the end of phase II are particularly encouraged, and co-products are welcomed.

- Hydrothermal liquefaction (conversion to jet and diesel blendstocks using sub- and supercritical fluids)

Hydrothermal Liquefaction (HTL) of wet organic waste streams using subcritical water to produce biofuels and bioproduct precursors is a promising technological pathway.[16] While BETO is already active in this area, this subtopic solicits additional proposals that utilize the following substances as solvents/reactive participants:

1. Subcritical water;[17, 18]
2. Supercritical water,[19-21] or;
3. Sub- or supercritical organic liquids, including supercritical CO_2 .[22]

Other organic substances are also welcomed as solvents, provided that they provide a net benefit in greenhouse gas reduction or cost advantages versus traditional waste disposal alternative such as incineration, anaerobic digestion, or landfilling. In all cases, the goal is to produce jet and diesel refinery blendstocks that align with BETO's 2017 and 2022 cost targets, as articulated in the office's Multi-Year

Program Plan.[9] Preference will be given to applications that propose a full chain of production for drop-in biofuels, and articulate a clear and credible path to market. Proposals that include co-products, particularly replacements for petrochemical feedstocks, in order to improve their techno-economic argument are also welcomed.

Questions – Contact: Mark Philbrick, mark.philbrick@hq.doe.gov

b. Non-Photosynthetic Carbon Dioxide Reduction and Biological Intermediate Upgrading

The potential environmental and economic benefits associated with carbon dioxide capture and utilization are drawing increased attention across industry, academia, and the general public. By capturing and subsequently utilizing CO_2, carbon capture and utilization (CCU) enables greater carbon management and more efficient use of existing fossil resources. Annually, the US transportation and power sectors combine to produce over 5 gigatons of CO_2 (1). Utilization of CO_2 not only improves the environmental impact of energy production, but it also incentivizes the monetization of a cheap and abundant carbon resource. Carbon capture is an emerging technology with several commercial-scale successes occurring earlier this year (2) (3), indicating that a future infrastructure to enable greater carbon capture and utilization is a real possibility.

Although there is a large supply of CO_2, one critical aspect of its utilization is its low energy content, which makes it relatively difficult for natural biological systems to efficiently reduce CO_2 to organic carbon. In fact, even the most robust photosynthetic biological systems are relatively inefficient and slow at utilizing CO_2; only about 5% of the energy hitting most plants in the form of light is theoretically used to fix carbon (4). However, once reduced, biological systems can much more easily manipulate simple organic molecules to synthesize more valuable products (5) (6). Leveraging this attribute of biological systems is a staple of the growing bioeconomy.

The US power grid is quickly changing as renewable resources make significant headway in contributing to our generation capacity. By 2018, the electricity generation of solar and wind across the US is projected to be over 870 GWh/day, or about 8% of all our electricity (7). As more renewables are deployed, curtailment of this power becomes a necessity. The power grid in California often sees midday periods where over 40% of the electricity is generated by solar and wind and when electricity supply outpaces demand, that power can be wasted (8) (9) (10) (11). Texas similarly has curtailment issues at times of high wind and low energy demand, setting up conditions where the price of electricity becomes negative (12). The ability to flexibly utilize surplus electricity on the grid during times of high generation could be a valuable grid management tool in a future with high renewable resource penetration and can serve as a strategy to better manage two novel "wastes": CO_2 and electricity.

The Department of Energy seeks grant applications that propose to demonstrate engineered systems that leverage electricity to power carbon dioxide reduction and employ biological processes to convert the reduced carbon intermediate to a final biofuel or enabling bioproduct.

Deployed systems would be required to show that input CO_2 will be sourced from either a waste gas point source or the atmosphere (i.e. CO_2 feedstock generation for such systems cannot be the intended purpose for consuming biomass or fossil resources). Engineered systems could exploit a catalytic, thermochemical, or electrochemical process to reduce CO_2. From there, the process could use any non-photosynthetic

biological mechanism to upgrade the reduced form of carbon into a biofuel or enabling bioproduct. Other items for applicants to consider:

- Examples of organic carbon intermediates generated from CO_2 include (but are not limited to): formic acid, methanol, carbon monoxide and methane.
- Hydrogen, ethanol, and methanol are not allowed as end products, but are acceptable as intermediates, if the proposal is clear how the intermediates will be incorporated into processes to produce biofuels or bioproducts by the completion of Phase II.
- While the final biofuel or bioproduct is the focus of this study, applicants must source their reduced carbon intermediate from CO_2 (i.e. biological processes that simply use a 1C organic feedstock are not in scope). This can be accomplished by a) acquiring the intermediate from a producer/partner who specifically generates the CO_2-derived intermediates or b) having the development of CO_2 reduction technology as a part of the scope-of-work. *Ideal applicants will already have some previously demonstrated capabilities in either the CO_2 reduction or biological upgrading portion of this effort.*
- Successful applications should propose technologies that, by the end of Phase II, could operate at a significant throughput of CO_2/intermediate per day at 100L reactor volume and preferably greater.
- Applicants should consider the robustness of any catalysts/biocatalysts used for the CO_2 reduction and upgrading.
- While applicants can assume that the electricity used for the reduction of CO_2 is both cheap/surplus and low-carbon, applications must address the energy efficiency of the system. Successful applications will minimize the ratio of required energy inputs to the energy potential of proposed outputs and justify greater electrical requirements with greater carbon efficiencies.
- By the end of Phase II, projects must present a preliminary technoeconomic analysis (TEA) which associates minimum fuel selling prices (MFSPs) to various electricity and carbon prices, and specifically what prices (perhaps even negative electricity and carbon prices) that offer fuel products at or below $3/GGE. Successful applications will outline how such a TEA will be performed and highlight data to be obtained in Phases I and II that would enable the needed analysis.
- Proposed systems should eventually (end of Phase II) function as modular units which can be deployed to defined sources of CO_2.

Questions – Contact: Ian Rowe, ian.rowe@ee.doe.gov

c. Other

In addition to the specific topics listed above, the DOE invites grant applications in other areas that fall within the scope and align with the objectives of the topic descriptions. We welcome other engineered systems which address the utilization of organic wet waste and inorganic gaseous waste streams.

Questions – Contact: Mark Philbrick, mark.philbrick@hq.doe.gov on organic wet waste systems or contact Ian Rowe, ian.rowe@ee.doe.gov on inorganic gaseous waste systems

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17. MEMBRANES AND MATERIALS FOR ENERGY EFFICIENCY

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

Separation technologies recover, isolate, and purify products in virtually every industrial process. Using membranes rather than conventional energy intensive technologies for separations could dramatically reduce energy use and costs in key industrial processes [1]. Separation processes represent 40 to 70 percent of both capital and operating costs in industry. They also account for 45 percent of all the process energy used by the chemical and petroleum refining industries every year. In response, the Department of Energy supports the development of high-risk, innovative membrane separation technologies and related materials. This includes membranes and materials to separate gas mixtures for buildings-relevant applications. Advancements are needed that will lead to new generations of organic, inorganic, and ceramic membranes. These membranes require greater thermal and chemical stability, greater reliability, improved fouling and corrosion resistance, and higher selectivity leading to better performance in existing industrial applications, as well as opportunities for new applications.

Materials for energy efficiency include both organic and inorganic types. Fundamental research into materials and processes that enable energy efficient high performance semiconductor solutions for computing at and to the limits of electro-static physical scaling for Moore's Law are especially encouraged. This could include quantum, neuromorphic and a number of other semiconductor device architectures. The research would be into the materials and processes with the potential for breakthrough manufacturing including atomically precise manufacturing. Atomically precise manufacturing (APM) --the production of materials, structures, devices, and finished goods in a manner such that every atom is at its specified location relative to the other atoms—is based on fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels. In APM there are no defects, missing atoms, extra atoms, or incorrect (impurity) atoms. This topic is fully aligned with the FY 2018 BES priorities to transform the understanding and control of matter and energy including emphasis on emerging high priorities in quantum materials and chemistry, catalysis science, and synthesis.

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 Toward Discovery and Development of Improved Ionomers for Polymer Electrolyte Membrane Fuel Cell Catalyst Layer

Much fundamental research remains to fully understand, predict, and control polymer electrolyte membrane (PEM) fuel cells. High power performance of PEMFCs is limited by local transport issues in the catalyst layer, believed to be due at least in part to the catalyst layer ionomer [1]. Today's commercial PEM technology typically relies on the same type of perfluorosulfonic acid ionomers in the catalyst layer as are used for the fuel cell membrane. However, the properties desired for the ionomer in the catalyst layer and the ionomer used in the membrane are different. While both applications require good protonic conductivity, the catalyst layer ionomer should have high gas permeance, while the membrane requires low gas permeability [2]. In addition, electrochemical tests have indicated that the sulfonate groups in PFSAs can inhibit the ORR, likely through competitive adsorption on the Pt [3]. Ionomers with lower sulfonate adsorption and higher gas permeability are sought. Novel ionomers suitable for application in the PEM fuel cell catalyst layer are solicited through this subtopic. Ionomers developed through this subtopic should have properties and characteristics required for application in PEM fuel cells, including:

- High proton conductivity in a range of temperature and humidity conditions
- Good compatibility with PFSA membranes enabling low resistance at the membrane-catalyst layer interface
- High permeability to gases, including O_2, H_2.
- High water permeance
- Low or no anion adsorption on Pt
- Chemical durability sufficient to pass the accelerated stress tests in the DOE MYRD&D plan

The goal of any proposed work under this subtopic should be to produce a new catalyst layer ionomer that can reduce the local mass transport losses in a low-Pt loaded electrode. Ex-situ testing of thin film properties such as conductivity and permeability, should be performed; however the catalyst layer ionomer should be demonstrated in an MEA. If such problems are addressed, PEMFCs are a leading candidate to power zero emission vehicles, with several major automakers already in the early stages of commercializing fuel cell vehicles powered by PEM fuel cells. PEM fuel cells are also of interest for stationary power applications, including primary power, backup power, and combined heat and power.

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b. Development of Innovative Gas Diffusion Layers for Polymer Electrolyte Membrane Fuel Cells

Fundamental research issues related to the gas diffusion layer (GDL) in PEM fuel cells remain including those related to the energy-water nexus. The GDL resides between the electrode and bipolar plate (BPP). The primary function of the GDL is to aid in reactant and product distribution to the anode and cathode, especially water. Easy movement of reactants and products during steady-state operation at all power levels is desired as well as during extreme and rapid transients facilitates cell operation at high current density by reducing mass transport resistance and minimizing liquid water build-up and blockage. Unhindered mass transport can result in smaller stacks for a given power level and, consequently, lower system cost. GDLs are porous structures usually fabricated from carbon paper or fibers treated to achieve the desired hydrophobicity/hydrophilicity and represent a non-trivial cost to the system (21% of stack cost for 1000 systems per year and 6% for 500,000 systems [2].

Proposals are sought to develop innovative GDL structures and chemistries that address mass transport and water management under the entire range of automotive operating conditions. Specific areas of interest include: tailored and stable hydrophobicity/hydrophilicity, GDL physical and chemical property

gradients for improved water management, integration of the GDL with the BPP, and non-carbon GDL materials. High thermal and electrical conductivity are also desirable.

Proposals must include the scientific rationale for the materials/structures being proposed including supporting experimental data and calculations, a discussion of potential cost impacts, supported estimates of stability, and a discussion of ex-situ and in-situ testing/characterization.

Ex-situ corrosion testing must recognize the guidelines described in Footnotes g (anode side) and i (cathode side) of Table 3.4.8 (BPP Targets https://energy.gov/sites/prod/files/2017/05/f34/fcto_myrdd_fuel_cells.pdf) presented in the 2016 DOE Multi-Year Research, Development, and Demonstration Plan. The anode guideline is "pH 3, 0.1ppm HF, 80°C, peak active current $<1x10^{-6}$ A/cm^2 (potentiodynamic test at 0.1 mV/s, -0.4V to +0.6V (Ag/AgCl)), de-aerated with Ar purge". The cathode conditions are "pH 3, 0.1ppm HF, 80°C, passive current $<5x10^{-8}$ A/cm^2 (potentiostatic test at +0.6V (Ag/AgCl)) for >24h, aerated solution". The 2020 goal for BPP anode-side corrosion is <1μA/cm^2 with no active peak and <1μA/cm^2 on the cathode side.

Phase I effort should demonstrate the feasibility of the concept by ex-situ corrosion testing as well as measurement of thermal and electrical conductivity and determination of mass transport properties. A preliminary cost analysis is required. Phase II should include in-situ cell performance testing and durability testing as well as a manufacturing assessment and a more detailed cost analysis.

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c. Innovative Approaches for the Improvement of Packing Densities of Hydrogen Adsorbents

Increasing the volumetric capacity of hydrogen storage is still a challenge and requires fundamental research to overcome. The current method of hydrogen storage onboard Fuel Cell Electric Vehicles (FCEVs) utilizes 700 bar compressed hydrogen gas stored within large, heavy and expensive carbon fiber overwrapped pressure vessels. Alternative methods of storage using materials that either chemically bind and release hydrogen, or reversibly adsorb hydrogen, have long been investigated as a means to lower the onboard storage pressure, reduce overall system and delivery costs, and lessen safety concerns. Novel approaches such as solid-state adsorbent materials, for example metal-organic frameworks (MOFs) or porous carbons are of particular interest because their high surface areas and low binding enthalpies allow for the storage of large amounts of hydrogen with excellent reversibility. Of particular importance for adsorbent-based systems is the volumetric capacity, as these materials tend to have low hydrogen storage densities.

The U.S. Department of Energy (DOE) publishes targets for wide-scale commercialization of FCEVs [1] that include over 20 properties pertaining to the function of a realistic storage system. Volumetric capacity in adsorbents is typically measured and reported with respect to the single crystal density of the material; however in a realistic system this capacity is significantly reduced due to packing inefficiencies inherent to filling a tank with a powdered or crystalline material. The volumetric system targets must be met taking the bulk density of the packed material into account, as well as other volumetric concerns from the tank itself and associated components. This penalty for low packing densities can reduce the volumetric capacity of an adsorbent material by a factor of two or more.

Applications are sought for the development of methods to densify adsorbent materials without compromising their hydrogen storage properties. Improvements in volumetric capacity must be demonstrated at a scaled-up level, while not adversely affecting storage temperatures and pressures, gravimetric capacity, or reversibility. These methods could encompass a wide variety of strategies, from mechanical densification of powders or crystals to synthetic alteration of materials to promote specific morphologies or particle sizes for improved packing. Efforts should not be material-specific, meaning that the underlying strategy must be demonstrated for multiple adsorbents (i.e., several different MOFs). Projects funded under this solicitation will be associated with DOE's Hydrogen Materials—Advanced Research Consortium (HyMARC). More information on the consortium can be found on its website (https://hymarc.org/) and at the DOE website [2].

Phase I of the proposed work should focus on the engineering or synthetic methods proposed to improve packing densities. Efforts must be demonstrated for more than one specific material, and discrete metrics must be proposed as benchmarks for success. DOE will require samples of the materials be analyzed by its adsorption measurement validation group at the National Renewable Energy Laboratory (NREL). Phase II of the effort should focus on the scale-up and demonstration of the strategy for a realistic storage system. This could potentially involve the use of newer materials developed through future HyMARC efforts, or existing materials which would subsequently be shown to approach the storage targets through the methods developed in Phase I.

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d. Membranes for Electrochemical Compressors

Efficient Compression of the smallest molecule also poses fundamental research challenges. Electrochemical systems offer the potential for high-pressure hydrogen compression with greater reliability than conventional mechanical systems due to their elimination of moving parts. Electrochemical hydrogen compressors (EHCs) utilize direct current and catalysts to oxidize hydrogen into protons that then pass through a proton exchange membrane (PEM) to the cathode. At the cathode, the protons are reduced, and accumulate to high pressures of hydrogen. The use of electrochemical cells in compressors is challenged by membrane stability under high pressure differentials, membrane tolerance to impurities, capital cost of membranes and catalysts, and risks of cell flooding due to membrane hydration requirements. [1] Research on electrochemical compression membranes to date has including the development of membrane synthesis approaches [2], novel polymeric components for membranes [3], and membrane electrode assembly designs that mitigate leakage and enhance durability [4]. Research accomplishments have also been leveraged from other electrochemical hydrogen applications, such as electrolyzers and fuel cells, due to the similarities in these technologies. [5] Development of advanced membrane materials is still necessary, however, for electrochemical cells to be used in high-pressure (875-bar) hydrogen compression.

Applications are sought for the development of a novel membrane that enables electrochemical hydrogen compression at > 1 kg/hour at 875 bar with an energy consumption of 1.4 kWh/kg, given hydrogen input at 100 bar. Phase I of this research will include synthesis of membrane samples, followed by bench-top evaluation of key performance characteristics, including polarization curves, Tafel plots, and evaluation of performance over time.

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e. Atomically Precise Manufacturing

At the Advanced Manufacturing Office workshop in Berkeley in 2015 [1], participants identified two specific positional assembly methods for achieving an atomically precise level of precision: (1) tip-based positional assembly using scanning probe microscopes, and (2) integrated nanosystems using molecular machine components. The first approach is also considered to include the methodology developed by Lyding of selective deprotection and atomic layer epitaxial deposition [2]. Both approaches have considerable challenges to implementation, including positional accuracy (which is influenced by factors such as component stiffness and thermal vibration), repeatability, working tip design and synthesis, suitable building block design, transport of molecules to the working tip, and scalability.

Advances in these positional assembly techniques will be considered for funding for high energy impact applications such as (but not limited to) atomically precise catalysts, molecular electronic computer circuits, quantum computer circuits, and high sensitivity molecular sensors. Responsive proposals will identify specific technological hurdles in their approach to positional molecular assembly, and show how the milestones and deliverables proposed for the project will overcome these hurdles. Physical demonstrations of the production of atomically precise structures or devices is the preferred deliverable, however the Phase I proposal may experimentally demonstrate overcoming issues at the subcomponent level that eventually lead to the desired advance in molecular assembly. For example, designing and building a critical molecular machine component would be responsive, if the proposal shows how this component would function as part of an integrated nanosystem for molecular assembly in a Phase II demonstration. Instrumentation advances such as atomically precise tip synthesis or improved scanning probe repeatability and positional accuracy would also qualify, if the proposal shows how these will lead to atomically precise manufacturing in a Phase II demonstration. Theoretical studies alone will not be considered responsive to this solicitation, although may be proposed in complement to experimental demonstrations.

Questions – Contact: David Forrest, david.forrest@hq.doe.gov

f. 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: Sven Mumme, Sven.Mumme@ee.doe.gov

References: Subtopic a:

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2. 2016, Fuel Cells Section, Multi-Year Research, Development, and Demonstration Plan, p. 58. https://energy.gov/sites/prod/files/2017/05/f34/fcto_myrdd_fuel_cells.pdf

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References: Subtopic b:

1. U.S. Department of Energy, 2016, DOE Hydrogen and Fuel Cells Program Record, 16020, p.9. https://www.hydrogen.energy.gov/pdfs/16020_fuel_cell_system_cost_2016.pdf

References: Subtopic c:

1. U.S. Department of Energy, Energy Efficiency & Renewable Energy, *DOE Technical Targets for Onboard Hydrogen Storage for light-Duty Vehicles.* https://energy.gov/eere/fuelcells/doe-technical-targets-onboard-hydrogen-storage-light-duty-vehicles

2. U.S. Department of Energy, Energy Efficiency & Renewable Energy, *HyMARC: Hydrogen Materials-Advanced Research Consortium.* https://energy.gov/eere/fuelcells/hymarc-hydrogen-materials-advanced-research-consortium.

References: Subtopic d:

1. Fishel, K., Qian, G., Eisman, G., Benicewicz, B.C., 2016, Electrochemical Hydrogen Pumping, Springer International Publishing, Switzerland, p. 14. http://www.benicewiczgroup.com/UserFiles/benigroup/Documents/BB114.pdf

2. Perry, K.A., Eisman, G.A., Benicewicz, B.C., 2008, Electrochemical Hydrogen Pumping Using a High-temperature Polybenzimidazole (PBI) Membrane, *Journal of Power Sources*, Vol. 177, Issue 2, pp. 478-484. http://www.sciencedirect.com/science/article/pii/S0378775307025700#aep-abstract-id12

3. Yang, B., Manohar, A.K., Surya Prakash, G.K., Narayanan, S.R., 2011, Electrochemical Hydrogen Pumping Using A Water-free Proton-Conducting Polymer Electrolyte Mambrane, The Electorchemical Society, Abstract #337. http://ma.ecsdl.org/content/MA2011-01/6/337.full.pdf

4. Strobel, R., Oszcipok, M., Fasil, M., Rohland, B., Jorissen, L., Garche, J., 2002, The Compression of Hydrogen in an Electrochemical Cell Based on a PE Fuel Cell Design, *Journal of Power Sources*, Vol. 105, Issue 2, pp. 208-215. http://www.sciencedirect.com/science/article/pii/S0378775301009417

5. Cohen, S., Porter, S., Chow, O., Henderson, D., 2009, *Hydrogen Generation From Electrolysis*, Final Report for DOE Award DE-FC36-04GO13030, DOE/GO/13030-1. https://www.osti.gov/scitech/servlets/purl/948808/

References: Subtopic e:

1. U.S. Department of Energy, Energy Efficiency & Renewable Energy, *Integrated Nanosystems for Atomically Precise Manufacturing Workshop – August 5-6, 2015*. https://energy.gov/eere/amo/downloads/integrated-nanosystems-atomically-precise-manufacturing-workshop-august-5-6-2015

2. Foresight Institute, 2007, *Technology Roadmap for Productive Nanosystems*. https://www.foresight.org/roadmaps/

18. SUBSURFACE PERMEABILITY MANIPULATION AND FLUID CONTROL

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), in collaboration with the Geothermal Technologies Office, is using high-risk, high-reward, basic research elements to advance the state of the art in adaptive control of subsurface fractures and fluid flow. This topic seeks applications in permeability manipulation and fluid control for geothermal energy production. From beneath the surface of the earth, we currently obtain about 80-percent of the energy our nation consumes each year. In the future we have the potential to generate gigawatts of baseload electrical power from domestic geothermal energy sources. The Department of Energy established the Subsurface Technology and Engineering RD&D (SubTER) initiative to more effectively harness subsurface resources while mitigating the impacts of developing and using these resources. One of the topic areas SubTER is emphasizing for targeted research and development is permeability manipulation and fluid control.

Related to this topic, the Geothermal Technologies Office is primarily interested in applications which enhance fluid flow, while some energy applications demand reducing or eliminating fluid flow. Applications responsive to this topic will describe a project that explores the feasibility of innovative concepts in subsurface permeability manipulation and fluid control. These projects should seek to develop a basic knowledge base and capabilities to manipulate subsurface flow through an integration of physical alterations, physicochemical fluid/rock interaction processes, and novel stimulation methods implemented at the field scale and show a pathway to for commercial application of these innovative concepts. In addition to providing details about the proposed Phase I project, the applicant should also describe how they plan to scale up to the principal R&D effort if successful in proceeding to Phase II.

Grant applications are sought in the following subtopic:

a. Innovations to Enhance Fluid Flow for Increased Geothermal Development

Enhanced Geothermal Systems (EGS) are engineered reservoirs, created where there is hot rock but little to no natural permeability or fluid saturation present in the subsurface. To develop EGS, enhancing subsurface permeability is typically achieved by injecting fluid into the subsurface at pressure under a safe, controlled, environmentally responsible, and well-engineered stimulation process that will cause pre-existing fractures or weaknesses in the rock fabric to open. The pressure increase causes displacements along the fracture planes and zones of rock heterogeneity, which results in increased permeability and allows fluid to circulate throughout the rock, heating up during circulation. Via a production well, this heated fluid then transports the heat to the surface, which can be used to generate electricity. The Department estimates that EGS technologies will enable an additional 100+ GW of baseload geothermal development.

Grant applications are sought to research, develop, and deploy novel stimulation techniques that will enable commercial deployment of EGS. The approaches (or combination of approaches) could include, but are not limited to: energetic approaches (e.g., high/low explosives or propellants), chemical approaches (e.g., acidization), and/or mechanical stimulation. New materials, propellants, and energetics can be proposed along with the possibility of developing waterless stimulation techniques that reduce, or eliminate, the use of water.

These techniques should aim to deliver precise stimulation at precise locations with the desired rate of energy release. Successful application of stimulation approaches could make the difference between an economical and sustainable EGS reservoir and one that may otherwise be abandoned. Due to the nature of geothermal reservoirs, the concepts proposed must be effective in high-temperature (> 250°C), high-pressure (> 1500 bar), and hard crystalline lithologies. Applicants are encourage to quantify their predicted improvement over current state of the art.

Questions – Contact: Josh Mengers, Joshua.Mengers@hq.doe.gov

b. Other

In addition to the specific subtopic listed above, the Department solicits applications in other areas that fall within the specific scope of the topic description above. This includes innovations which impede or eliminate fluid flow in the subsurface.

Questions – Contact: Josh Mengers, Joshua.Mengers@hq.doe.gov

References:

1. Lawrence Berkeley National Laboratory, Earth Sciences Division, Subsurface Crosscut:, SubTER: Subsurface and Engineering Research, Development, and Demonstration, *Permeability Manipulation and Fluid Control*. https://eesa.lbl.gov/subter/home/permeability/

2. U.S. Department of Energy, Subsurface Technology and Engineering RD&D Crosscutting Team, Subsurface Control for a Safe and Effective Energy Future. http://energy.gov/downloads/subter-crosscut-white-paper

19. 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, conversion of coal wastes and coal plus other opportunity fuel mixtures (such as coal plus municipal solids) to produce electricity and/or liquid fuels, power plant improvement technologies related to controls and sensors, and sealant development with long-term stability for SOFC stacks. The 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. Proposals that can utilize stranded assets are encouraged.

Questions – Contact: Doug Archer, douglas.archer@hq.doe.gov

b. Conversion of Coal Wastes and Coal Plus Other Opportunity Fuel Mixtures, Such as Coal Plus Municipal Solids, to Produce Electricity and/or Liquid Fuels

Applications are invited to study the conversion of coal wastes and coal plus other opportunity fuel mixtures, such as coal plus municipal solids, to produce electricity and/or liquid fuels. The research will conduct physical experiments to study conversion kinetics, emissions characteristics, and optimization of process parameters to improve product yield and quality and minimize pollutant emissions. A techno-economic analysis quantifying the benefits of the proposed technical approach is a desirable deliverable. A process model based on experimental data and a conceptual design of the conversion reactor is also a desirable research product. Novel reaction pathways and reactor concepts for conversion of wastes to energy, such as, FastOx gasification (1), pyrolysis, or plasma induced conversion reactions are of interest. Since one need of the synthesis gas is for use to produce liquid transportation fuels, hydrogen production

is favored, whereas methane production would be a liability. Technologies amenable to modularization are of special interest to DOE, as are technologies that could be used effectively at mine-mouth, coal preparation locations, military installations, or research park facilities.

Questions – Contact: Arun Bose, arun.bose@netl.doe.gov

c. Advanced Controls with Embedded Sensing (ACES)

Fossil energy (FE)-based systems are able to achieve higher efficiencies, lower emissions, and improved reliability and availability (lower total operating costs), through advanced controls R&D, enabled by real-time sensor measurements and data. However, due to inherent challenges of FE-based systems (including high-temperatures and harsh environments where survivability and durability of sensors is a longstanding, critical issue), there are unobservable states and operating parameters that are inferred using software models or determined via proxy using periphery sensor measurements, resulting in operating schemes that, in some cases, are implemented using inadequate and/or incomplete information. Embedded sensor technology offers a promising solution to achieve enhanced process control by enabling instrumentation to be removed from direct contact with the harsh environments, and included in components with complex geometry. Additionally, embedded sensors within structures also allow for better insight into real-time component health monitoring and scheduling of maintenance.

Applications are sought that conduct advanced controls research with use of embedded sensor technology for the purpose of gaining new understanding of previously unobservable states and process engineering parameters, enabling changes to energy process control systems. Objectives for this research topic include the realization of a fully instrumented energy system process that features embedded sensor technology that is relevant to fossil energy (featuring oil, natural gas, or coal as primary fuel source) with real-time, dynamic control algorithms. Therefore, it is expected that the proposed sensor system and respective methodology to fabricate and assemble a component with embedded sensor technology will have been established prior to the time of application.

The use of embedded sensors within proposals will venture beyond direct substitution of a single measurement signal that is already accessible through traditional information and will seek non-trivial understanding and control of physical phenomena where little to no actionable information has been historically available. Examples include (but are not limited to) the use of embedded sensor technology to: i) mitigate detrimental process control scenarios and properly define the performance envelope for system components, ii) develop methodologies that merge in-situ component health monitoring into dynamic control schemes for targeted maintenance and repair, iii) observe the impact of process input parameters on degradation and life cycle management of system components, and iv) optimize the operation of a reactor through improved resolution of physical state measurement, such as multipoint sensing of temperature through sensor(s) embedded in the reactor wall.

Questions – Contact: Sydni Credle, sydni.credle@netl.doe.gov

d. Sealant Development with Long-Term Stability for SOFC Stacks

Among power generation systems, solid oxide fuel cells (SOFC) which operate in the temperature range between 700 and 900°C have higher potential efficiency and more fuel flexibility with carbon storage capability. However, the internal fuel leakage can lower fuel utilization within SOFC systems resulting in less efficiency. In addition, the direct mixing of fuel and air causes low Nernst potential and accelerates

cell degradation due to local combustion. In order to get a higher efficiency and longer durability, a seal plays a critical role in preventing both fuel leakage and direct mixing of fuel and air. Therefore, the development of seal materials is one of the key challenges for SOFC stacks.

Grant applications are sought for research and development of seal materials that can be stable for at least 40,000 hours at SOFC operating temperatures and withstand numerous thermal cycles between room temperature and operating temperature. The seal materials have to meet the chemical and physical criteria as follows: be an electrical insulator to the SOFC stack, match coefficient of thermal expansion (CTE) to other SOFC components (10-12 ppm/K), be chemically compatible to other SOFC components (no poisoning), and have chemical stability at operating temperature in oxidizing and wet reducing atmospheres. The applicant must provide the set of seal materials that can meet the criteria which was described above based on a thermodynamic calculation, a complete description of how those materials meet the criteria through a scientific explanation or a literature search and experimental work plan on a few selected seal materials. The seal materials have to be tested with a SOFC cell electrochemically including leakage test at operating condition for at least 3,000 hours with 50 times thermal cycles.

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

References: Subtopic a:

1. Armor, J.N., 2013, Emerging Importance of Shale Gas to Both the Energy & Chemicals Landscape, *Journal of Energy Chemistry*, Vol. 22, Issue 1, pp. 21-26. http://www.sciencedirect.com/science/article/pii/S2095495613600029?via%3Dihub

2. National Academy of Sciences, Engineering, and Medicine, 2016, *The Changing Landscape of Hydrocarbon Feedstocks for Chemical Production: Implications for Catalysis: Proceedings of a workshop*, Proceedings of a Workshop, Washington, DC, The National Academies Press, doi: 10.17226/23555. https://www.nap.edu/catalog/23555/the-changing-landscape-of-hydrocarbon-feedstocks-for-chemical-production-implications

3. American Chemistry Council (ACC), Economics & Statistics Department American Chemistry Council, 2017, *The Potential Economic Benefits of an Appalachian Petrochemical Industry*, p. 28. https://www.americanchemistry.com/Appalachian-Petrochem-Study/

4. Sulogna, R., Elsevier B.V., 2017, Consider Modular Plant Design, *Chemical Engineering Progress*, Vol. 113, Issue 5, pp. 28-31, ISSN: 0255-2701. https://www.aiche.org/resources/publications/cep/2017/may/consider-modular-plant-design

References: Subtopic b:

1. White, R., and Roberts, M., 2017, FastOx Gasification: An Integrated Solution to Zero Waste, *Materials for Energy, Efficiency and Sustainability,* TechConnect Briefs 2017, ISBN 978-0-9975117-9-6 https://techconnect.org/proceedings/paper.html?volume=TCB2017v2&chapter=10&paper=950

2. Sulogna, R., Elsevier B.V., 2017, Consider Modular Plant Design, *Chemical Engineering Progress*, Vol. 113, Issue 5, pp. 28-31, ISSN: 0255-2701. https://www.aiche.org/resources/publications/cep/2017/may/consider-modular-plant-design

References: Subtopic c:

1. U.S. Department of Energy, National Energy Technology Laboratory, *NETL Research*. https://www.netl.doe.gov/research.

2. U.S. Department of Energy, National Energy Technology Laboratory (NETL), 2016, Crosscutting Research & Analysis Program: Sensors and Controls Portfolio, p. 66. https://www.netl.doe.gov/File%20Library/Research/Coal/cross-cutting%20research/CCR-Sensors-and-Controls-2016.pdf

References: Subtopic d:

1. Chou, Y.-S., Choi, J.-P., Xu, W., Stephens, E., Koeppel B., and Stevenson, J., 2014, *Compliant Glass Seals for SOFC Stacks*, Pacific Northwest National Laboratory, Richland, WA, p. 46. http://www.pnnl.gov/main/publications/external/technical_reports/PNNL-23397.pdf

2. U.S. Department of Energy, Office of Fossil Energy, Clean Coal Research Program, 2013, Solid Oxide Fuel Cells, Technology Program Plan, p. 70 http://www.netl.doe.gov/File%20Library/Research/Coal/energy%20systems/fuel%20cells/Program-Plan-Solid-Oxide-Fuel-Cells-2013.pdf

20. ADVANCED FOSSIL ENERGY SEPARATIONS AND ANALYSIS 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 Separations and Analysis 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 systems and natural gas recovery systems.

The only areas considered under this topic include research and technology issues and opportunities for supercritical water technologies to treat fracking water, advanced shale gas recovery technologies for horizontal well completion optimization, novel concepts for online, real-time monitoring of liquid phase selenium in pulverized coal power plant wastewaters, and coal beneficiation. The 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 and scope 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. Supercritical Water Technologies to Treat Fracking Water

A supercritical fluid is any substance at a temperature and pressure above its critical point, where distinct liquid and gas phases do not exist. It can effuse through solids like a gas, and dissolve materials like a liquid. In addition, close to the critical point, small changes in pressure or temperature result in large changes in density, allowing many properties of a supercritical fluid to be "fine-tuned" (1). In a range of industrial and laboratory separations processes supercritical fluids are used as a substitute for organic solvents. Most recently, carbon dioxide and water are the most commonly used supercritical fluids, with carbon dioxide being used in power generation for higher efficiencies with smaller footprint (2)

Water is highly polar at room temperature and is a solvent that can dissolve salts and other inorganics but becomes completely non-polar above the critical point and can precipitate out the salts. The Department of Energy Fossil Energy Office is seeking novel proposals that are modular and economic to treat fracking water which has high levels of dissolved solids (greater than sea water (~33,000 ppm) in many instances) by using the supercritical properties of water. The process desired should be such that the biologics and organics are destroyed and the inorganics are removed for the subsequent use of the water in cooling processes or for further treatment to make it potable. Additional advantages of having such a process available for fracking water is that heavy metals that come out of fracking can be separated for value addition.

Most supercritical fluid technology has been confined to the laboratory since it is expensive. The key requirement for this process will be that it has to be competitive or improve upon the energy requirement of conventional reverse osmosis (RO) techniques (3) that are currently used. It is anticipated that widespread commercial application of such supercritical application to clean water requires a reactor design capable of resisting fouling and corrosion under supercritical conditions including novel techniques to recuperate any heat losses to keep the process competitive with RO. Technologies amenable to modularization are of special interest to the DOE, as are technologies that are efficient and could be used effectively at coal mining locations.

In Phase I of this project it is expected that a demonstrable process that can achieve the target of getting the water down to 1000 ppm levels will be put together. It is also expected that fundamental questions listed below will be answered, with clear analysis that takes economics into consideration. The questions include:

1. Can the energy parity with RO can be achieved? Would it be through heat or pressure recovery in some

way or incineration of organics or both or some other way?

2. How is the proposed solution going to offset the capital costs for sustaining super critical conditions? Can the system proposed be cost competitive in a situation where produced water from Enhanced Oil Recovery (EOR) is cleaned for re-injection?

3. Could you recover fractionally or selectively precipitate metals, salts etc. into separate pure streams for adding value? If so, is there a cost competitive model that shows benefits from such recovery that includes costs of separations?

4. How difficult is the challenge of corrosion and degradation of materials under super critical conditions and is this problem such that it retracts this process when compared to anti fouling in RO membranes?

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

b. Increasing Recovery of Oil and Natural Gas Resources

DOE is interested in developing novel technologies that can: (1) improve our ability to characterize hydraulic fractures, and further, (2) that can advance the application of enhanced recovery methods to unconventional oil and natural gas reservoirs. Advances in either of these two areas could improve recovery of hydrocarbons in place in shale reservoir rocks. In the first case, finding ways to directly characterize the height, length and orientation of hydraulic fractures will provide a long-sought point of reference for optimizing hydraulic fracture treatments. Micro-seismic fracture monitoring is currently the best alternative for approaching this solution but it remains a less than perfect option. In the second case, catalyzing the development and testing of new technologies for increasing the volume of recoverable oil, condensate and natural gas, through the use of injectants like CO_2, is critical to maximizing the recovery of unconventional resources.

Area 1 - Advanced Hydraulic Fracture Diagnostics for Unconventional Oil and Natural Gas Wells

This topic invites proposals for research that is focused on developing novel technologies for more accurately characterizing the orientation and dimensions of hydraulic fractures, in support of efforts to increase the efficiency of fracturing and increase recovery efficiency in unconventional oil and natural gas wells.

The current categories of diagnostic tools (Cipolla and Wright, 2000) include a variety of methods for near-wellbore fracture diagnostics (e.g., production and temperature logs, tracers, borehole imaging) as well as a variety of far-field techniques (e.g., microseismic fracture mapping), but none of these succeed in consistently providing a fully detailed and accurate description of the character of created fractures.

DOE has several projects currently underway that seek to expand the tools available for fracture diagnostics. These include a combination of highly sensitive borehole sensors coupled with proppant-sized acoustic emitters that can signal from within a created fracture, electromagnetic logging tools that can image the dimensions of a fracture filled with conductive proppant, enhanced logging methods and permanent downhole seismic sensors.

DOE is interested in building upon its existing research portfolio by developing new ways to reduce the cost and/or enhance the accuracy of existing or under-development technologies and methods for hydraulic fracture diagnostics, or by researching entirely new solutions.

Specific concepts could include innovative and breakthrough technologies for improved subsurface characterization, visualization, and diagnostics, including:

- Near-wellbore fracture diagnostic methods
- Far-field fracture diagnostic methods
- Intelligent proppant systems.

Area 2 - Innovative Technologies to Enhance Gas or Oil Recovery (EGR/EOR) from Tight Formations
Conventional enhanced oil recovery techniques are being applied to unconventional reservoirs to improve low primary recovery factors. For example, EOG has successfully tested miscible gas injection in the Eagle Ford play and is expanding its pilot program. In the Bakken Shale play, a lab testing by a North Dakota research consortium has shown promise for the use of CO_2 to increase oil recovery, although initial field tests have not as yet borne out this lab-predicted potential. While many operators are seeking to apply improved well design and hydraulic fracturing techniques to increase per well recoveries beyond the relatively low percentages of in-place hydrocarbons witnessed, there may still be significant potential for enhancing recovery of liquids and gas from tight reservoirs using injected fluids.
Proposals are sought for research to develop and test new methods (or to repurpose existing methods) for enhancing oil and gas recovery from tight formations. Such proposals may include:

- Core tests using recovered core from tight oil plays that evaluate the ability of injectants to enhance recovery
- Modeling of enhanced recovery processes within stimulated reservoir volumes with hydraulic and natural fractures
- Field pilot tests of novel processes in established or emerging plays

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

c. Novel Concepts for Online, Real-time Monitoring of Liquid Phase Selenium in Pulverized Coal Power Plant Wastewaters

Selenium has been identified as a toxic pollutant in the Clean Water Act (CWA) list of Priority Pollutants 307(a)(1) which are further referenced and defined in the Code of Federal Regulations 40 CFR 401.15.1. Effluent Guidelines are national regulatory standards issued by the U.S. Environmental Protection Agency (EPA) for wastewater discharged to surface waters and municipal sewage treatment plants.

In 2015, U.S. EPA finalized new effluent limitation guidelines (ELGs) pertaining to total dissolved solids, mercury, selenium, nitrates, and arsenic in effluent streams from steam power generation plants. The specific ELG selenium guidelines for power plant flue gas desulfurization wastewaters are as follows:

Flue Gas Desulfurization Wastewater (Existing Sources)		**Flue Gas Desulfurization Wastewater (New Sources + Incentive Program)**	
Selenium, ppb		Selenium, ppb	
30-day Average	12	30-day Average	N/A
Daily Maximum	23	daily Maximum	5

In 2017, the US EPA issued a stay on the November 2018 compliance date to further review the regulations.

The capture, measurement, and monitoring of selenium in power plant effluent streams remains a needed area of further research. The amount and form of selenium in power plant wastewaters can vary depending upon changes in fuel or flue gas particulate and desulfurization control equipment operation. The removal of selenium from power plant wastewaters using convention means can be problematic in many instances. Biological systems are subject to upset conditions if the bacteria doing the work die off, or if changes in loading, pH, or temperature exceed limits. Further, some types of chemical/physical treatment may not be effective for selenate removal. Therefore, it is important to have on-line, real-time monitoring of liquid phase selenium.

The use of available commercial online monitoring analyzers can be problematic and in need of development to eliminate plugging caused by supersaturation of sulfates, to operate with higher suspended solids content, to improve the analyzer availability and reliability, and to eliminate other interferences in the effluent stream.

Proposals are sought to develop novel concepts for real-time, online liquid phase selenium measurements in power plant effluent streams. The selenium real time, on-line analyzer development is to involve designs which are capable of long term operation without corrosion from dissolved chlorides, plugging, and without the need for frequent calibration or upkeep. Analyzers should be suitable for use in the presence of suspended solids, and capable of measuring total selenium along with the primary speciated forms of selenium; selenate and selenite. The selenium analyzer should target near-term field testing and be capable of measuring selenium at concentrations, flow rates, pressures, and temperatures that are present in power plant wastewaters.

Questions – Contact: Robie Lewis, robie.lewis@hq.doe.gov

d. Coal Beneficiation

In the mining industry beneficiation in extractive metallurgy, is any process that improves (benefits) the economic value of the ore by removing the gangue minerals, which results in a higher-grade product (concentrate) and a waste stream (tailings). Coal beneficiation can not only improve the quality of raw coal by either reducing the extraneous matter that gets extracted along with the mined coal or reducing the associated ash or both, but also can provide opportunities to liberate other higher value products that are contained in raw coal.

Area 1: Improved Coal Preparation Processes

Coal preparation which includes washing, cleaning, processing and beneficiation, is the method by which mined coal is upgraded in order to satisfy size, purity specifications, or enhance unique qualities defined by a given market to improve efficient utilization of domestic resources. Coal preparation operations make it possible to meet coal specifications by removing impurities from run-of-mine (ROM) coals prior to shipment to power stations.

Coal preparation or beneficiation offers many attractive benefits for coal-fired power generation. These include low cost transportation, improved properties for coal utilization, and reduced particulate emissions and gaseous pollutants. Novel technologies need to be developed. Specific technical areas include fine

particle cleaning, fine particle dewatering and inherent moisture reduction, dry separation processes, and low rank coal upgrading.

Area 2: Coal Beneficiation for Liberation of Rare Earth Elements
Efforts shall be directed to the liberation of REE-containing minerals (i.e., <5-10 micron) from coal and coal by-product materials. Efforts shall be focused on coal preparation or beneficiation, using current/conventional grinding technologies, as well as modification to equipment, procedures, additives, etc., to primarily optimize REE liberation, separation and extraction from coal-based resources, as well as to assist in the generation of alternate co-product materials (i.e., micronized coal particles, carbon, scandium, magnetite, etc.) during the separation and extraction of REEs. REE drivers include: national security, environmental impact, economic markets, and development of domestic infrastructure.

Area 3: Coal Beneficiation for Production of Nano-materials
Efforts shall be directed to coal beneficiation for production of nano-materials for development of carbon nanotubes for reinforcement of metal composites and/or concrete, carbon fiber reinforced polymers (CFPR), and nanotube filaments for 3D printing fluids and nano-enabled textiles. Carbon nano-material drivers include development of high value market products as carbon-based electronics, printed supercapacitors based on graphene aerogels, etc., and advancements to bio- and medical imaging, optoelectronics, and the aerospace, automotive, energy (wind), etc., industries.

Questions – Contact: Barbara Carney, Barbara.carney@netl.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

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21. 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. Technology Transfer Opportunity: Membraneless Seawater Desalination with a Bipolar Electrode

Researchers at The University of Texas at Austin have developed a novel, membraneless desalination process. The process uses a microfluidic device to flow high salinity water to a microelectrode positioned at the intersection of an inlet channel and two outlet channels. Under an applied voltage, and in the presence of this flow of saltwater, the microelectrode generates an electric field gradient across the intersection of the channels, which preferentially directs ions into one outlet channel, while the partially desalted water flows to the other outlet channel. The concept, called electrochemically mediated desalination (EMD), potentially can be scaled and made massively parallel. That is, while the flow rate through an individual microchannel is small, stackable arrays of these devices may be able to generate meaningful volumes of fresh water from high-salinity feed, while using less energy than reverse osmosis (RO). Unlike RO, the process has no membrane or the associated maintenance costs. The required voltage is low and the required electrical current is both low and DC, which should integrate well with renewable energy sources.

Licensing Information:
The University of Texas at Austin
Contact: Les Nichols (nichols@otc.utexas.edu, (512) 471-0275)
TTO Tracking Number: UT Tech ID 6210 CRO
Patent Status: U.S. Pat. App. 14/136,541
Type of License: Non-exclusive
USPTO Link: http://appft.uspto.gov/netacgi/nph-Parser?Sect1=PTO1&Sect2=HITOFF&d=PG01&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.html&r=1&f=G&l=50&s1=%2220140183046%22.PGNR.&OS=DN/20140183046&RS=DN/20140183046
Website: https://research.utexas.edu/otc/available-technologies/at-display/?pk=1005

Questions – Contact: Raul Miranda, 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.

22. 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

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. 2H, 18O, CH4, CO2, 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 or Paul Bayer, 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 or Paul Bayer, paul.bayer@science.doe.gov

References: Subtopic a:

1. BERAC, Paul Adams, Lawrence Berkeley Laboratory, 2017, DOE BER Workshop Report: Technologies for Characterizing Molecular and Cellular Systems Relevant to Bioenergy and Environment, p.19. https://science.energy.gov/~/media/ber/berac/pdf/201704/Adams_BERAC_Apr_2017.pdf

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

References: Subtopic b:

1. U.S. Department of Energy, 2016, Office of Biological & Environmental Research: Climate and Evironmental Sciences Division (CESD), Subsurface Biogeochemical Research (SBR) Program. http://science.energy.gov/ber/research/cesd/subsurface-biogeochemical-research/.

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23. 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**

An objective of the Climate and Environmental Sciences Division within the Office of Biological and Environmental Research is to use data from field campaigns and long-term observations to quantify local atmospheric aerosol, cloud, and precipitation processes, including aerosol formation, chemical evolution, and optical properties; initiation of cloud droplets, ice crystals, and precipitation; and feedbacks involving the terrestrial-aerosol-cloud system (Reference 1). 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).

While existing technologies can measure 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 deployment at field sites and that has lower weight and power requirements for deployment at remote field sites with limited power or for deployment on small aerial platforms.
This topic is specifically focused on developing technologies for robust field-deployable measurements of aerosol chemical composition; instruments capable of deployment on small aerial platforms for measurement of cloud condensation nuclei, ice nuclei, or particles in mixed-phase clouds; and field-deployable aerosol absorption measurements.

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) describe the purpose and benefits of any proposed teaming arrangements with government laboratories or universities, and (2) 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 are sought in the following subtopics:

a. Aerosol and Cloud Measurements from Small Aerial Platforms
Small aerial platforms, including unmanned aerial systems (UAS), tethered balloons, and kites, provide an innovative approach for making atmospheric measurements in conditions that are logistically difficult for ground-based measurements, that are too dangerous or cost-prohibitive for manned aircraft, or under operating conditions (e.g., slow airspeeds or low altitudes) that are more difficult for large or manned platforms (Reference 3-4). The Atmospheric Radiation Measurement (ARM) Facility is currently operating

tethered balloon systems (Reference 5) and is developing capabilities for mid-size UAS flights (Reference 6). While small aerial platforms are gaining increased use in the scientific, civil, and defense arenas, there is still a lack of sophisticated observing capabilities for important aerosol and cloud variables that have been miniaturized for deployment on such platforms.

Instrument packages developed to measure aerosol and cloud properties have been successfully deployed from research aircraft in a wide range of atmospheric conditions. However, traditional instrument packages typically are too large and heavy and/or require too much power to be used on small aerial platforms, such as UAS, tethered balloons, or kites. A need exists for instrument packages capable of installation on a small aerial platform with capabilities to measure properties of aerosols, cloud droplets, and/or glaciated hydrometeors (Reference 3-4).

Grant applications are sought to develop lightweight and low power (suitable for sampling from UAS, tethered balloons, or kite platforms) instruments for (1) a fast spectrometer for measurement of cloud condensation nuclei number concentrations over supersaturation ranges of the order 0.02% – 1%, and (2) a spectrometer/counter for ice nuclei (IN) number concentrations over effective local temperatures down to -38 °C.

Instruments must be capable of operating on light-weight airborne platforms such as UAS's and tethered balloons with little or no temperature or pressure controls. Particular aerial platforms of interest for instrument deployment include the Skydoc #26 aerostat (http://www.skydocballoon.com/aerostats.html) and the Navmar TigerShark UAS (https://www.nasc.com/Tigershark.php). We are particularly interested in instruments that weigh less than 6 kg and require less than 150 W of power and that are capable of operating in Arctic conditions (temperatures down to -40 degrees C).

Questions – contact: Rickey Petty, rick.petty@science.doe.gov (platform related) or Ashley Williamson, ashley.williamson@science.doe.gov (sensor related)

b. Robust Field-Deployable Measurements of Aerosol Composition

Atmospheric aerosol particles may be caused by natural as well as anthropogenic sources and may form either from emissions of primary particulate matter or through formation of secondary aerosols from gaseous precursors. Aerosol chemical composition is quite variable in space and time, depending on the emission sources and chemical processing and removal in the atmosphere (Reference 2). Knowledge of the composition of aerosol particles is an important factor in understanding their sources, formation, impact on cloud microphysics and the earth's radiation budget. Long-term measurements of aerosol composition, in concert with measurement of cloud parameters and background meteorology, are critical to improving the understanding and numerical modeling of aerosol and cloud formation processes.

Major aerosol components of interest include, in particular, secondary inorganic sulfate and nitrate compounds, mineral dust and sea spray, and complexes that contain, e.g., oxidized organic material with other residues. Aerosol chemical composition is historically measured using a variety of techniques, typically more than one analytical method being required to measure all components efficiently. While many research-grade instruments are used for short-term studies involving intensive field campaigns, issues of cost, manpower, and durability limit the methods available for long-term continuous measurements of aerosol composition. Most long term networks, including the Interagency Monitoring of Protected Visual Environments (IMPROVE) network, use filter-based samplers to collect (typically over a

period of 24 hours) time-integrated samples followed by offline chemical analysis. This strategy allows relatively simple unattended and robust field operation suitable for unattended sites while allowing state of the art analytical techniques even when the samples are acquired at remote locations. It also allows minimization of the field portion of the operating costs, but requires considerable operational costs to maintain the analytical infrastructure. A further tradeoff is that bulk samples allow typically low detection limits at the expense of time resolution.

DOE ARM has made chemical composition measurements both at ARM permanent sites and at locations sampled during ARM Mobile facility campaigns, using a suite of instruments including mass spectral instruments (either single particle or short-time integrated) for near real-time data collection, time resolved collection for later analysis, or short-term wet chemical collection with a Particle Into Liquid Sampler (PILS). In contrast to the daily sampling network strategy involving filters as described above, DOE has attempted to use techniques that retain higher time resolution to resolve atmospheric processes which impact aerosol composition. One limitation of several techniques is insensitivity of some methods to some species of interest (especially those characterized by very low vapor pressure, water-insoluble or otherwise difficult to isolate). Even for the measurements with satisfactory detection capability, a practical limitation for long-term deployments is the need to operate with minimal expert attention while measuring an array of desired species in an automated, low-cost, and reliable manner while maintaining the necessary accuracy and detection limits. Specific points of weakness are the need for frequent expert calibration and maintenance of instrumentation, requirements for extensive post-collection chemical analysis or labile calibrants, or need for extensive manual data analysis.

Therefore, grant applications are sought to develop new measurement technologies and/or to improve instruments using current measurement principles, with a goal to allow long-term, continuous measurements of key atmospheric aerosol components listed above, including non-refractory organics (commonly called OA), nitrate, sulfate, ammonium, mineral dust and at certain sites sea salt.

Measurements need to be autonomous or semi-autonomous with operations, calibrations and maintenance routinely conducted by general instrument technicians rather than experts in aerosol instrumentation. While prototype systems need not be immediately able to operate in autonomous mode, such operation should be anticipated or at least compatible with the system design and operating principle. Other desirable characteristics of robust field deployable systems include:

- Size: standard rack-mountable instrument (or smaller footprint).
- Power: ideally able to be powered from of a variety of different international power supplies, e.g. 50 or 60 Hz, 110 or 220 V.
- Shipping: custom shipping container or recommended procedure for protecting the instrument when shipping internationally.
- Routine Operations
- Low level of daily maintenance required to ensure high data quality.
- Low level of training required for continuous measurements at remote field site locations.
- Calibrations: as automated as possible so that a high level of scientific expertise is not required to maintain the instrument at the field site to ensure high quality data. Some examples include, but are not limited to:
- Automated valve switching for the routine sampling of a calibrant that does not require any manual switching from ambient sampling lines

- Calibrations that a general technician can be trained to do routinely and do not require scientific expertise.
- If solutions are required, that they are prepared autonomously and do not require wet chemistry skills/labor to be done in the field, e.g. the preparation of high precision chemical standards.
- Maintenance and Serviceability: spare parts and consumables are easy (not time-consuming) to procure, store, and ship to remote locations. For example, limited use for spares that require special offline upkeep, storage or shipping requirements (e.g., hazardous chemicals and/or radioactive materials).

Grant applications should specify the proposed analytes, and document anticipated performance characteristics which represent improvements over other available techniques. Applications should specifically address expected requirements for maintenance and calibration. Detection limits should be appropriate to the analytes, but adequate to measure expected fractions of ambient aerosols at relatively clean (< 5 μg/m3 average) locations. Applications must provide convincing documentation (experimental data, calculations, and simulation as appropriate) to show that the sensing method is both sensitive (i.e., low detection limit), precise, and highly selective to the target analyte(s), (i.e., free of anticipated physical/chemical/biological interferences). Approaches that leave significant doubt regarding sensor functionality for realistic multi-component aerosol samples and realistic field conditions will not be considered.

Questions – contact: Ashley Williamson, ashley.williamson@science.doe.gov

c. Field-Deployable Aerosol Absorption Measurements

Atmospheric aerosols exert a dominating influence on both cloud formation and the earth's radiation balance, yet the processes that govern cloud-aerosol interactions are poorly understood and represent major sources of uncertainty in predictive models. 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, i.e., 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 that, in turn, affects 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, wildfire smoke, 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 7).

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. 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.

The following technical specifications are strongly desired:

- A sensitivity goal of 1 Mm^{-1} (2σ 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 ~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
- Potential 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: Ashley Williamson, ashley.williamson@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: Rickey Petty, rick.petty@science.doe.gov (platform related) or Ashley Williamson, ashley.williamson@science.doe.gov (sensor related).

References:

1. U.S. Department of Energy, 2012, Climate and Environmental Sciences Division Strategic Plan, DOE/SC-0151. http://science.energy.gov/ber/research/cesd/

2. Stocker, T.F., Qin, D., Plattner, G.-K., Tignor, M., et al., IPCC, 2013, Climate Change 2013: The Physical Science Basis, Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, p.1535, doi:10.1017/CBO9781107415324. http://www.climatechange2013.org/report/full-report/

3. U.S. Department of Energy, 2015, Climate and Environmental Sciences Division, Aerial Observation Needs Workshop, p. 50, DOE/SC-0179. https://science.energy.gov/~/media/ber/pdf/workshop%20reports/CESD_AerialObsNeeds_Workshop_2015web.pdf

4. U.S. Department of Energy, Ivey, M., Petty, R., Verlinde, J., et al., 2013, *Polar Research with Unmanned Aircraft and Tethered Balloons*, A Report from the Planning and Operational Meeting on Polar Atmospheric Measurements Related to the U.S. Department of Energy ARM Program Using Small Unmanned Aircraft Systems and Tethered Balloons, p. 36, DOE/SC-ARM-TR-135. http://www.arm.gov/publications/tech_reports/doe-sc-arm-tr-135.pdf?id=6

5. Dexheimer, D., Sandia National Laboratories, 2016, Tethered Balloon System Operations at ARM AMF3 Site at Oliktok Point, AK, 2016 Atmospheric Radiation Measurement (ARM)/Atmospheric System Research (ASR) joint User Facility/PI meeting, p. 12. http://asr.science.energy.gov/meetings/stm/2016/presentations/143.pdf

6. Schmid, B. and Ivey, M., 2016, *ARM Unmanned Aerial Systems Implementation Plan*, DOE ARM Climate Research Facility, p. 28, DOE/SC-ARM-16-054. https://www.arm.gov/publications/programdocs/doe-sc-arm-16-054.pdf

7. U.S. Department of Energy, Biological and Environmental Research Climate and Environmental Sciences Division, 2016, *Absorbing Aerosols Workshop Report*, p. 40, DOE/SC-0185. (http://science.energy.gov/~/media/ber/pdf/workshop%20reports/CESD-AbsorbingAerosol2016.pdf

24. 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 light 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 subtopic 01b “Advanced Data Analytic Technologies for System Biology and Bioenergy”.

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

b. Other

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

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

References:

1. U.S. Department of Energy, Office of Biological and Environmental Research, 2015, Biological Systems Science Division, Strategic Plan, p. 18. http://genomicscience.energy.gov/pubs/BSSDStrategicPlan.pdf

2. BER Structural Biology Resources at Synchrotron and Neutron Facilities. http://www.BERStructuralbioportal.org

25. 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

b. Other

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

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

References:

1. U.S. Department of Energy, 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

2. U.S. Department of Energy, Office of Biological and Environmental Research, 2015, *New Bioimaging Technologies for Plant and Microbial Systems*, p, 16. https://science.energy.gov/~/media/ber/pdf/community-resources/bioimaging_technologies.pdf

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

26. TECHNOLOGY TRANSFER OPPORTUNITIES: BIOLOGICAL AND ENVIRONMENTAL RESEARCH

Maximum Phase I Award Amount: **$225,000**	*Maximum Phase II Award Amount:* **$1,500,000**
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.

DOE's Office of Biological and Environmental Research (BER) Genomic Science Program supports fundamental research and technology development to achieve a predictive systems-level understanding of complex biological systems to advance DOE missions in energy and the environment. Development of innovative approaches for sustainable bioenergy production will be accelerated by systems biology understanding of non-food plants that can serve as dedicated cellulosic biomass feedstocks or microbes capable of deconstructing biomass into their sugar subunits and synthesizing next generation biofuels (either from cellulosic biomass or through direct photosynthetic conversion). The Genomic Science program's research also brings the -omics driven tools of modern system biology to bear on analyzing

interactions between organisms that form biological communities and with their surrounding environments.

BER established three Bioenergy Research Centers (BRCs) in 2007 to pursue the basic research underlying a range of high-risk, high-return biological solutions for bioenergy applications. Advances resulting from the BRCs are providing the knowledge needed to develop new biobased products, methods, and tools that the emerging biofuel industry can use. The three Centers are based in the Southeast, the Midwest, and the West Coast, with partners across the nation. DOE's Lawrence Berkeley National Laboratory leads the DOE Joint BioEnergy Institute (JBEI) in California, DOE's Oak Ridge National Laboratory leads the BioEnergy Science Center (BESC) in Tennessee, and the University of Wisconsin-Madison leads the Great Lakes Bioenergy Research Center (GLBRC).

The goal for the three BRCs is to understand the biological mechanisms underlying biofuel production from cellulosic biomass so that these mechanisms can be improved, and used to develop novel, efficient bioenergy strategies that can be replicated on a mass scale. Detailed understanding of many of these mechanisms form the basis for the BRCs' inventions and tech-transfer opportunities, which enable the development of technologies that are critical to the growth of a biofuels industry.

Successful applicants will propose R&D that will lead to biofuel or bioproduct commercialization utilizing one of the TTOs listed below. Applications that propose technologies related to a TTO but that do not directly utilize a TTO will not be funded. Applications should include sufficient preliminary data and scientific detail so that expert reviewers will understand both the potential benefits and the challenges that may be encountered in carrying out the proposed research. Challenges should be identified, and solutions should be proposed that will explain how the PI's team will overcome the challenges. Applications should address potential risks such as biocontainment challenges as well as strategies to mitigate those risks.

Questions – Contact: Ramana Madupu, ramana.madupu@science.doe.gov

Grant applications are sought in the following subtopics: a-p total 17 including 6 BESC and 11 GLBRCs TTOs

a. Mutualistic Microbes for Plant Productivity- SAFE Bio-Fertilizer

ORNL researchers have studied the impact of a constructed multiple-microbial member community for a bio-fertilizer for increased plant productivity. The bio-fertilizer is a mix of naturally occurring microbes (fungi and bacteria) that are symbionts that can advance food and energy (SAFE) crops, coined as SAFE bio-fertilizer. Initial greenhouse studies showed that the SAFE bio-fertilizer had a significant higher biomass yield on both poplar and corn plants. Field crop studies in both poplar and corn confirmed the increased plant growth and additional benefits from the soil microflora such as increased pathogen resistance and increased crop drought tolerance. The bio-fertilizer can be readily applied to seeds, plant surfaces, or soils, and is stable at the field-scale. Application of SAFE bio-fertilizer is flexible in both formulation and agnostic to agriculture practice. Experimental validated advantages observed across different poplar and corn plant systems in the greenhouse at ORNL, and cases with completed field studies, include (1) superior germination frequencies for faster crop establishment (poplar and corn, field studies), (2) increased growth and biomass (poplar and corn, field studies), (3) increased plant defense against pathogens, (4) improved drought tolerance (poplar, field studies), and (5) improved soil heath (corn, field studies).

Licensing Information:
Oak Ridge National Laboratory
Contact: Jennifer Caldwell (caldwelljt@ornl.gov, 865-574-4180)
TTO Tracking Number: UTB ID 201503575
Patent Status: US Patent Application 14/852,073 filed on 9/11/2015
Type of License: Available for either exclusive or nonexclusive licensing
USPTO Link: N/A
Website: https://www.ornl.gov/partnerships/mutualistic-microbes-plant-productivity

b. Improved Enzymes for Biomass Conversion

Transferring CelA technology. This technology deals with a Hyperthermophillic enzyme system and methods to improve the performance of this enzyme and mixture of enzymes that contain the CelA enzyme.

Licensing Information:
NREL/BESC
Contact: Eric Payne (eric.payne@nrel.gov, 303-275-3166)
TTO Tracking Number: internal ref 12-28
Patent Status: Issued U.S. patent 9,249,432
Type of License: TBD
USPTO Link: http://appft1.uspto.gov/netacgi/nph-Parser?Sect1=PTO1&Sect2=HITOFF&d=PG01&p=1&u=/netahtml/PTO/srchnum.html&r=1&f=G&l=50&s1=20140017735.PGNR.
Website:

c. Use of Extremophiles and their Enzymes for the Production of Biofuels, Biomaterials and other Commodity Chemicals

A collaboration between UGA and NCSU researchers led to the development of a portfolio of technologies that take advantage of characteristics of P. furiosus (a hyperthermophile) to metabolize CO2 into chemical commodities. The portfolio includes isolated recombinant enzymes, as well as microbial constructs and methods of using the same. The portfolio includes IP co-owned by the two institutions as well as "UGA-only" IP and may include know how and information about the genetics of the microorganism.

Licensing Information:
North Carolina State University, The University of Georgia
Contact: Kultaran Chohan, Ph.D., LL.M., CLP (kultaran_chohan@ncsu.edu, 919-513-1322)
TTO Tracking Number: UGA Dockets: 1563, 1576, 1889, 1964, 2154. NCSU Dockets: 13003, 12192, 14124
Patent Status: US Patent 9,249,440; US Patent 9,587,256; US Patent 8,927,254
Type of License: Either, at licensee's choice. Candidate licensee must identify field of use for the license/option when approaching TTO.
USPTO Link: http://patft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-tool.html&r=0&f=S&l=50&TERM1=Adams&FIELD1=INNM&co1=AND&TERM2=Georgia&FIELD2=ASNM&d=PTXT
Website:

d. (This technology transfer opportunity is no longer available. Applications will not be accepted for this subtopic.)

e. Genetic Regulation for Lignin Reduction and Flavonoid Enhancement in Sorghum Plants (outside of forage uses)

ORNL researchers have studied natural variation in lignin content in a population of Poplar trees to understand the genetic basis of cell wall recalcitrance effecting the conversion of biomass into biofuels and bioproducts. This research resulted in the identification of a gene with major effects on lignin biosynthesis, the key polymer hindering efficient biomass digestibility. This gene regulates carbon flow entering the phenylpropanoid, tyrosine, flavonoid and tryptophan pathways. Variants of the gene function by redirecting carbon flux from lignin biosynthesis toward flavonoid or tryptophan biosynthesis resulting in highly increased accessibility to cellulose. In addition to utility in biofuels production, this genetic regulator has application in forage crops where low lignin and high flavonoid content are both highly valued traits for improved digestibility and reduced proteolysis, respectively. The newly identified gene can be manipulated in Sorghum and this Technology Transfer Opportunity is specific to the application of this ORNL technology in Sorghum plants.

Licensing Information:
Oak Ridge National Laboratory
Contact: Jennifer Caldwell (caldwelljt@ornl.gov, 865-574-4180)
TTO Tracking Number: UTB ID 201403346
Patent Status: US Patent Application 14/720,023 filed on 5/22/2015
Type of License: Available for exclusive licensing for the field of use for Sorghum plants.
USPTO Link: http://appft1.uspto.gov/netacgi/nph-Parser?Sect1=PTO1&Sect2=HITOFF&d=PG01&p=1&u=/netahtml/PTO/srchnum.html&r=1&f=G&l=50&s1=20150353948.PGNR.
Website: https://www.ornl.gov/partnerships/genetic-regulation-lignin-reduction-and-flavonoid-enhancement-plants

f. Ethanol Tolerant Yeast for Improved Production of Ethanol from Biomass

UW–Madison researchers have developed a method to impart ethanol tolerance to yeast. The toxicity of alcohol to microbes such as yeast is a bottleneck in the production of ethanol from biomass-derived sugars through fermentation. The Elongase 1 gene encodes ELO1, an enzyme involved in the biosynthesis of unsaturated fatty acids in yeast. This gene could be incorporated into an industrial yeast strain to increase the amount of ethanol produced from biomass. An industrial fermentation yeast strain with increased ethanol tolerance could be widely applicable in reducing costs and energy consumption.

Licensing Information:
University of Wisconsin – Madison
Contact: Mark Staudt (mstaudt@warf.org, 608-265-3084)
TTO Tracking Number: P100228US02
Patent Status: 8178331
Type of License: Exclusive
USPTO Link: http://patft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&u=%2Fnetahtml%2FPTO%2Fsearch-adv.htm&r=2&f=G&l=50&d=PTXT&p=1&S1=8,178,331&OS=8,178,331&RS=8,178,331

Website: http://www.warf.org/technologies/summary/P100228US02.cmsx

g. Organic Acid-Tolerant Microorganisms and Uses Thereof for Producing Organic Acids

UW–Madison researchers have genetically modified microorganisms to better tolerate organic acids like 3-hydroxypropionic acid, acrylic acid and propionic acid. In the modified bacteria, the acsA gene is replaced or deleted. This leads to increased organic acid tolerance. The modified microorganisms are cyanobacteria such as Synechococcus. They can be used for industrial production of organic acids.

Licensing Information:
University of Wisconsin – Madison
Contact: Jennifer Gottwald (jennifer@warf.org, 608-262-5941)
TTO Tracking Number: P120017US02
Patent Status: 8,715,973; 8,846,354; 8,846,329
Type of License: Exclusive
USPTO Link: http://patft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&u=%2Fnetahtml%2FPTO%2Fsearch-adv.htm&r=5&f=G&l=50&d=PTXT&p=1&S1=8,715,973&OS=8,715,973&RS=8,715,973
Website: http://www.warf.org/technologies/summary/P120017US02.cmsx

h. Multifunctional Cellulase and Hemicellulase

UW–Madison researchers have engineered a multifunctional polypeptide capable of hydrolyzing cellulose, xylan and mannan. It is made of the catalytic core of Clostridium thermocellum Cthe_0797 (also called CelE), a linker region and a cellulose-specific carbohydrate binding module(CBM3). C. thermocellum is a well-known cellulose-degrading bacterium whose genome has been sequenced, annotated and published. Multifuncional enzymes could simplify the enzyme cocktail needed for biomass conversion, thereby reducing costs.

Licensing Information:
University of Wisconsin – Madison
Contact: Jennifer Gottwald (jennifer@warf.org, 608-262-5941)
TTO Tracking Number: P120371US02
Patent Status: 9145551
Type of License: Exclusive
USPTO Link: http://patft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&u=%2Fnetahtml%2FPTO%2Fsearch-adv.htm&r=1&f=G&l=50&d=PTXT&p=1&S1=9145551&OS=9145551&RS=9145551
Website: http://www.warf.org/technologies/clean-technology/biofuels-renewable-fuels/summary/powerful-new-enzyme-for-transforming-biomass-p120371us02.cmsx

i. Selective Aerobic Alcohol Oxidation Method for Conversion of Lignin into Simply Aromatic Compounds

UW–Madison researchers have developed a metal-free, aerobic oxidation method that selectively transforms the benzylic alcohol in lignin to the corresponding ketone. The process uses a nitric acid (HNO_3) catalyst combined with another Brønsted acid. The reaction leaves unchanged at least a portion of unprotected primary aliphatic alcohols in the lignin or lignin subunit.

The reaction may be carried out in any suitable polar solvent and in the presence of additional reagents including TEMPO and derivatives.

Licensing Information:
University of Wisconsin – Madison
Contact: Jennifer Gottwald (jennifer@warf.org, 608-262-5941)
TTO Tracking Number: P130104US01
Patent Status: 8969534
Type of License: Exclusive
USPTO Link: http://patft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&u=%2Fnetahtml%2FPTO%2Fsearch-adv.htm&r=2&f=G&l=50&d=PTXT&p=1&S1=8,969,534&OS=8,969,534&RS=8,969,534
Website: http://www.warf.org/technologies/clean-technology/bio-based-renewable-chemicals/summary/selective-conversion-of-lignin-into-simple-aromatic-compounds-p130104us01.cmsx

j. Modifying Flowering Time in Maize

UW-Madison researchers have found a gene in maize that affects flowering time. By modulating this gene, GRMZM2G171650, the onset of flowering in maize may be delayed or accelerated. Standard vector and transgenic methods can be employed to overexpress or suppress the gene, or introduce it into new crop lines. The gene was identified by studying more than 500 different maize lines. The researchers mapped single nucleotide polymorphisms (SNPs) correlating to early or late flowering traits. A large concentration of such SNPs was located in GRMZM2G171650, a transcription factor on chromosome 3. The gene was of previously unknown function in corn. The expression of this gene could be altered to optimize biomass crops for growth in different climates and conditions.

Licensing Information:
University of Wisconsin – Madison
Contact: Emily Bauer (ebauer@warf.org, 608-262-8638)
TTO Tracking Number: P130256US02
Patent Status: 14/296352
Type of License: Exclusive
USPTO Link: http://appft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-bool.html&r=1&f=G&l=50&co1=AND&d=PG01&s1=14%2F296352&OS=14/296352&RS=14/296352
Website: http://www.warf.org/technologies/summary/P130256US02.cmsx

k. Oxygen-Responsive Bacterial Gene Switch

UW-Madison researchers have identified six novel variants of a known bacterial promoter sequence that can be used in industrial microbes to regulate gene expression based on O2 levels. The expression variants are exquisitely sensitive to industrially-relevant changes in O2 levels, allowing for regulation of gene expression by an endogenous inducer. The variations are within the transcriptional repressor ArcA. These variants would allow for precise control of gene expression through fermentation growth conditions.

Licensing Information:
University of Wisconsin – Madison
Contact: Jennifer Gottwald (jennifer@warf.org, 608-262-5941)

TTO Tracking Number: P130380US02
Patent Status: 14/497466
Type of License: Exclusive
USPTO Link: http://appft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-bool.html&r=1&f=G&l=50&co1=AND&d=PG01&s1=14%2F597466&OS=14/597466&RS=14/597466
Website: http://www.warf.org/technologies/summary/P130380US02.cmsx

l. Recombinant Yeast Having Enhanced Xylose Fermentation Capabilities and Methods of Use

A UW–Madison researcher has developed an S. cerevisiae strain that is 80 percent more effective at fermenting xylose. He discovered that knocking out several genes (hog1, isu1, gre3, ira1/2) enables dramatically faster xylose fermentation under the anaerobic conditions favored by industry. Industrial yeast strains are most efficient when they can utilize all available carbon sources, including xylose, so these modifications would enhance industrial yeast strains.

Licensing Information:
University of Wisconsin – Madison
Contact: Jennifer Gottwald (jennifer@warf.org, 608-262-5941)
TTO Tracking Number: P140199US02
Patent Status: 14/683724
Type of License: Exclusive
USPTO Link: http://appft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-bool.html&r=1&f=G&l=50&co1=AND&d=PG01&s1=14%2F683724&OS=14/683724&RS=14/683724
Website: http://www.warf.org/technologies/summary/P140199US02.cmsx

m. Constructs and Methods for Genome Editing and Genetic Engineering of Fungi and Protists

UW-Madison researchers have developed an efficient genome editing system for industrial yeast and other prototrophic fungi. The system includes constructs and protocols to facilitate precise and predictable editing or replacement of sequences by using both selectable and counter-selectable markers. The ability to manipulate prototrophic and diploid strains is important for applications in the biofuels and other fermentation industries, and this technology could be a broadly applicable tool for this.

Licensing Information:
University of Wisconsin – Madison
Contact: Jennifer Gottwald (jennifer@warf.org, 608-262-5941)
TTO Tracking Number: P140240US03
Patent Status: 14/826566
Type of License: Nonexclusive
USPTO Link: http://appft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-bool.html&r=1&f=G&l=50&co1=AND&d=PG01&s1=14%2F826566&OS=14/826566&RS=14/826566
Website: http://www.warf.org/technologies/research-tools/gene-expression/summary/high-throughput-genome-editing-and-engineering-of-industrial-yeast-other-fungi-p140240us03.cmsx

n. Antimicrobial Ferulic Acid and Derivatives and Uses Thereof

UW–Madison researchers have identified an antimicrobial agent produced as a byproduct of biomass processing. The agent is a diferulate compound called poacic acid (and sometimes also called '8-5-DC'). It has been shown to target and destroy the cell walls of several species of fungus and yeast.

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Contact: Mark Staudt (mstaudt@warf.org, 608-265-3084)
TTO Tracking Number: P140248US02
Patent Status: 14/703337
Type of License: Exclusive
USPTO Link: http://appft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-bool.html&r=1&f=G&l=50&co1=AND&d=PG01&s1=14%2F703337&OS=14/703337&RS=14/703337
Website: http://www.warf.org/technologies/agriculture/pesticides-inoculants/summary/natural-antimicrobial-agent-derived-from-biomass-p140248us02.cmsx

o. Enzymes for Producing Non-Straight-Chain Fatty Acids

UW-Madison researchers have developed a method to produce furan-containing fatty acids (FFAs), an important, yet poorly understood class of compounds, using the photosynthetic bacterium Rhodobacter sphaeroides. The inventors used an R. sphaeroides mutant with increased expression of genes that are activated in the presence of the reactive oxygen species singlet oxygen. In R. sphaeroides and other phototrophs, singlet oxygen is a byproduct of light energy capture in integral membrane complexes of the photosynthetic apparatus. Cells having an increased transcriptional response to singlet oxygen increase their production of FFAs resulting in an accumulation of these useful fatty acids. In addition, the inventors were also able to identify another potentially important compound, methylated unsaturated fatty acid (M-UFA), an intermediate in the production of FFA. The present invention provides a bio-based method for producing M-UFA and FFA at commercially relevant quantities.

Licensing Information:
University of Wisconsin – Madison
Contact: Jennifer Gottwald (jennifer@warf.org, 608-262-5941)
TTO Tracking Number: P140318US02
Patent Status: 14/755213
Type of License: Exclusive
USPTO Link: http://appft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-bool.html&r=1&f=G&l=50&co1=AND&d=PG01&s1=14%2F755213&OS=14/755213&RS=14/755213
Website: http://www.warf.org/technologies/materials-chemicals/biochemicals/summary/bio-based-production-of-non-straight-chain-and-oxygenated-fatty-acids-for-fuels-and-more-p140318us02.cmsx

p. Method for Selectively Preparing Levoglucosenone (LGO) and Other Anhydrosugars from Biomass in Polar Aprotic Solvents

UW–Madison researchers have developed a new method to produce levoglucosenone (LGO) from cellulosic biomass under mild reaction conditions. Conventionally, LGO is derived from materials such as waste paper via high temperature pyrolysis. However, the process is hindered by low yield. Attempts to

improve yield using expensive, toxic ionic liquids are undesirable. In this methodology, the biomass material is reacted in a mixture comprising a polar aprotic solvent (e.g., tetrahydrofuran or THF) and an acid in the absence of water. The LGO can be separated out by routine downstream processes such as distillation and evaporation. Glucose, levoglucosan, furfural and 5-hydroxymethylfurfural also are produced in small quantities. LGO is an important, non-petroleum building block chemical with potential uses in a wide range of industrial processes. For example, it can be converted to 1,6-hexanediol to be utilized in the production of polyurethanes and polyesters. This methodology allow for LGO production using less energy.

Licensing Information:
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Contact: Jennifer Gottwald (jennifer@warf.org, 608-262-5941)
TTO Tracking Number: P150101US01
Patent Status: 9376451
Type of License: Exclusive
USPTO Link: http://patft.uspto.gov/netacgi/nph-Parser?Sect1=PTO2&Sect2=HITOFF&u=%2Fnetahtml%2FPTO%2Fsearch-adv.htm&r=1&f=G&l=50&d=PTXT&p=1&S1=9,376,451&OS=9,376,451&RS=9,376,451
Website: http://www.warf.org/technologies/clean-technology/bio-based-renewable-chemicals/summary/high-yield-method-to-produce-lgo-from-biomass-p150101us01.cmsx

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 and accelerator facilities, and at 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. In an upgrade currently underway, the CEBAF electron beam energy was doubled from 6 to 12 GeV. 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; a beam luminosity upgrade is currently underway. NP is supporting the development of a future Facility for Rare Isotope Beams (FRIB) currently under construction at Michigan State University. The NP community is also exploring opportunities with 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, and of the fundamental properties of nucleons and neutrinos. This research is made possible 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; a local program of basic and applied research 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; non-accelerator experiments, such as large stand alone detectors and observatories for rare events. Of 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.

27. 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 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 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 Nuclear Physics (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.

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. Large Scale 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 computing facilities, such as local computing resources, major DOE funded computing resources, and private or 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, 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 data-intensive high performance computing tasks, such as user analyses in which repeated passes over large datasets are needed; and (4) distributed authorization and identity management systems, enabling single sign-on access to data distributed across many sites.

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b. Software-Driven Network Architectures for Data Acquisition

The building blocks of the experimental data acquisition system 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; (5) collect event data from the individual elements to be assembled into events; and (6) 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 nuclear physics 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; (b) trigger decision systems that may be fully software based or have hardware assists (e.g. FPGA accelerators); (c) data flow systems that are capable of responding to trigger accepts by reading data from the digitizers and making it available to interested clients; (d) free running data flow systems into which time stamps are injected for later data correlation; (e) scalable event builders that accept data from the data flow system and produce events for online analysis and, if rate permits, logging; (f) protocols and middle-ware that can tie this system together and provide relatively high level interfaces to user software; and 2) 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.

Questions – Contact: Michelle Shinn, 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.

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 (e.g., python/pandas, r/dplyr), 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.

Questions – Contact: Michelle Shinn, 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.

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 templatized C++ code into high performance implementations for heterogeneous architectures.

Utilizing High Performance Computing (HPC) and Leadership Computing Facilities (LCFs) is of growing relevance and importance to experimental NP as well. 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.

Questions – Contact: Michelle Shinn, 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.

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 or the NP SBIR/STTR Topic Associate for Software and Data Management: Frank E (Ted) Barnes, Ted.Barnes@science.doe.gov

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28. 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 detectors described in Topic 30 (Nuclear Instrumentation, Detection Systems and Techniques).

This topic is related to Topic 30 (Nuclear Instrumentation…): to develop innovative readout electronics for use with the nuclear physics detectors. 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 nuclear and particle physics and adjacent markets such as medicine, homeland security, the environment and industry.

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.

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

b. Front-End Application-Specific Integrated Circuits

Grant applications are sought to develop front-end application-specific integrated circuits (ASICs) for amplifying and processing data from highly-segmented 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) front-end ASICs capable of operating in cryogenic environment to allow for increased resolution; (4) integrated circuits for very high dynamic range; (5) integrated circuits for very high timing resolution, and (6) 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.

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

c. Next Generation Pixel Sensors

Active Pixel Sensors (APS) in CMOS (complementary metal-oxide semiconductor) technology have largely replaced Charge Coupled Devices 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 µm) 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} cm^{-2} 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 ~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.

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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.); (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); and (3) miniaturization techniques for connectors and cables with 5-10 times the density of standard inter-density connectors.

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.

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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.

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

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29. 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 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 basic 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 with the Facility for Rare Isotope Beams (FRIB) linac under construction at Michigan State University, and technologies relevant to the development of a proposed future Electron Ion Collider (EIC). A major focus in all of the above areas is superconducting radio frequency (SRF) acceleration or superconducting magnets and related technologies. Relevance to nuclear physics must be explicitly described, as discussed in more detail below. 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.

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 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 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 Nuclear Physics (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.

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 room-temperature 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 ultra-high vacuum seals, terminations, high reliability, lower cost radio frequency windows with improved dielectric properties such as loss tangents better than 0.01% at 1 GHz yet exhibiting a small dc conductivity to overcome charging by beams or field emission, RF power couplers, and high beam current, low-impedance bellows; (2) fast ferroelectric microwave components that control reactive power for fast tuning of cavities or fast control of input power coupling; (3) SRF cavity joining techniques that create vacuum seals without resorting to the use of bolted flanges in order to minimize particulates; (4) alternative cavity fabrication techniques to produce seamless SRF cavities of various geometries (*e.g.*, elliptical, quarter, half wave resonators and crab cavities) at 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 $E_{acc} \sim 20$ MV/m, or equivalently, $R_s < 5$ nW and $E_{peak} > 60$ MV/m, with correspondingly lower Q's at higher temperatures such as 4.5 K; and (5) 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 are also sought to develop improved superconducting materials or processes applied to such materials that have lower RF losses, operate at higher temperatures, and/or have higher RF critical fields than sheet niobium. Approaches of interest involving atomic layer deposition (ALD) synthesis should identify appropriate precursors. Processes should create high quality, NbN, Nb_3Sn, or MgB_2 films with anti-diffusion dielectric overlayers as needed, depending on the deposition technique. Demonstration of deposition should be on an actual RF cavity surface, e.g., elliptical, quarter wave, or crab geometry to allow for subsequent testing of SRF performance.

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b. Radio Frequency Power Sources

Grant applications are sought for a microwave power device, e.g., klystron, inductive output tube, tunable/phase stabilized magnetron or solid state amplifiers (especially class F devices) offering improved efficiency >80%, while delivering up to 12.5 kW, 50 kW or 500 kW Continuous Wave (CW) at 952.6 MHz. In the case of vacuum tube devices, the net tube power efficiency (including focusing magnet power) must meet the above efficiency. Similar devices are sought for MW-class power output with the same efficiency requirements operating at 563 MHz and 650 MHz. Note: In the case of the MW-class RF devices, if the same technology is to be employed at the three frequencies listed above, then a design solution may be proposed for only the most challenging frequency and brief comments made on how to modify the design for the other two frequencies.

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c. 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° or less of phase and 0.1% amplitude RMS jitter) and electron acceleration structures (0.1° 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) multi-cell, superconducting, 0.2-1.5 GHz accelerating structures that have sufficient higher-order mode damping for use in energy-recovering linac-based devices with ~1 A of electron beam; (3) passive or active methods for preserving beam quality by damping beam break-up effects in the presence of otherwise unacceptably large, higher-order cavity modes – one example of which would be a very high bandwidth feedback system; and (4) 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.

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

d. Particle Beam Sources and Techniques

Grant applications are sought to develop (1) methods and/or devices for improving emission capabilities of photocathode sources, such as improving charge lifetime, bunch charge, average current, emission current density, emittance, or energy spread; and (2) 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 cooling medium to high energy bunched proton or ion beams are of great interest for next generation colliders, like the proposed Electron-Ion Collider (EIC) for nuclear physics experiments. Therefore, grant applications are sought for (1) design, modeling, and component development for a fast beam-switching kicker with 0.5 ns duration and 10 to 20 kW power in the range of 5-100 MHz repetition rate. The transverse kick should be at least 200 kV ± 1% during the pulse with sub-100 ps rise and fall times (10-90%).

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e. 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 (≤ 1 mA) beam currents, the specifications for polarization and quantum efficiency are the same as listed above, and (2) devices, systems, and sub-systems for flipping the helicity of polarized electron beams at frequencies > 2 kHz, with very small helicity-correlated changes in beam intensity, position, angle, and emittance.

Grant applications also are sought for (1) advanced software and hardware to facilitate the manipulation and optimized control of the spin of polarized beams; (2) advanced beam diagnostic concepts, including beam polarimeters, particularly non-invasive devices; (3) absolute polarimeters for spin polarized ^{3}He beams with energies up to 160 GeV/nucleon; and (4) novel concepts for producing polarized particle beams of interest to nuclear physics research, including electrons, positrons, protons, deuterons, and ^{3}He.

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f. Rare Isotope Beam Production Technology

Grant applications are sought to develop (1) techniques for secondary radioactive beam collection, and fast release for subsequent re-ionization in order to enable multi-user capability at in-flight rare isotope beam facilities.

(Additional needs for high-radiation applications can be found in subtopic f "Technology for High Radiation Environments" of Topic 30, Nuclear Physics Instrumentation, Detection Systems and Techniques.)

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g. Accelerator Control and Diagnostics

As accelerator facilities advance in their capabilities, it is important that diagnostics and controls keep pace. Grant applications are sought by the accelerator community to develop (1) advanced beam diagnostics 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.

For facilities that produce high average power beams, grant applications are sought for (1) measurement devices/systems for CW beam currents in the range 0.01 to 100 μA, with very high precision ($<10^{-4}$) and short integration times; (2) non-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) instrumentation for 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 (an especially challenging region is for intensities of 10^2 to 10^5 with beam energy from 25 keV to 1 MeV/u); and (2) diagnostics for time-dependent, multicomponent, interleaved heavy ion beams. The diagnostic system must separate time-dependent constituents (total period for switching between beams >10 ms), where one species is weaker than the other, and is ~5% of a 30 - 100 ms cycle. The more intense beam would account for the remainder. Proposed solutions which work over a subset of the total energy range are acceptable.

In consideration of the above interests, grant applications are sought for (1) beam diagnostic devices that have increased sensitivity through the use of superconducting components (for example, filters based on high T_c superconducting technology or Superconducting Quantum Interference Devices); and (2) beam diagnostics enabled by non-traditional bulk materials such as diamond, graphene, thin films, large refractive index materials, photonic crystals and other nano-structured materials.

For accelerator controls, grant applications are sought to (1) enhance Control System Studio (CS-Studio). CS-Studio is an Eclipse-based collection of tools to monitor and operate large scale control systems from the accelerator community to the highly distributed Internet of Things. One of the primary concerns with CS-Studio remains its reliance on the Eclipse Rich Client Platform (RCP) which offers a look and feel similar to the running platform. Using Java 9 modules and JavaFX directly represents a potential replacement for CS-Studio. Grant applications are sought to develop: (a) a Java application framework to enable the

development of data visualization and controls tools, and (b) 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 remove the close coupling with specific technologies like Eclipse's RCP and develop 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. Proposals should indicate familiarity with complex accelerator systems and the interfaces between the beamline diagnostics and the control systems in use, e.g., EPICS, Control System Studio, etc.

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h. 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 (≥ 20 cm) superconducting dipole (≥ 2 T pole-tip field) with a field-exclusion region of about 3 cm in radius along the dipole bore; and (2) radiation-resistant high field (≥ 8 T pole tip field), large aperture (≥ 20 cm radius) compact (yoke thickness of ≤14 cm outer diameter – inner diameter) quadrupole. Also of interest are proposals for development of (3) techniques for efficient compensation of the external field generated by a quadrupole in item (2) above (in a region of about 3 cm in radius outside the quadrupole along its length for passage of the electron beam); (4) cost-effective materials and manufacturing techniques; and (5) high-efficiency cooling methods and cryogenic systems; (d) power supplies and other related hardware. 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.

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

i. Other

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

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

References:

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30. 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 is interested in supporting projects that may 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 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) Upgrade 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, 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. This topic also seeks state-of-the-art targets for applications ranging from spin polarized and unpolarized nuclear physics experiments to stripper and production targets required at high-power, advanced rare isotope beam facilities.

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 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 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 (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.

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) Ultra-violet and optical photon detectors and photosensitive devices:

- Ga-based (GaAs, GaInP etc.) Silicon Photomultiplier (SiPM) equivalents with the goal of large arrays of radiation-tolerant photodetection, especially in blue and UV wavelengths.

(2) Particle identification 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 with broad particle identification capabilities over a large momentum range and/or large area that can trigger at a high rate in noisy (very high rate, low-energy background) environments and that are also magnetic field tolerant;

Questions – Contact: Michelle Shinn, 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.

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 sought in the general field of micro-pattern gas detectors. This includes:

- New developments in micro-channel plates; micro-strip, Gas Electron Multipliers (GEMs), Micromegas and other types of micro-pattern detectors which significantly increase their position resolution, energy resolution, or significantly decrease their cost. Innovations such as commercial and cost

effective production of GEM foils or thicker GEM structures, and high resolution multidimensional readout such as 2D readout planes are desired.

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 (< 200ps FWHM), high energy loss resolution (1-2%), and high total energy resolution (1-2%), including associated readout electronic and data acquisition systems.

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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; and
- 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.

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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 photons and charged particles over a wide range of energies (from a few keV to up to many GeV). These include crystalline (such as BGO, BaF_2, LaBr. LSO etc.) 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 materials for practical devices.

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).

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e. Specialized Targets for Nuclear Physics Research

Grant applications are sought to develop specialized targets, including:

- A positron production target capable of converting hundreds of kilowatts of electron beam power (10 MeV at 10 mA) over a sufficiently short distance to allow for the escape of the produced positrons. Of particular interest would be moving and/or cooled high-Z targets of uniform, stable thickness (2-8 mm), which may be immersed in a 0.5-1.0 T axial magnetic field.
- Polarized ^{3}He gaseous targets based on optical pumping and spin exchange that will withstand high intensity laser pumping and electron beam currents beyond the current state of the art.

Grant applications are sought to develop the technologies and sub-systems for the targets required at high-power, rare isotope beam facilities that use heavy ion drivers for rare isotope production. Targets for heavy ion fragmentation and in-flight separation are required that are made of low-Z materials and that can withstand very high power densities and are tolerant to radiation for:

- Preparation of targets of radioisotopes, with half-lives in the range of hours, to be used off-line in both neutron-induced and charged-particle-induced experiments.

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f. 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:

- Radiation tolerant infrared video cameras: It would be beneficial for beam delivery and remote handling operations to have cost-efficient video cameras using infrared sensors that also have high resistance to radiation. With beam dump and/or target temperatures in the 300°C range, such a camera should be sensitive in the 5 µm and longer spectral range. The camera should operate at

standard frame rates with video graphics array sensor resolutions of (640 × 480 pixel) or better, with a radiation tolerance for prolonged operation in the presence of neutron fluxes of about 10^5 *n* cm^{-2} s^{-1}, and a total absorbed dose of ~ 1MRad/yr.

- Radiation resistant magnetic field probes based on new technologies: An issue in all high-power target facilities and accelerators is the limited lifetime of conventional nuclear magnetic resonance probes in high-radiation environments (0.1-10 MGy/y). The development of radiation-resistant magnetic field probes for 0.2-5 Tesla and a precision of $\Delta B/B<10^{-4}$ is highly desired.
- 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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g. 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 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 (Isotope Program) 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 Isotope Program 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.

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). This includes advanced accelerator and beam transport technologies (e.g. the application of high-gradient particle accelerating structures, high-energy/high-current cyclotrons) or other technologies that could lead to compact sources and target approaches needed to optimize isotope production. 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}Cu/^{67}Cu, ^{44}Sc/^{47}Sc, or ^{186}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}He is used for cryogenics, homeland security, and medical applications. Proposals are sought for efforts leading to terrestrial production of ^{3}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).

The development of high quality, robust targets is required to utilize the higher-current and power-densities available from commercially available accelerators; of particular concern is the design and fabrication of encapsulated salt targets and liquid metal targets. These targets could be subjected to energies up to ~70 MeV with intensities of between 100 μA and 750 μA. 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 are 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. An

area of significant interest is 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.

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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, 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, including 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 uCi/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}At, ^{225}Ra, ^{225}Ac, and ^{227}Ac from contaminant metals, including thorium, radium, lead, lanthanides, and/or bismuth; b) improve ion-exchange column materials needed for generating ^{212}Pb from ^{224}Ra, ^{213}Bi from ^{225}Ac and/or ^{225}Ra; 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. Among those listed, advanced methods for the preparation of high purity ^{225}Ra and ^{225}Ac from irradiated thorium targets are of particular interest. 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.

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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.

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