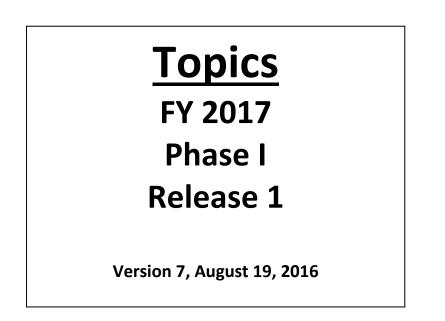


# **U.S. Department of Energy**

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



### 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

## <u>Schedule</u>

Event	Dates
Topics Released:	Monday, July 18, 2016
Funding Opportunity Announcement Issued:	Monday, August 15, 2016
Letter of Intent Due Date:	Tuesday, September 06, 2016
Application Due Date:	Monday, October 17, 2016
Award Notification Date:	Monday, January 09, 2017*
Start of Grant Budget Period:	Tuesday, February 21, 2017*

#### \* Dates Subject to Change

Table of Changes				
Version	Version Date Change			
Ver. 1	July 18, 2016	Original		
Ver. 2	July 20, 2016	Point of Contact added for Topic 4 subtopic a		
Ver. 3	July 26, 2016	Website added for Topic 21 subtopics a-d		
Ver. 4	July 28, 2016	<ul> <li>Modification to Topic 15 topic description</li> <li>Reference added to Topic 15 subtopic b</li> <li>Correction to Reference 1 under Topic 15 subtopic c</li> <li>Reference added to Topic 15 subtopic e</li> </ul>		
Ver. 5	August 3, 2016	<ul> <li>Title modification to Topic 5</li> <li>Modification to Topic 5 subtopic a description</li> <li>Removal of Topic 5 subtopic c</li> <li>Title modification to Topic 6</li> <li>Modification to Topic 23 topic description</li> <li>Modification to Topic 24 topic description</li> <li>Modification to Topic 25 topic description</li> <li>Modification to Topic 25 subtopic f description</li> <li>Modification to Topic 26 topic description</li> <li>Modification to Topic 27 topic description</li> </ul>		
Ver. 6	August 10, 2016	DOE National Energy Research Scientific Computing Center (NERSC) resources have been added to the following areas:         • Topic 2 subtopic b subtopic description         • Topic 5 topic description         • Topic 6 topic description         • Topic 10 topic description         • Topic 15 topic description         • Topic 17 topic description         • Topic 18 topic description		
Ver. 7	August 19, 2016	Corrected laboratory contact for Topic 23 subtopic c		

<ul> <li>Changed point of contact for Topic 14 subtopic c</li> </ul>		• Changed point of contact for Topic 14 subtopic c
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### **Notifications**

Beginning in FY 2017, the DOE SBIR/STTR Programs will no longer accept Fast-Track (combined Phase I/II) applications. Only Phase I applications will be accepted under the associated Funding Opportunity Announcement that will be issued on August 15, 2016.

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#### DOE GRANT APPLICATION PREPARATION SUPPORT – PHASE 0 ASSISTANCE PROGRAM

To increase the number of high-quality SBIR/STTR Phase I applications submitted to the DOE by womenowned 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 <a href="http://www.dawnbreaker.com/doephase0/">http://www.dawnbreaker.com/doephase0/</a>.

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.

#### **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.

#### 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?

Initially we anticipate making a maximum of one award per TTO subtopic. This will insure that an awardee is able to sign an option agreement that includes exclusive rights in its intended field of use. If we receive applications to a TTO that address different fields of use, it is possible that more than one award will be made per TTO.

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

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

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

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

#### PROGRAM AREA OVERVIEW: OFFICE OF 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 highspeed 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 <u>here</u>.

#### 1. 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.

Scientific instruments and supercomputer facilities generate, consume, process, and store both raw and analyzed data enabling the discovery of new knowledge. Efforts are underway to scale these computers to support extreme-scale computationally intensive science applications and to deal with increasing volumes and velocities of experimental and observational data. This topic addresses the need for higher level middleware services and analysis tools that are needed to turn raw data into actionable knowledge

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

Questions - contact Richard Carlson, richard.carlson@science.doe.gov

#### b. Big Data 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 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-/time-effective commercial grade technologies in the following categories:

 BigData management software-enabling technologies – this includes 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 systems; 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

 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). This 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, <u>thomas.ndousse-fetter@science.doe.gov</u>

#### c. Other

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

Questions – contact: Richard Carlson, <u>richard.carlson@science.doe.gov</u>

#### References: Subtopic a:

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- Calyam, P., Pu, J., Mandrawa, W., & Krishnamurthy, A., 2010, Ontimedetect: Dynamic Network Anomaly Notification in PerfSONAR Deployments, In Proceedings - 18th Annual IEEE/ACM International Symposium on Modeling, Analysis and Simulation of Computer and Telecommunication Systems, MASCOTS 2010, IEEE, pp. 328-337. (<u>https://uncch.pure.elsevier.com/en/publications/ontimedetectdynamic-network-anomaly-notification-in-perfsonar-de</u>)
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#### **References: Subtopic b:**

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- 8. University of Chicago, Nimbus: An open source toolkit for Infrastructure-as-a-Service for clouds, Homepage. (<u>http://www.nimbusproject.org/</u>)
- 9. Department of Energy, VACET, The Visualization and Analytics Center for Enabling Technologies (VACET), Homepage. (<u>http://www.vacet.org/about.html</u>)
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- 11. Department of Energy, SciDAC, Monroe, D., From Data to Discovery, SciDAC Data Management Center. (<u>http://www.scidacreview.org/0602/html/data.html</u>)
- 12. The Apache Software Foundation, 2016, Welcome to Apache Hadoop!, Homepage. (<u>http://hadoop.apache.org/</u>)
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#### 2. 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 accerators, and multi-level memory subsystems have made a significant impact on the HPC systems performance and usability. Programming tools and services are required that can hide this hardware complexity without impacting performance.

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, additive manufacturing (3D Printing) processes and Smart Manufacturing are strongly 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). 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 or small scale clusters, 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 (SC) 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.

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 <a href="http://www.nersc.gov/users/accounts/allocations/request-form/">http://www.nersc.gov/users/accounts/allocations/request-form/</a>.

Questions - contact: Randall Laviolette, <u>Randall.Laviolette@science.doe.gov</u>

#### 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 DOE's Open Science (DOE-SC) Computing facilities, the National Energy Research Scientific Computing Center (NERSC), the Argonne Leadership Computing Facility (ALCF), or the Oak Ridge Leadership Computing Facility (OLCF). Applicants wishing to run at the NERSC (<u>http://www.nersc.gov</u>) facility should send email to "<u>consult@nersc.gov</u>" and inquire about the Education/Startup allocation program. Descriptions of the allocation programs available at the ALCF can be found at <u>http://www.alcf.anl.gov/user-guides/how-getallocation</u>. Questions concerning allocations on the ALCF can be sent to David Martin"<u>dem@alcf.anl.gov</u>". Descriptions of the allocation programs available at the OLCF are available at <u>http://www.olcf.ornl.gov/support/getting-started/</u>. Questions concerning allocations on the OLCF can be sent to Jack Wells "<u>wellsjc@ornl.gov</u>". Proprietary work may be done at the ALCF and OLCF facilities using a cost recovery model.

#### **References Subtopic a:**

- 1. Michael, F., 2011, Minding the Missing Middle, HPCC Conference Summary, Newport, RI., HPCWire. (<u>http://www.hpcwire.com/hpcwire/2011-03-31/minding\_the\_missing\_middle.html</u>)
- Kirkley, J., 2011, Making Digital Manufacturing Affordable: A Vendor Perspective, EnterpriseTech. (<u>http://www.digitalmanufacturingreport.com/dmr/2011-06-</u> <u>14/making digital manufacturing affordable: a vendor perspective.html</u>)

- Trader, T., 2011, Digital Manufacturing, Why There's Never Been a Better Time, EnterpriseTech. (<u>http://www.enterprisetech.com/2011/06/20/digital manufacturing why theres never been a bett</u> <u>er time/</u>)
- Executive Office of the President National Science and Technology Council, 2012, A National Strategic Plan for Advanced Manufacturing, p.51. (<u>http://www.whitehouse.gov/sites/default/files/microsites/ostp/iam\_advancedmanufacturing\_strateg\_icplan\_2012.pdf</u>)
- 2012, Solid Print Making Things with a 3D Printer Changes the Rules of Manufacturing, The Economist, Manufacturing and Innovation: A Third Industrial Revolution. (<u>http://www.economist.com/node/21552892</u>)
- 6. 2012, Special Report: What is SMART Manufacturing, Time Magazine, p.6. (<u>https://www.rockwellautomation.com/resources/downloads/rockwellautomation/pdf/about-us/company-overview/TIMEMagazineSPMcoverstory.pdf</u>)
- 7. "Journal Report: Unleashing Innovation Manufacturing", Wall Street Journal, June 11 2013. (<u>http://www.reskem.com/unleashing-innovation-manufacturing-wall-street-journal-special-report/</u>)

#### **References Subtopic b:**

- 1. "Workshop for Independent Software Developers and Industry Partners" Workshop Summary, Chicago IL, March 31, 2011. (<u>http://outreach.scidac.gov/scidac-overview/</u>)
- McIntyre, C., 2009, US Manufacturing-Global Leadership Through Modeling and Simulation, High Performance Computing Initiative, Compete. Council on Competitiveness, p. 4. (<u>http://www.compete.org/storage/images/uploads/File/PDF%20Files/HPC%20Global%20Leadership%20030509.pdf</u>)
- 3. DOE Software Developed or Extended under the Scientific Discovery through Advanced Computing (SciDAC) program. (<u>http://outreach.scidac.gov/scidac-overview/init/default/scidac\_current?mode=all</u>)
- 4. DOE Office of Science, Scientific Discovery through Advanced Computing (SciDAC), Project Website. (<u>http://www.scidac.gov</u>)

#### **3. 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 rely on High Performance Computing (HPC) systems to enable large scale information processing for a multitude of areas such as business, utility, financial, education, 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 the worldwide network,

and ensuring effective cybersecurity monitoring, situational awareness, logging, reporting, preventions, remediation, etc, is an increasingly important task.

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, critical infrastructure, or user facilities. 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. 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-, and wireless-based solutions; internet; internet-of-things; basic research; natural language processing; social networks; 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:**

- Department of Energy, 2015, The 2015 Cybersecurity for Scientific Computing Integrity Workshop, DOE Workshop Report. (<u>http://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/ASCR\_Cybersecurity\_For\_Scientific\_Computing\_Integrity\_Report\_2015.pdf</u>)
- Campbell, S., Mellander, J., 2015, Experiences with Intrusion Detection in High Performance Computing, p. 9. (<u>https://cug.org/5-publications/proceedings\_attendee\_lists/CUG11CD/pages/1-program/final\_program/Monday/03B-Mellander-Paper.pdf</u>)
- Malin, A.B., Van Heule, G.K, 2013, Continuous Monitoring and Cyber Security for High Performance Computing, Report LA-UR-13-21921. (<u>http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-13-21921</u>)

 Catlett, C., 2008, A Scientific Research and Development Approach To Cyber Security, Final Report Submitted to the Department of Energy, p. 36. (<u>http://science.energy.gov/~/media/ascr/pdf/program-</u> <u>documents/docs/Cyber security science dec 2008.pdf</u>)

#### 4. COLLABORATIVE DEVELOPMENT PROJECTS

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

The ASCR program office is actively engaged in the development of next generation leadership class supercomputers. This topic solicits proposals that require a collaborative team of small businesses combining there different expertise's to develop more complex and operational subsystems or software modules for these emerging supercomputers. A collaborative team approach, with up to 5 small businesses forming this team, will receive funding under this topic.

#### a. Photonic Memory Controller Module (P-MCM)

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 (copper traces, connectors, switches, etc) with photonic based components would greatly increase the I/O and memory 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 Memory Controller Module that meets the following specifications.

- Server class multiprocessor chip
- High Density stacked Memory Modules: 10 stacked memory modules at 0.5 TB/s I/O rate each
- Simultaneous access from Multi-core processor chip to 10 memory modules (5 TB/s aggregate I/O rate)
- WDM optical transceivers matched to the I/O memory rates
- Reconfigurable optical interconnect fabric
- Low loss Optical connectors and/or integrated Micro Optical Bench assemblies

The photonic components of the P-MCM must be capable of operating on 0.5 pJ/b of power (not counting the CPU or memory module electrical power) while allowing any CPU core to access data from any memory module. Memory modules may be located up to 1 meter distant from the CPU core.

It is expected that a collaborative team of businesses will work together to design and build this P-MCM 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 should clearly delineate the roles of each small business team member and what portion of the effort each will perform. Each proposal must have business specific budget & budget justification forms, biographical data for the PI and senior personnel involved in the project, and commercialization plan. The maximum Phase I and Phase II

award amount is for each small business of the collaborative team. The cover sheet for each submission must clearly show all businesses involved in the collaboration.

If a grant is awarded, each member of the collaborative team must submit an Intellectual Property Management Plan at the time of award. Details of the requirements of the Intellectual Property Management Plan and a model are available at <a href="http://science.energy.gov/sbir/applicant-and-awardee-resources/">http://science.energy.gov/sbir/applicant-and-awardee-resources/</a>.

The Intellectual Property Management Plan should be negotiated and established between the team members and provide for the management and disposition of Intellectual Property arising from the project in accordance with the terms of the Award under which Intellectual Property was developed, for example the treatment of confidential information, background intellectual property, inventions and data produced under the project, any necessary licensing, or the handling of any disputes between the members.

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

#### **References:**

- Bahadori, M., Rumley, S., Nikolova, D., Bergman, K., 2016, Comprehensive Design Space Exploration of Silicon Photonic Interconnects, IEEE Journal of Lightwave Technology, Vol. 34, Issue 12, p. 2975-2987. (<u>http://lightwave.ee.columbia.edu/files/Bahadori2015b.pdf</u>)
- Rumley, S., Nikolova, D., Hendry, et al., 2015, Silicon Photonics for Exascale Systems [Invited Tutorial], Journal of Lightwave Technology, Vol. 33, Issue 3, p. 547-562. (<u>http://lightwave.ee.columbia.edu/files/Rumley2015.pdf</u>)
- Biberman, A., Bergman, K., 2012, Optical interconnection networks for high-performance computing systems[invited], Reports on Progress in Physics, Vol. 75, p.15. (<u>http://lightwave.ee.columbia.edu/files/Biberman2012.pdf</u>)
- 4. Brunina, D., Liu, D., Bergman, K., 2013, An Energy-Efficient Optically Connected Memory Module for Hybrid Packet- and Circuit-Switched Optical Networks, IEEE Journal of Selected Topics in Quantum Electronics, Vol. 19, Issue 2, p. 7. (<u>http://lightwave.ee.columbia.edu/files/Brunina2012e.pdf</u>)
- Pepeljugoski, P., Kash, J., Doany, F., et al., 2010, Low Power and High Density Optical Interconnects for Future Supercomputers, Optical Fiber Communication (OFC), collocated National Fiber Optic Engineers Conference, 2010 Conference on (OFC/NFOEC), IEEE, p.1-3. (<u>http://ieeexplore.ieee.org/xpl/login.jsp?tp=&arnumber=5465516&url=http%3A%2F%2Fieeexplore.ieee.org%2Fxpls%2Fabs\_all.jsp%3Farnumber%3D5465516</u>)
- 6. The Optical Society (OSA), 2016, OSA Industry Development Associates (<u>http://www.osa.org/en-us/corporate\_gateway/</u>)
- 7. The American Institute for Manufacturing Integrated Photonics (AIM Photonics), Home page. (<u>http://www.aimphotonics.com/</u>)

#### **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.

#### 5. ANCILLARY TECHNOLOGIES FOR ADVANCED LIGHT SOURCES

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 is specifically focused on the development of superconducting helical undulators with superimposed focusing gradient for high-efficiency tapered x-ray free electron lasers (FELs); undulator tapering techniques for high-efficiency FELs, and non-invasive x-ray flux monitoring on light source optical elements. Grant applications that are not beyond the state-of-the-art nor do not fall within the topic 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 <a href="http://www.nersc.gov/users/accounts/allocations/request-form/">http://www.nersc.gov/users/accounts/allocations/request-form/</a>.

Grant applications are sought in the following subtopics:

#### a. Superconducting Helical Undulator with Superimposed Focusing Gradient for High Efficiency Tapered X-Ray FELs

Undulator tapering can significantly improve the x-ray FEL efficiency of energy transfer from electrons to X-ray photons **[1]**. Recent studies **[2]**, at photon energies around 8 keV, indicate that although a tapered superconducting planar undulator, with focusing quadrupoles in between the undulator sections is feasible **[3]**, a superior performance, achieving multi-TW peak power, is obtained using superconducting helical undulators with transverse focusing gradient superimposed on the main undulator field, short magnet sections and short breaks between sections.

Grant applications are sought for feasibility studies of a prototype helical NbTi superconducting undulator with superimposed transverse focusing gradient technology with emphasis on performance, tunability, focusing properties, and practical viability for x-ray FELs applications. The sought out prototype characteristics are: undulator period 1.8-2 cm, undulator parameter 3, quadrupole focusing average beta function 4-6 m, undulator section length 1 m, undulator break length 15 cm. Matching phase shifters and beam position monitors must be included in the breaks. A systematic design study needs to be carried out, including iterative optimization of undulator features and geometry, FEL performance optimization, and experimental development effort. The expectation is that the results from Phase I will lead to Phase-II developments of a prototype magnet scalable to the full cell design.

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

#### b. Undulator Tapering Techniques for High-Efficiency Free Electron Laser Sources

The x-ray FEL efficiency, measured as a fraction of the electron beam power converted into light, is typically below 0.1% for most of the x-FEL facilities presently in operation. Undulator tapering techniques can be used to improve the conversion efficiency by 1-2 orders of magnitude. Grant applications are sought for the development and scaled demonstration of a robust tapered x-FEL schemes, with the conversion efficiency above 10%. Such high efficiency x-FEL schemes can result in a significant increase in peak and average power available to the users, but need to be tested at laboratory scale

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

#### c. Subtopic Has Been Removed

#### d. Non-Invasive X-Ray Flux Monitoring on Optical Elements

Most scientific instruments at synchrotron and free-electron laser facilities are complicated arrangements of individual optical components. These instruments often require a substantial fraction of the operational time to be allocated for optical alignment and troubleshooting. Non-invasive x-ray flux monitoring directly on the optical elements is expected to facilitate the alignment and troubleshooting as well as to provide real-time diagnostics of the optics performance. While in the soft x-ray regime (photon energies < 3 keV) monitoring x-ray-induced photocurrent on x-ray optics in vacuum may provide reliable measure of the incident and/or absorbed flux, in the regime of hard x-rays (photon energies > 3 keV) non-invasive (i.e., without the use of stand-alone x-ray detectors) characterization of the flux incident, transmitted or reflected from individual optical components remains limited.

Solutions including integration of hard x-ray flux monitoring capabilities to frequently used types of nontrivial optical elements (i.e., elements which operation is based on the effects of x-ray refraction, reflection or diffraction, such as x-ray mirrors, capillaries, refractive lenses, Fresnel zone plates, multilayers and diffracting crystals) are sought. The proposed solutions must provide quantitative measurement of the xray flux incident or reflected from or transmitted through the optical element with signal-to-noise ratio of better than  $1x10^3$  at an incident x-ray flux as small as  $1x10^9$  photons/second and greater in a non-invasive manner, i.e., avoiding additional attenuation of x-rays or any distortion of the radiation wavefront other than those resulting from the primary function of the optical element. The solutions may include x-ray optical elements with integrated flux monitoring capability or enclosures for existing optical components with an arrangement, which enables detection of the x-ray flux without deterioration of the performance of the optical components installed and operated in these enclosures.

The principle of non-invasive detection/monitoring of the incident/reflected/transmitted flux can be based on measurements of x-ray-induced photoemission, fluorescence, scattered radiation or other effects resulting from the interaction of x-rays with the material of the optical element [1-3].

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

#### e. Other

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

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

#### References: Subtopic a:

- Kroll, N., Morton, P., & Rosenbluth, M., 1981, Free-electron Lasers with Variable Parameter Wigglers, IEEE Journal of Quantum Electron, Vol. 17, p. 1436–1468. (<u>http://iopscience.iop.org/article/10.1088/0022-3727/26/7/002/meta</u>)
- Emma, C., Fang, K., Wu, J., & Pellegrini, C., 2016, High Efficiency, Multiterawatt X-ray Free Electron Lasers, Physical Review Accelerators and Beams, Vol. 19, 020705. (<u>https://journals.aps.org/prab/pdf/10.1103/PhysRevAccelBeams.19.020705</u>)
- Emma, P., et al., 2014, A Plan for the Development of Superconducting Undulator Prototypes for LCLS-II and Future FELs, in FEL 2014 Conference proceedings, Basel, Switzerland, THA03. (<u>https://portal.slac.stanford.edu/sites/ad\_public/FEL\_RandD/scu\_rd/shared\_docs/General%20Present\_ations/FEL14-SCU-Paper-THA03.PDF</u>)

#### References: Subtopic b:

- Kroll, N., Morton, P., & Rosenbluth, M., 1981, Free-electron Lasers with Variable Parameter Wigglers, IEEE Journal of Quantum Electron, Vol. 17, p. 1436–1468. (<u>http://iopscience.iop.org/article/10.1088/0022-3727/26/7/002/meta</u>)
- Orzechowski, T.J., et al., 1986, High-Efficiency Extraction of Microwave Radiation from a Tapered-Wiggler Free-Electron Laser, Physical Review Letters, Vol. 57, American Physical Society, p. 2172. (<u>http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.57.2172</u>)
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- Duris, J., Murokh, A., Musumeci, P., 2015, High Efficiency Energy Extraction from a Relativistic Electron Beam in a Strongly Tapered Undulator, New Journal of Physics, Vol. 17, 063036. (<u>https://arxiv.org/pdf/1605.01448.pdf</u>)
- Emma, C., Fang, K., Wu, J., and Pellegrini, C., 2016, High Efficiency, Multiterawatt X-ray Free Electron Lasers, Physical Review Accelerators and Beams, Vol. 19, 020705. (<u>https://journals.aps.org/prab/pdf/10.1103/PhysRevAccelBeams.19.020705</u>)

#### References: Subtopic d:

- Afanas'ev, A.M., Imamov, R.M., & Mukhamedzhanov, E.Kh., 1992, Asymmetric X-ray Diffraction, Crystallography Reviews, Vol. 3, p. 157-230. (<u>http://www.tandfonline.com/doi/abs/10.1080/08893119208032970</u>)
- Yang, S.-H., Gray, A.X., Kaiser, A.M., et al., 2013, Making Use of X-ray Optical Effects in Photoelectron-, Auger Electron-, and X-ray Emission Spectroscopies: Total Reflection, Standing-wave Excitation, and Resonant Effects, Journal of Applied Physics, Vol. 113, 073513. (<u>http://scitation.aip.org/content/aip/journal/jap/113/7/10.1063/1.4790171</u>)
- Stupin, S., 2016, Self-detection of X-ray Fresnel Transmissivity Using Photoelectron-induced Gas Ionization, Applied Physics Letters, Vol. 108, Issue 4, 041101 (<u>http://scitation.aip.org/content/aip/journal/apl/108/4/10.1063/1.4940908</u>)

#### 6. ELECTRON OPTICS FOR ULTRAFAST ELECTRON MICROSCOPY (UEM) FOR ADVANCED LIGHT SOURCES

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, electron microscopes, and the Spallation Neutron Source (SNS). This topic seeks exclusively the development of electron optics capabilities beyond the present state-of-the-art in electron microscopy to support these user facilities. Grant applications that do not fall within the topic 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 <u>http://www.nersc.gov/users/accounts/allocations/request-form/</u>.

Grant applications are sought in the following subtopic:

#### a. Electron Optics for MeV Ultrafast Electron Microscope (UEM)

Electron microscopy and nano-characterization capabilities are important in materials sciences and are used in numerous research projects funded by the Department. The 2014 Report of the Basic Energy Sciences Workshop on electron scattering and diffraction [1] recommended the development of an Ultrafast Electron Diffraction and Microscopy Instrument to enable revolutionary advances in the study of electron interaction with matter. Such a capability would be complementary to x-ray free electron lasers due to the difference in the nature of electron and x-ray scattering, enabling space-time mapping of lattice vibrations and energy transport, facilitating the understanding of molecular dynamics of chemical reactions, the photonic control of emergence in quantum materials, and the dynamics of mesoscopic materials.

To capture irreversible processes in materials science and biology, such as direct imaging of biologically important conformational transitions of macromolecules and glass phase transitions in real time, a single-shot ultrafast electron microscope (UEM) with atomic spatial resolution and sub-nanosecond temporal resolution is required. The number of electrons needed for such single-shot MeV UEM should 10 millions or more. What is needed is the development of electron-optical components and accessories for such single-shot MeV UEM. Novel electron optics, including electron lenses, correction elements and magnets for single-shot MeV UEM, need to be designed and simulated with state-of-the-art software to achieve the desired set of column specifications (magnification, high spatial and temporal resolution, beam current, correction/deflection elements etc.). In particular, this includes the design of the 4 MeV objective lens and computation of its 3rd order optical properties using high-accuracy field solvers such as the second-order finite element method (SOFEM). Simulations need to include the computation of the magnetic flux distribution in the magnetic circuit and coil windings, taking into account relativistic effects and magnetic saturation in state-of-the-art magnetic materials. The simulations should yield a design suitable for a prototype UEM that targets performance with sub-ns temporal resolution and atomic (0.3 nm) spatial resolution for a 4 MeV electron beam with a relative energy spread of 10<sup>-5</sup>.

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

#### References: Subtopic a:

 U.S Department of Energy, 2014, Future of Electron Scattering and Diffraction, Report of the Basic Energy Sciences Workshop on electron scattering and diffraction. (<u>http://science.energy.gov/~/media/bes/pdf/reports/files/Future\_of\_Electron\_Scattering.pdf</u>)

#### 7. INSTRUMENTATION FOR ADVANCED NANOMETER SCALE OPTICAL 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 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 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, exciton dynamics and charge transport in 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

Information on carrier transport and dynamics phenomena associated with materials and nanostructures is often available from optical spectroscopies involving interactions with electromagnetic radiation ranging from the infrared spectrum to ultraviolet. Fast laser technologies can provide temporally resolved chemical information via optical spectroscopy or laser-assisted mass sampling techniques. These approaches provide time resolution ranging from the breakage or formation of chemical bonds to conformational changes in nanoscale systems but generally lack the simultaneous spatial resolution required to analyze individual molecules or nanostructures.

Grant applications are sought that make significant advancements in spatial resolution towards the singlenanometer for spectroscopic imaging instrumentation available to the research scientist. The nature of the advancement may span a range of approaches including sub-diffraction limit illumination or detection, selective sampling, and coherent or holographic signal analysis. Conventional Nearfield Scanning Optical Microscopy (NSOM) probes and techniques do not have sufficient spatial resolution, spectral range and optical coupling efficiency. An optical tip technology is needed that is potentially scalable to manufacturing, and will yield low-cost, high performance, robust instruments that are affordable by the larger scientific community.

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. 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. (http://science.energy.gov/bes/community-resources/reports/).

 BESAC Subcommittee, 2012, From Quanta to the Continuum: Opportunities for Mesoscale Science, A Report for the Basic Energy Sciences Advisory Committee Masoscale Science Subcommittee. (http://science.energy.gov/bes/community-resources/reports/)

# 8. 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 collaboration with a successful user of neutron sources. To this end, the STTR program would be an appropriate vehicle for proposal submission. Alternatively, applicants are encouraged to demonstrate applicability by providing a letter of support from 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 would be to examine the strategic plans and annual activity reports from neutron scattering facilities at: <u>http://neutrons.ornl.gov/sites/default/files/NScD-Strategic-Plan-2014.pdf</u> and <u>http://www.ncnr.nist.gov/</u>.

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 <a href="http://www.nersc.gov/users/accounts/allocations/request-form/">http://www.nersc.gov/users/accounts/allocations/request-form/</a>.

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 focusing optics, neutron guides, neutron lenses, neutron polarization devices including <sup>3</sup>He polarizing filters, and neutron spin flippers for the current and future neutron scattering facilities using time-of-flight techniques.

Questions – contact James Rhyne <u>james.rhyne@science.doe.gov</u> or Thiyaga Thiyagarajan, <u>P.Thiyagarajan@science.doe.gov</u>

#### b. Advanced Sample Environment

Develop instrumentation and techniques for advanced sample environment [6,7] for neutron scattering studies. These *in-situ* environments should simulate conditions relevant to energy-related materials and should provide a novel means of achieving controlled chemical and gaseous environment and extreme sample conditions of temperature, pressure, electric and magnetic fields or combinations thereof.

Questions – contact James Rhyne <u>james.rhyne@science.doe.gov</u> or Thiyaga Thiyagarajan, <u>P.Thiyagarajan@science.doe.gov</u>

#### 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 2017.

Questions – contact James Rhyne <u>james.rhyne@science.doe.gov</u> or Thiyaga Thiyagarajan, <u>P.Thiyagarajan@science.doe.gov</u>

#### **References:**

- 1. U.S. Department of Energy, Office of Science, 2015, User Facilities, Neutron Scattering Facilities. <u>http://science.energy.gov/bes/suf/user-facilities/neutron-scattering-facilities/</u>
- United States National Nanotechnology Initiative, 2005, X-rays and Neutrons: Essential Tools for Nanoscience Research Workshop Report, Report of the National Nanotechnology Initiative Workshop. (<u>http://www.nano.gov/node/68</u>).
- International Atomic energy Agency (IAEA), 2012, Proceedings of the Twentieth International Collaboration on Advanced Neutron Sources (ICANS-XX) (<u>http://www.icansxx.com.ar/proceedings.php</u>)
- 4. Anderson, I.S, McGreevy, R.L., Bilheux, H.Z., 2009, Neutron Imaging and Applications: A Reference for the Imaging Community, Springer. (<u>http://www.springerlink.com/content/978-0-387-78692-6</u>)
- Majkrzak, C., & Wood, J.L., 1992, Neutron Optical Devices and Applications, Proceedings of the SPIEthe International Society for Optical Engineering Proceedings of SPIE Series, Vol. 1738, p.492. ISBN: 0819409111. (<u>http://books.google.com/books/about/Neutron\_optical\_devices\_and\_applications.html?id=XdhRAAA\_AMAAJ</u>)
- Klose, et al., 2004, Physica B: Condensed Matter, Proceedings of the Fifth International Workshop on Polarized Neutrons in Condensed Matter Investigations, Vol. 356, Issue 1-4, p. 280. (<u>http://www.sciencedirect.com/science/journal/09214526/356/1-4</u>)

- Crow, J., et al, 2003, Workshop Report, SENSE: Sample Environments for Neutron Scattering Experiments Workshop, Tallahassee, FL, September 24-26, p.35. (<u>http://neutrons-old.ornl.gov/workshops/tallahassee\_workshops\_2003/SENSE\_report\_1-14-04.pdf</u>)
- 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, (<u>http://scitation.aip.org/content/aip/journal/rsi/78/1/10.1063/1.2426878</u>)

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

Maximum Phase I Award Amount: \$225,000	Maximum Phase II Award Amount: \$5,000,000
Accepting SBIR Applications: YES	Accepting STTR Applications: YES

Materials researchers using synchrotron and x-ray free electron laser (XFEL) light sources at National Laboratories have a need for advanced spectrometers and detectors for x-ray scattering experiments. The light source staff and user community engage in detector research to push the state of the art of x-ray scattering and imaging techniques. They often advance a detector technology to a level approaching a prototype stage and use it for a particular experiment. They have thus created some type of working detector or detector components. However, they are not equipped to fully develop the detector as a product or transfer their technology readily into a stand-alone system for use by other researchers at another beam line or facility.

This topic seeks to identify and perform the necessary research and development to commercialize promising light source spectrometer and detector technology into products that are readily available throughout the light source community. The proposed technology must already be near the prototype level and the proposal should focus on the development of the technology into a user friendly and fully implemented product that can be purchased by researchers and light source facilities.

A successful Phase I proposal and project will identify a research group at a National Laboratory or university that has invented and used a new detector or spectrometer capability. The technology must be near the prototype stage as demonstrated by successful data acquisition in a materials research experiment at a synchrotron or XFEL beam line. (This topic is not for new x-ray sensor research.) The SBIR/STTR development project will involve a collaboration with an experienced materials science light source user capable of utilizing the detector capability in new x-ray techniques applied to materials research experiments. The experiments must be capable of obtaining competitive beam time at a light source user facility.

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

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

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

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

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

Grant applications are sought in the following subtopics:

#### a. Detector and Spectrometer Systems for X-ray Scattering

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

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

#### b. Other

Detector and spectrometer systems consistent with the topic description and which enable Synchrotron and XFEL materials research experiments not included in sub-topic (a).

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

#### **References:**

- U.S. Department of Energy, Office of Science, 2012, Neutron and X-ray Detectors, Report of the Basic Energy Sciences Workshop on Neutron and X-ray Detectors, p. 92. (<u>http://science.energy.gov/~/media/bes/pdf/reports/files/NXD\_rpt\_print.pdf</u>)
- Denes, P., and Schmitt, B., 2014, Pixel Detectors for Diffraction-limited Storage Rings, Journal of Synchrotron Radiation, Vol. 21, p. 1006–1010. (<u>http://www.ncbi.nlm.nih.gov/pmc/articles/PMC4181641/</u>)
- 3. Blaj, G., et. al., 2015, X-ray Detectors at the Linac Coherent Light Source, Journal of Synchrotron Radiation, Vol. 22, p. 577-583. (<u>http://journals.iucr.org/s/issues/2015/03/00/yi5006/yi5006.pdf</u>)

 Giewekemeyer, K., et. al., 2014, High Dynamic Range Coherent Diffractive Imaging: Ptychography Using the Mixed-Mode Pixel Array Detector, Journal of Synchrotron Radiation, Vol. 21, p. 1167-1174. (<u>http://scripts.iucr.org/cgi-bin/paper?mo5086</u>)

#### **10.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 greenhouse gas (GHG) emission reduction 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 climate change 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 <a href="http://www.nersc.gov/users/accounts/allocations/request-form/">http://www.nersc.gov/users/accounts/allocations/request-form/</a>.

Grant applications are sought in the following subtopics:

#### a. Specialty Steels and Alloys

Grant applications are sought to develop improvements in radiation-resistant, high-temperature steels and alloys with practical applications for Generation IV reactor systems, such as high-temperature gas- or liquid-cooled systems at 400-850°C. In general, this will be interpreted to mean that those materials which have improved creep strength can be formed and joined, are compatible with one or more high-temperature reactor coolants, and could reasonably be expected to eventually receive ASME Section III qualification for use in nuclear construction.

Questions – Contact: William Corwin, <u>william.corwin@nuclear.energy.gov</u>

#### 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, <u>william.corwin@nuclear.energy.gov</u>

#### 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, <u>sue.lesica@nuclear.energy.gov</u>

#### 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: Sue Lesica, <u>sue.lesica@nuclear.energy.gov</u>

#### **References:**

- 1. U.S. Department of Energy, 2010, Nuclear Energy Research and Development Roadmap, Report to Congress. (<u>http://energy.gov/sites/prod/files/NuclearEnergy\_Roadmap\_Final.pdf</u>).
- 2. U.S. DOE Office of Nuclear Energy, Science and Technology, Fuel Cycle Research and Development Program. (<u>http://www.energy.gov/ne/nuclear-reactor-technologies/fuel-cycle-technologies</u>).
- 3. U.S. DOE Office of Nuclear Energy, Science and Technology, Generation IV Nuclear Energy Systems, Nuclear Reactor Technologies. (<u>http://www.energy.gov/ne/nuclear-reactor-technologies</u>)
- 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 (<u>http://info.ornl.gov/sites/publications/files/Pub26178.pdf</u>).
- 5. U.S. DOE Office of Nuclear Energy, Light Water Reactor Sustainability (LWRS) Program. (<u>http://www.energy.gov/ne/nuclear-reactor-technologies/light-water-reactor-sustainability-lwrs-program</u>)

#### **11.ADVANCED MATERIALS AND COMPONENTS 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

Many significant materials innovations and advancements have been realized since the introduction of solidstate lighting products for general illumination applications nearly a decade ago. During this period, the worldwide lighting industry has begun an unprecedented transformation away from legacy lighting products using electric lamp technologies developed a century ago and with efficacies barely over a few lumens per watt and lasting only a few hundred hours. Today's solid-state lighting (SSL) devices routinely exceed 100 lumens per watt for 50,000 hours but are thought to be capable of doubling these values with the advent of new advanced materials and components. This extraordinary transformation has been made possible by significant materials advancements and new components used to manufacture Light Emitting Diodes (LEDs) and Organic Light Emitting Diodes (OLEDs). Many scientific and engineering disciplines have contributed to this successful lighting transformation and significant energy conservation opportunity ranging from basic physics, chemistry and mathematics to applied engineering disciplines, materials science and even biology.

While these technological advancements have unquestionably helped to make the solid-state transformation in general illumination a reality, development of advanced new materials are required to harvest the full economic and performance potential of these transformative SSL technologies. Even though the rapid evolution of SSL price and performance targets has been remarkable over the past decade, the industry and DOE believe that there are still many notable opportunities for even more significant cost reductions and product performance improvements. It is expected that these improvements will be made possible with the advent of new advanced materials across the wide spectrum of SSL products and components.

The special scientific challenges associated with making these predicted advancements possible in any of the numerous materials systems that make energy efficient and cost competitive SSL products possible are of interest under this topic. The following subtask descriptions highlight a few opportunities that are of special interest to the DOE and are included in the Department's Solid-State Lighting (SSL) program that is explained more fully on the program's comprehensive website: <a href="http://www1.eere.energy.gov/buildings/ssl/">http://www1.eere.energy.gov/buildings/ssl/</a>. Many technical reports, roundtable summaries, program roadmaps and summaries of current and past SSL projects may be downloaded at this website. Through this SBIR-STTR opportunity, grant applications are sought that address these advanced materials and components challenges that will build upon sound basic scientific knowledge leading to commercially successful intellectual property or intermediate components used specifically in the evolution of energy efficient, high color quality and cost effective SSL sources. General descriptions of areas for advancement are included in the following subtopics and proposals submitted for consideration should address the subtopic that best describes the end product's application space.

The intent of this broad topic is to encourage innovative material science development or composite solutions that will enable SSL products to perform closer to their theoretically predicted maxima in the long run and meet or exceed the aggressive device performance goals established by the DOE in the SSL R&D Plan available for download at <u>http://www1.eere.energy.gov/buildings/ssl/</u>. Responsive proposals must succinctly address and reference one or more of the key R&D challenges described fully in the DOE's SSL R&D Plan. Innovations that address manufacturing technology and cost of SSL Products while simultaneously addressing the fundamental materials challenges such as those described here as they pertain to general illumination applications are welcome. Applications that primarily address other related photonic materials or devices not directly relating to general illumination in buildings such as automotive lighting, projection or displays will not be accepted. The key metric for judging responsiveness of all proposals will be the commercialization potential identified in the applications, quantitative comparison to existing materials or components used in SSL and the prospect of making a substantive, long term and positive impact on the rapidly evolving SSL industry resulting in the production of higher quality SSL products at affordable life cycle cost. Proposals that include substantial technical risk are encouraged provided that 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 benefit the small business or participating technology transfer office.

Grant applications are sought in the following subtopics:

#### a. Efficiency and Performance Advancements of Down Converting Materials Systems

Many constituent materials are used today in the manufacture of phosphor-converted LEDs (pcLEDs) and phosphorescent OLEDs. While these components perform very well, there are important opportunities for device performance improvement and manufacturing cost reductions. Materials systems with good thermal stability and high quantum yield are used today in commercial pcLEDs and in future products that may use quantum dots or nanocrystals instead of conventional phosphors. The SSL industry has worked with DOE to identify a number of high priority, materials oriented research and development opportunities that are summarized in the references. For example, certain fundamental photonic processes such as nonradiative loss mechanisms in nanocrystals or QDs remain incompletely understood particularly at the high temperatures and power densities of interest to SSL. Color control, lifetime and spectrum of rare earth containing phosphors used for pcLEDs remains a challenge and despite their achievement of very high quantum yields, these materials typically fail at the temperatures and power levels thought to be targets for future SSL products. Also, there are important gaps in existing down-conversion spectrum in both color and efficiency especially at certain pump wavelengths. Consequently, some pcLEDs are less comparable to more familiar legacy lighting products whose emission spectrum is more continuous. For OLEDs, certain limitations in phosphorescent emitter efficiency remain and limit power densities, color, spectrum and service lifetime. Encapsulation materials and techniques that offer a balanced relationship between optical performance, stability, shelf life and exposure to environmental conditions associated with modern building illumination requirements, continues to discourage widespread use of OLEDs. While constituent materials used in either system are relatively low, manufacturing costs are high due to the special techniques, tools and manpower requirements of each. Thus, targeted materials system improvements or new constituent component technology or intermediate products are sought that will overcome these and other down converting approaches whose price and performance targets are more fully described in the DOE SSL Program R&D Plan.

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

#### b. Optical Performance of Photonic Materials

All SSL sources have special optical performance requirements that often conflict with other requirements. Many current SSL products use carefully engineered optical solutions that produce a viable balance between high performance demands and low manufacturing cost. In many cases however, new solutions are believed to enable even better optical performance, especially for beam management at little or no additional cost. Examples include optical out coupling enhancements for both LEDs and OLEDs that are derived from imaginative or novel geometrical optical designs such as graded index matching or better index of refraction matching for polymeric encapsulating materials like silicon. Out coupling efficiency and beam management can also be effected by using novel materials or structures such as diffractive optical elements or sophisticated computer generated diffusers to improve optical performance of devices. Combining recently developed physics-based mathematical modeling with advanced computational power may also be used to develop new products or tools that allow more of the generated light from the SSL source to reach the desired illuminated surface. Specific materials development or intermediate products or components that achieve notable optical performance improvement that is both easy and inexpensive to manufacture yet whose performance can be quantitatively predicted are sought under this subtopic.

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

#### c. Emitter and Substrate Materials

The state-of-the-art emitter materials systems for both LEDs and OLEDs have become somewhat standardized especially in the extensively researched and mass-produced III-Nitride alloy system used widely today as the workhorse for SSL. Despite their good efficiency, there remains ample room for fundamental materials improvement in both technologies. In LED systems for example, a number of technical challenges such as droop and materials defects arise as a consequence of the lattice constant mismatch between the emitter film and the deposition substrate. These conspire to limit device efficiency, lifetime and yield. It is possible that alternative alloys or structures could reduce the deleterious effects at both molecular levels as well as in the resulting crystalline structures. Alternative lower cost substrate materials or structures that produce more ideal growth conditions and reduction in cost by improving reproducibility, color and yield are also possible. In OLED systems, stable, long-life blue emitters, effects of compositional impurities, environmental contamination, current introduction and electrode transparency still remain among the more fundamental materials challenges that limit achievement of maximum efficacy, extraordinary lifetime and low cost of manufacture. For OLED substrates, current distribution, electron or hole injection, and optical properties may provide opportunities to improve OLED performance in flexible designs that are more easily and cost effectively manufactured using less complex tools and for a wider variety of applications in general illumination. It is expected that by increasing our scientific knowledge and understanding of these and similar fundamental materials effects in SSL, development of new and advanced materials, components or IP that would further improve and advance market penetration of any SSL technology beyond today's levels can be achieved and is well matched to the SBIR-STTR program.

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

#### **References:**

- U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, 2016, Solid-State Lighting 2016 Research & Development Plan, Prepared for Lighting Research and Development Building Technologies Program at the Department of Energy. (<u>http://energy.gov/eere/ssl/downloads/solidstate-lighting-2016-rd-plan</u>)
- U.S. Department of Energy Solid-State Lighting Program, 2015, DOE Solid-State Lighting Program Overview Brochure, Modest Investments, Extraordinary Impacts. (<u>http://energy.gov/eere/ssl/downloads/solid-state-lighting-program-overview-brochure</u>)
- 3. U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, 2014, DOE Joint Solid-State Lighting Roundtables on Science Challenges, p.20. (<u>http://energy.gov/eere/ssl/downloads/doe-joint-solid-state-lighting-roundtables-science-challenges</u>)

## **12.INSTRUMENTATION FOR ADVANCED CHEMICAL IMAGING**

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 chemical imaging 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 imaging techniques that combine molecular-scale spatial resolution and ultrafast temporal resolution to explore energy flow, molecular dynamics, breakage, or formation of chemical bonds, or conformational changes in nanoscale systems.

Grant applications are sought in the following subtopics:

### a. High Spatial Resolution Ultrafast Spectroscopy

Chemical information associated with molecular-scale processes is often available from optical spectroscopies involving interactions with electromagnetic radiation ranging from the infrared spectrum to x-rays. Ultrafast laser technologies can provide temporally resolved chemical information via optical spectroscopy or laser-assisted mass sampling techniques. These approaches provide time resolution ranging from the breakage or formation of chemical bonds to conformational changes in nanoscale systems but generally lack the simultaneous spatial resolution required to analyze individual molecules. Grant applications are sought that make significant advancements in spatial resolution towards the molecular scale for ultrafast spectroscopic imaging instrumentation available to the research scientist. The nature of the advancement may span a range of approaches including sub-diffraction limit illumination or detection, selective sampling, and coherent or holographic signal analysis.

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

### b. Time-Resolved Chemical Information from Hybrid Probe Microscopies

Probe microscopy instruments (including AFM and STM) have been developed that offer spatial resolution of molecules and even chemical bonds. While probe-based measurements alone do not typically offer the desired chemical information on molecular timescales, methods that take advantage of electromagnetic interactions or sampling with probe tips have been demonstrated. Grant applications are sought that would make available to scientists new hybrid probe instrumentation with significant advancements in chemical and temporal resolution towards that required for molecular scale chemical interactions. The nature of the advancement may span a range of approaches and probe techniques, from tip-enhanced or plasmonic enhancement of electromagnetic spectroscopies to probe-induced sample interactions that localize spectroscopic methods to the molecular scale.

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

#### **References:**

- U.S. Department of Energy, 2006, Office of Science Notice DE-FG01-05ER05-30, Basic Research for Chemical Imaging, BES Chemical Imaging Research Solicitation. (http://science.energy.gov/~/media/grants/pdf/foas/2005/DE-FG01-05ER05-30.pdf).
- 2. National Research Council, 2006, Visualizing Chemistry, The Progress and Promise of Advanced Chemical Imaging, National Academies Press. (<u>http://www.nap.edu/catalog.php?record\_id=11663</u>).

### **13.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, <u>mark.pederson@science.doe.gov</u>

### 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, <u>mark.pederson@science.doe.gov</u>

### **References:**

- Executive Office of The President National Science and Technology Council, 2011, Materials Genome Initiative for Global Competitiveness, p. 18. (www.whitehouse.gov/sites/default/files/microsites/ostp/materials\_genome\_initiative-final.pdf)
- Galli, G., and Dunning, T., U.S. Department of Energy, 2009, Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale, Scientific Grand Challenges, p. 117. (<u>http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/BES\_exascale\_report.pdf</u>)
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- 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, p. 54. (<u>http://science.energy.gov/~/media/bes/pdf/reports/files/PreSICE\_rpt.pdf</u>)
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- Subcommittee on Theory and Computation of the Basic Energy Sciences Advisory Committee, U.S. Department of Energy, 2005, Opportunities for Discovery: Theory and Computation in Basic Energy Sciences, Report based on BESAC Deliberations. (http://science.energy.gov/~/media/bes/besac/pdf/Theory-and-Computation rpt.pdf)

## **14. BIOFUELS AND BIOPRODUCT PRECURSORS FROM WET ORGANIC WASTE STREAMS**

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

Organic waste streams contain substantial amounts of chemical energy. Resource streams including 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. Thus, 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 and bioproduct 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]. A 2015 DOE workshop also elicited input on the potential of anaerobic membrane bioreactors (AnMBRs) and microbial electrochemical cells (MxCs) to contribute to this aim, particularly at the distributed scales at which these feedstocks occur [8]. Finally, a 2014 DOE waste-to-energy workshop yielded participant recommendations to target both alternative anaerobic digestion reactor designs, and options to bypass biogas production in converting wet organic feedstocks to biofuels and bioproducts [9]. This topic is in direct response to those and other stakeholder inputs. While some specifics vary by subtopic, the following criteria will apply to all applications:

- Proposed systems must utilize wet organic waste streams as the primary feedstock to produce fuels.
   Wet waste streams are defined in the Bioenergy Technologies Office Multi-Year Program Plan [10]. For purposes of this Small Business Innovation Research topic, biogas is specifically excluded as a feedstock.
- 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).
- 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 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, interspecies electron transfer, improved understanding of heterogeneous microbial and archeal 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.
- In all cases, 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 mediumchain fatty acids, such as succinic, muconic, and lactic acids. Proposals that strive to complete the

conversion of relevant feedstocks to jet or diesel fuels by the end of phase II are particularly encouraged.

- Hydrogen, ethanol, and methanol are not allowed as 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 solely produce biopower will be considered non-responsive.

Grant applications are sought in the following subtopics:

a. Anaerobic Membrane Bioreactors (AnMBRs) and Microbial Electrochemical Cells (MxCs) as Enablers for Wastewater Integrated Biorefineries (IBRs)

AnMBRs have the potential to extend the economic viability of anaerobic digestion to smaller scales, which would enable expanded deployment of distributed energy recovery from relevant waste streams [11-13]. MxCs hold forth the possibility of producing biofuels and bioproduct precursors from waste feedstocks [8, 14, 15]. Combinations of the two could simultaneously produce petroleum replacements, clean water, and valuable nutrients, a meaningful extension of the notion of IBRs that fits well with larger visions of future Bioeconomies

This subtopic seeks applications that produce biofuels and bioproducts from wet organic feedstocks using combinations of MxCs and AnMBRs [13, 16, 17]. Proposals that effectively address the challenge of energy-efficient fouling reduction in AnMBRs are especially welcomed, as are applications that set forth a credible path for scaling of MxCs to industrial relevance. Proposals may utilize either MxCs or AnMBRs alone, but all applications must demonstrate positive energy balances, as detailed above. Applications that include the production of clean water as a valuable byproduct will also be viewed favorably.

Questions – contact: Dan Fishman, daniel.fishman@ee.doe.gov

### b. 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 [9]. 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 [18]. Applications should address specific mechanisms to inhibit 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 [19-22]. Again, applications that propose to complete conversion of relevant feedstocks to jet or diesel fuels by the end of phase II are particularly encouraged.

Questions – contact: Dan Fishman, <u>daniel.fishman@ee.doe.gov</u>

#### c. Other

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

Questions – contact: Dan Fishman, <u>daniel.fishman@ee.doe.gov</u>

### References: Subtopic a:

- Alibardi, L., Cossu, R., Saleem, M., and Spagni, A., 2014, Development and Permeability of a Dynamic Membrane for Anaerobic Wastewater Treatment, Bioresource Technology, Vol. 161, p. 236-244. (<u>http://www.ncbi.nlm.nih.gov/pubmed/24709537</u>)
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- Logan, B.E., and Rabaey, K., 2012, Conversion of Wastes into Bioelectricity and Chemicals by Using Microbial Electrochemical Technologies, Science, Vol. 337, Issue 6095, p. 686-690. (<u>http://science.sciencemag.org/content/337/6095/686</u>)
- Mohan, S.V., Velvizhi, G., Modestra, J.A., and Srikanth, S., 2014, Microbial Fuel Cell: Critical Factors Regulating Bio-catalyzed Electrochemical Process and Recent Advancements, Renewable & Sustainable Energy Reviews, Vol. 40, p.779-797. (<u>https://www.researchgate.net/publication/264977622 Microbial fuel cell Critical factors regulatin</u> <u>g bio-catalyzed electrochemical process and recent advancements</u>)
- Ren, L., Ahn, Y., and Logan, B.E., 2014, A Two-Stage Microbial Fuel Cell and Anaerobic Fluidized Bed Membrane Bioreactor (MFC-AFMBR) System for Effective Domestic Wastewater Treatment, Environmental Science & Technology, Vol. 48, Issue 7, p. 4199-4206. (<u>http://pubs.acs.org/doi/pdf/10.1021/es500737m?src=recsys&</u>)
- Tian, Y, Ji, C, Wang, K and Le-Clech, P., 2014, Assessment of an Anaerobic Membrane Bioelectrochemical Reactor (AnMBER) for Wastewater Treatment and Energy Recovery, Journal of Membrane Science, Vol. 450, p242-248. (<u>http://www.engr.psu.edu/ce/enve/logan/publications/2014-Katuri-etal-ES&T.pdf</u>)

### **References: Subtopic b:**

- Lee, W.S., Chua, A.S.M., Yeoh, H.K., and Ngoh, G.C., 2014, A Review of the Production and Applications of Waste-derived Volatile Fatty Acids, Chemical Engineering Journal, Vol. 235, p. 83-99. (<u>http://repository.um.edu.my/32642/1/2014 Lee VFA production and application review.pdf</u>)
- Vajpeyi, S and Chandran, K., 2015, Microbial Conversion of Synthetic and Food Waste-derived Volatile Fatty Acids to Lipids, Bioresource Technology, Vol. 188, p. 49-55. (<u>http://www.ncbi.nlm.nih.gov/pubmed/25697838</u>)

- Yun, J.H., Sawant, S.S., and Kim, B.S., Production of Polyhydroxyalkanoates by Ralstonia Eutropha from Volatile Fatty Acids, Korean Journal of Chemical Engineering, Vol. 30, Issue 12, p. 2223-2227. (<u>http://link.springer.com/article/10.1007/s11814-013-0190-9</u>)
- Gaeta-Bernardi, A and Parente, V., 2016, Organic Municipal Solid Waste (MSW) as Feedstock for Biodiesel Production: A Financial Feasibility Analysis, Renewable Energy, Vol. 86, p. 1422-1432. (<u>http://www.sciencedirect.com/science/article/pii/S0960148115302251</u>)
- Tice, R.C., and Kim, Y., 2014, Methanogenesis Control by Electrolytic Oxygen Production in Microbial Electrolysis Cells, International Journal of Hydrogen Energy, Vol. 39, Issue 7, p. 3079-3086. (<u>http://www.eng.mcmaster.ca/civil/facultypages/Tice-Kim-2014-IJHE.pdf</u>)

## **References: All Subtopics:**

- Environmental Protection Agency, 2014, EPA. Regulation of Fuels and Fuel Additives: RFS Pathways II, and Technical Amendments to the RFS Standards and E15 Misfueling Mitigation Requirements Federal Register, 2014; Vol. 79, Issue 138, p. 42128-42167. (<u>https://www.epa.gov/sites/production/files/2015-08/documents/2014-16413.pdf</u>)
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- Shen, Y., Linville, J.L., Urgun-Demirtas, M., et al., 2015, An Overview of Biogas Production and Utilization at Full-scale Wastewater Treatment Plants (WWTPs) in the United States: Challenges and opportunities towards energy-neutral WWTPs, Renewable & Sustainable Energy Reviews, Vol. 50, p. 346-362. (<u>https://epic.uchicago.edu/research/publications/overview-biogas-production-andutilization-full-scale-wastewater-treatment</u>)
- WERF, 2014, Utilities of the Future Energy Findings, Final Report, Water Environment Research Federation, Alexandria, VA, p. 86. (<u>https://www.americanbiogascouncil.org/pdf/waterUtilitiesOfTheFuture.pdf</u>)
- 5. U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, 2015, Integrated Biorefineries. (<u>http://www.energy.gov/eere/bioenergy/integrated-biorefineries</u>)
- U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, 2015, Energy Positive Water Resource Recovery Workshop Report, April 28-29, p.58. (<u>http://www.energy.gov/eere/bioenergy/energy-positive-water-resource-recovery-workshop-report</u>)
- Water Environment & Reuse Foundation (WERF), 2011, Energy Production and Efficiency Research -The Roadmap to Net-Zero Energy, WER Foundation, Alexandria, p. 8. (<u>https://www.werf.org/CMDownload.aspx?ContentKey=cf3ed15a-e53b-44a3</u>)
- U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, 2015, Hydrogen, Hydrocarbons, and Bioproduct Precursors from Wastewaters Workshop. (<u>http://energy.gov/eere/fuelcells/hydrogen-hydrocarbons-and-bioproduct-precursors-wastewatersworkshop</u>)

- Energetics Incorporated, 2015, Waste-to-Energy Workshop Summary, U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, p. 53. (http://energy.gov/sites/prod/files/2015/08/f25/beto\_wte\_workshop\_report.pdf)
- U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, 2015, Bioenergy Technologies Office Multi-Year Program Plan: March 2015 Update, p. 244. (<u>http://www.energy.gov/eere/bioenergy/downloads/bioenergy-technologies-office-multi-year-program-plan-march-2015-update</u>)

# **15. 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. Many barriers must be overcome before membrane technology becomes widely adopted. Technical barriers include fouling, instability, low flux, low separation factors, and poor durability. 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. Non-atomically-precise membranes may be proposed under subtopic e providing the respondent is able to articulate a significant impact of their membrane technology compared to best-in-class commercial products. Proposals on materials and membranes related to battery applications also will be accepted. Note that references in the other subtopics are ALL relevant for topic e. In addition, for wide band gap consider technologies described in PowerAmerica also called the Next Generation Power Electronics National Manufacturing Innovation Institute which is focused on commercializing WBG applications such as industrial motor systems, consumer electronics & data centers and conversion of renewable power.

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 <a href="http://www.nersc.gov/users/accounts/allocations/request-form/">http://www.nersc.gov/users/accounts/allocations/request-form/</a>.

Grant applications are sought in the following subtopics:

### a. Atomically Precise Membranes

This subtopic is focused on the advancement of manufacturing processes that are able to produce atomically precise membranes with exceptional selectivity for separations. Atomically precise is defined

as: materials, structures, devices, and finished goods produced in a manner such that every atom is at its specified location relative to the other atoms, and in which there are no defects, missing atoms, extra atoms, or incorrect (impurity) atoms. Spiroligomers and engineered proteins are examples of atomically precise structures. Polymers are not; although the individual molecules in a conventional polymer are atomically precise, their relative positions are not atomically precise; therefore, conventional polymers are not considered to be atomically precise.

We seek to promote the development of a new class of strong, thin, and atomically precise membrane materials for separations that provide a 10X permeance improvement over state-of-the-art polymer membranes. They would have thicknesses generally below 10 nm for high permeance, incorporate atomically precise molecular pores for 100% selectivity, be atomically flat to prevent fouling, and heavily cross-linked for environmental stability. These membranes offer the potential to provide game-changing process energy advances. From a strategic perspective, the development of gram-scale and kilogram-scale atomically precise manufacturing processes would bring a new capability to produce materials near their theoretical strength limits—more than an order of magnitude beyond that of current state of the art material production methods.

The application space of special interest includes, but is not restricted to, chemical separations, desalination, and gas separations. Atomically precise membranes that have channels for purposes other than molecular, atomic, or ion transport will also be considered. In desalination, a rate increase of 2-3 orders of magnitude over reverse osmosis is projected for a system with not only controlled pore size but also engineered pore edge composition [1]. In principle, a series of membranes of sufficient selectivity could separate air into its raw components of N<sub>2</sub>, O<sub>2</sub>, Ar, CO<sub>2</sub>, Ne, He, etc. for significant energy savings in a wide range of cryogenic, chemical, and combustion processes [2, 3] and for greenhouse gas reduction.

We seek grant applications to advance scalable technologies that provide order-of-magnitude increments over the performance of current industrial membrane applications. The focus of the proposal must be on methods to produce atomically precise membranes for near 100% selectivity; or in the case of transport that is non-molecular in nature, 2X improvement or better in transport property metric over the comparative state-of-the-art. Consideration must be given to addressing the issues of fouling, stability, scalability, and cost. The choice of membrane material should be appropriate to the target separation or transport in a commercial setting. Target separations with high energy impact are preferred, that result in a minimum of 50% energy savings over competitive state of the art materials. Paper or computation-only studies do not qualify for this subtopic. We require the synthesis and testing of candidate materials. This can include the demonstration of overcoming a key technical barrier to synthesis or scale up. The proposal should include a plan for experimental measurements and supporting calculations to show that cost-competitive energy savings can be achieved with practical economies of scale. The proposal should provide a path to scale up in potential Phase II follow on work.

Questions – contact: David Forrest, <u>david.forrest@hq.doe.gov</u>

### b. Wide Bandgap Semiconductors

Gallium Nitride (GaN) wafers of 30-60 micrometers thickness and of various dopant compositions are used in a wide variety of applications, such as the amplifier in power electronics and as the light amplifier in "white" light LEDs and UV lasers (eliminating the need for sum-frequency conversion). The GaN wafers are difficult to prepare, however, as it is difficult to prepare bulk GaN crystals and obtain wafers, and it is difficult to grow GaN wafers directly. A near commercial process developed in China applies a chemical vapor deposited layer of GaN to a sapphire or gallium arsenide substrate and physically removes the GaN wafer from the substrate. The process is difficult and time consuming, and the resulting GaN wafers require chemical and mechanical polishing for epitaxially-ready GaN wafers. This subtopic solicits new methods of GaN wafer production that will translate to a high production commercial wafer process. The innovation in production process is expected to produce GaN wafers that require minimal chemical and mechanical polishing for epitaxially-ready GaN wafers are encouraged to collaborate with industry, including manufacturers, suppliers, and end users, to commercialize successful new technology.

Questions – contact: Brian Valentine, Brian.Valentine@ee.doe.gov

c. Innovative Approaches Toward Discovery and Development of Novel, Durable Supports for Low-Platinum Group Metal (PGM) Catalysts for Polymer Electrolyte Membrane Fuel Cells

Catalyst support composition and structure changes are known to affect electrode performance and durability. This subtopic seeks approaches that address support performance and chemical and structural stability by development of novel carbon-based or non-carbon support compositions and/or structures. The focus of this subtopic is novel catalyst support research with the potential to improve catalyst performance and durability, especially under transient operating conditions, while decreasing cost. DOE is specifically seeking research and development (R&D) on novel supports for low-PGM catalysts.

Concepts should possess appropriate properties such as high surface area, high protonic/electronic conductivities, and facile reactant/product transport. Catalyst deposition and stable anchoring of the catalyst on the support should be discussed. Possible effects of the support on the catalytic activity through modified dispersion or through catalyst-support interactions should be described. Applicants should clearly state the status of their current catalyst support technology as it relates to the state-of-the-art and provide sufficient justification that the approach has the potential to meet or exceed relevant DOE targets, including performance at high power density in air, durability, and cost [1].

The work plan should include a discussion of the catalytic activity testing required to show viability, including rotating disk electrode (RDE) and membrane electrode assembly (MEA) testing, and should demonstrate a pathway toward scientific advancement, which may include development of a better understanding of the catalyst-support interaction, and structural degradation, leading to novel strategies to extend electrode durability.

Questions – contact: Bahman Habibzadeh, <u>bahman.habibzadeh@ee.doe.gov</u>, or Donna Ho, <u>donna.ho@ee.doe.gov</u>

### d. Metal Hydride Materials for Compression

Reversible metal hydride materials have great potential to improve the reliability of compressors at hydrogen refueling stations at reasonable cost, but are challenged by efficiency. To achieve the pressures of interest at refueling stations (875 bar), metal hydrides typically require heating well above 100°C as well as substantial cooling to temperatures ranging from 20 to -10°C. Few materials are capable of such pressures, and many are significantly impacted by hysteresis effects that diminish their performance over time. Even at pressures below 200 bar, the efficiency of metal hydride compression is significantly lower than that of mechanical compression.

Research is needed in the discovery of new metal hydride materials for high-pressure compression. Combinatorial approaches to materials discovery have been extremely productive in the study of metal hydrides for hydrogen storage applications. Such approaches have included molecular modeling with new force fields, high throughput synthesis apparatuses, and novel high throughput screening techniques with conventional tools. Phase I proposals are sought to develop a technique that will enable high throughput discovery of metal hydrides for high-pressure hydrogen compression. This includes both high throughput combinatorial synthesis and high throughput characterization. High throughput characterization techniques designed in Phase I should be capable of predicting or evaluating materials' pressurecomposition-temperature (PCT) curves, and support the development of predictive models. Combinatorial synthesis techniques should target a material class with previously demonstrated potential. Follow on Phase II funding would involve the use of the Phase I tool to screen and down select materials of interest, along with the synthesis and experimental characterization of down-selected materials. Materials of interest are those capable of 875 bar discharge, scale-up to at least 10 kg-H<sub>2</sub>/day, and cycle lives of at least 100,000 cycles. The suction pressure can be defined by the applicant based on the integration of the metal hydride with the station. If the metal hydride is the sole compressor, it should be capable of receiving a suction pressure of 100 bar. If the metal hydride is a follow-on stage to a mechanical stage of compression, the applicant should describe the inlet temperature and pressure for which the hydride material is being designed.

Questions – contact: Neha Rustagi, <u>neha.rustagi@ee.doe.gov</u>

#### e. 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: Tina Kaarsberg, <u>Tina.Kaarsberg@ee.doe.gov</u>

### References: Subtopic a:

- Cohen-Tanugi, D., and Grossman, J.C., 2015, Nanoporous Graphene as a Reverse Osmosis Membrane: Recent Insights from Theory and Simulation, Desalination, Vol. 366, p. 59-70. (<u>http://www.rle.mit.edu/gg/wp-content/uploads/2016/03/04\_NanoporousGraphene.pdf</u>)
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### References: Subtopic b:

1. U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, 2016, <u>http://energy.gov/eere/amo/power-america</u>

### References: Subtopic c:

 U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, 2016, Technical Plan – Fuel Cells, Multi-Year Research, Development and Demonstration Plan, p. 49 (http://energy.gov/sites/prod/files/2016/06/f32/fcto myrdd fuel cells 0.pdf)

### References: Subtopic d:

- Lototskyy, M.V., et. al., 2014, Metal Hydride Hydrogen Compressors: A Review, International Journal of Hydrogen Energy, Vol. 39, Issue 11, p. 5818-5851. (<u>http://www.sciencedirect.com/science/article/pii/S0360319914002389</u>)
- Klebanoff, L., and Keller, J., 2012, Final Report for the DOE Metal Hydride Center of Excellence, Sandia National Laboratories, Albuquerque, New Mexico, SAND2012-0786. (<u>https://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/metal\_hydride\_coe\_final\_report.pdf</u>

### References: Subtopic e:

1. U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, 2016, <u>http://energy.gov/eere/amo/power-america</u>

## **16. SUBSURFACE TECHNOLOGY AND ENGINEERING RESEARCH AND DEVELOPMENT**

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 support of the DOE Office of the Under Secretary for Science and Energy's Subsurface Technology and Engineering Research, Development and Demonstration (SubTER) Crosscut Initiative, seeks to developing advanced methods to access the subsurface.

While subsurface sources constitute the Nation's primary source of energy (providing more than 80 percent of total U.S. energy needs today), they are also critical to the Nation's low-carbon and secure energy future. Next generation advances in subsurface technologies will enable access to more than 100 gigawatt-electric (GWe) of clean, renewable geothermal energy, as well as safer development of domestic natural gas supplies. The subsurface provides hundreds of years of safe storage capacity for carbon dioxide (CO<sub>2</sub>) and opportunities for environmentally responsible management and disposal of hazardous materials and other energy waste streams. The subsurface can also serve as a reservoir for energy storage for power produced from intermittent generation sources, such as wind and solar. These opportunities are directly linked to Administration priorities and to broader societal needs. Clean energy deployment and CO<sub>2</sub> storage are critical components of the President's Climate Action Plan and are necessary to meet the 2050 greenhouse gas (GHG) emissions reduction target of 83 percent below 2005 levels. Increasing domestic hydrocarbon resource recovery in a sustainable and environmentally sound manner is also an Administration goal that enhances national security and fuels economic growth. Thus, discovering and effectively harnessing subsurface resources while mitigating impacts of their development and use are critical pieces of the Nation's energy strategy moving forward.

Grant applications are sought in the following subtopics:

a. Development of Advanced Methods to Access the Subsurface in High-Temperature and High-Pressure Environments

Grant applications are sought to research, develop, and deploy new and original processes, techniques, tools, and/or sensors that support the SubTER crosscut initiative's thrust areas of wellbore integrity and drilling technologies. Geothermal energy resources are often more difficult to access compared to other

subsurface energy resources due to deep drilling through high-temperature, high-pressure, hard crystalline lithologies.

Responsive applications to this subtopic could include techniques to address wellbore instability, reduce lost circulation, or drill in the presence of CO<sub>2</sub> (or other gasses). The innovations sought range from well log/petrophysical analyses to new packers, liners, and other completion tools.

Applicants must quantify and support their predicted improvement over current state of the art. The technologies of interest must have a pathway toward operations in high temperature (> 250°C) and high pressure (> 1500 bar) environments.

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.

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

### **References:**

- Lawrence Berkeley National Laboratory, Earth Sciences Division, Wellbore Integrity and Drilling Technologies, Subsurface Crosscut, SubTER: Subsurface and Engineering Research, Development, and Demonstration. (<u>http://esd.lbl.gov/subter/home/wellbore-integrity/</u>)
- Finger, J., and Blankenship, D., 2010, Handbook of Best Practices for Geothermal Drilling, Sandia National Laboratories, Albuquerque. (<u>http://www1.eere.energy.gov/geothermal/pdfs/drillinghandbook.pdf</u>)
- Rivenbark, Mark, et al., 2011, Deep Geothermal Well Completions: A Review of Downhole Problems and Specialized Technology Needs, Proceedings 36th Workshop on Geothermal Reservoir Engineering, Stanford, California, p. 4. (https://pangea.stanford.edu/ERE/pdf/IGAstandard/SGW/2011/rivenbark.pdf)

## **17.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 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 large scale industrial and utility fossil energy power generation and natural gas recovery systems. These include R&D activities in carbon capture and storage, CO<sub>2</sub> utilization, coal and biomass utilization, advanced separation (CO<sub>2</sub>, H<sub>2</sub>, O<sub>2</sub>, REE), oil & gas, unconventional resources (oil shale,

methane hydrates, etc.), gasification (IGCC, Coal and Biomass), algae to fuels, solid oxide fuel cells, turbines, sensors and controls for coal-fired power plants, and high-performance materials for power plants.

The only areas considered in this opportunity announcement include research and technology issues and opportunities in shale gas conversion to liquid fuels and chemicals, solid oxide fuel cell (SOFC) anode modifications for gradual on-cell reforming, carbon dioxide capture – enabling advanced process systems, and CFD model development for direct fired supercritical carbon dioxide power cycles. 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 <a href="http://www.nersc.gov/users/accounts/allocations/request-form/">http://www.nersc.gov/users/accounts/allocations/request-form/</a>.

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, 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.

Questions – Contact: Doug Archer, <u>douglas.archer@hq.doe.gov</u>

### b. SOFC Anode Modifications for Gradual On-Cell Reforming

Direct Internal Reforming SOFC (DIR-SOFC) is a process in which some hydrocarbons (i.e. methane) can be directly used as fuels instead of hydrogen and carbon monoxide by feeding it straight to the anode side of the SOFC. DIR-SOFC could simplify the use of fuel cells operating on hydrocarbons and significantly improve efficiency by avoiding the losses associated with external reformers. DIR-SOFC requires an anode material with good catalytic reforming and electrochemical reactivity. Although the current state-of-the-art SOFC anode consisting of nickel and yttrium-stabilized zirconia (YSZ) has excellent catalytic properties and stability for the H<sub>2</sub> oxidation at the usual operation conditions, the use of Ni-YSZ anode with carbon-containing fuels results in the deposition of large quantities of carbon on the nickel surface, resulting in a marked irreversible reduction of cell performance.

Grant applications are sought for research and development to modify SOFC anodes for DIR-SOFC operation. This requires an anode material that has good catalytic properties for reforming reaction and electrochemical reactions while preventing carbon formation at the anode side due to the high operating temperature and lead to the loss of cell performance and poor durability. The applicant must be able to demonstrate that the performance of the proposed anode materials match those of the current state-of-the-art Ni-based anodes. Approaches of interest include, but are not limited to:

- Modifying the Ni-YSZ anode by adding a layer of catalyst that has high activity towards the hydrocarbon reforming reactions
- Developing carbon-resistant anodes for gradual on-cell reforming
- Developing alternative anodes for the direct utilization of hydrocarbons

Questions – Contact: Patcharin Burke, Patcharin.Burke@netl.doe.gov

### c. CO<sub>2</sub> Capture – Enabling Advanced Process Systems

Advanced carbon capture processes are enabling gas separations from post combustion capture, gasification, and other industrial sources. It has been recognized that the capital costs of these systems is a barrier to project development and financing. To realize large scale deployment of these technologies it will be necessary to address key process challenges, enable modular manufacturing and utilize advanced manufacturing to realize improvements to the process components which optimize gas transfer rates at the lowest costs in these transformational carbon capture systems.

1. Novel mitigation methods to decrease the quantity of aerosols that lead to large solvent loses through direct elimination of aerosols or methods to reduce the formation of aerosols during the capture process.

2. Novel reclamation methods that can be applied specifically to aqueous or non-aqueous solvent systems that remove heat stable salts, metals, and degradation products of amines and reduce the current energy penalty compared to distillation.

3. Novel manufacturing processes to enable the use of advanced materials such as non-aqueous solvents, metal organic frameworks (MOFs), and polymeric materials together to enhance capture performance and reduce cost while considering ways to optimize heat exchangers directly into the absorption process.

Applications should be aware of how these technologies compare to currently available systems, how the process improvements will impact the capital and operating costs of the systems, address issues with materials of construction, availability of materials, and lifecycle of the process impacts on cost of capture.

Questions – Contact: John Litynski, John.Litynski@hq.doe.gov

### d. CFD Model Development for Direct Fired Supercritical CO<sub>2</sub> Power Cycles

Supercritical  $CO_2$  (SCO2) power cycle operate in manners similar to other turbine cycles, but they use  $CO_2$  as the working fluid in the turbomachinery. The cycles are operated above the critical point of  $CO_2$  so that it does not change phases (from liquid to gas), but rather undergoes drastic density changes over small ranges of temperature and pressure.

Direct fired SCO2 cycles combust fossil fuels with oxygen and the resulting steam/CO<sub>2</sub> mixture is used to drive the turbine. Typical conditions are around 300 bar pressure, 700°C preheat temperature and 1100°C combustion temperature with either natural gas or coal derived syngas fuel reacting with oxygen in a highly CO<sub>2</sub> diluted environment. It is not clear whether current turbulence modeling approaches, including Reynolds Averaged Navier-Stokes and Large Eddy Simulation and their associated assumptions and modeling constants are valid at these conditions. Also, existing combustion modeling approaches such as chemical equilibrium, embedded flamelets, thickened flames and others may not be applicable at these conditions where Reynolds numbers are very high due to the high density and dissipative turbulence length scales are very small. Furthermore, the mode of combustion might be very different from current experience and may include a mix of auto ignition, flame propagation and distributed reaction.

Grant applications are sought which validate and develop CFD combustion and turbulence modeling approaches which are suitable for to direct fired supercritical power cycles.

Questions – Contact: Steve Richardson, <u>Steven.Richardson@netl.doe.gov</u>

### 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, <u>douglas.archer@hq.doe.gov</u>

### References: Subtopic a:

- Zhu, Q., Wegener, S.L., Xie, C., et al., 2013, Sulfur as a Selective 'Soft' Oxidant for Catalytic Methane Conversion Probed by Experiment and Theory, Nature Chemistry, Vol. 5, Issue 2, p. 104-109. (<u>http://www.ncbi.nlm.nih.gov/pubmed/23344430</u>)
- Armor, J.N., 2013, Emerging Importance of Shale Gas to Both the Energy & Chemicals Landscape, Journal of Energy Chemistry, Vol. 22, Issue 1, p. 21-26. (<u>http://dx.doi.org/10.1016/S2095-4956(13)60002-9</u>)
- Ghose, R., Hwang, H.T., and Varma, A., 2013, Solution Combustion Synthesized Catalytic Materials for Oxidative Coupling of Methane, 23rd North American Catalysis Society Meeting, O-W-Fre-11. (<u>https://nam.confex.com/nam/2013/webprogram/Paper8439.html</u>)
- Schwach, P., Hamilton, N.G., Schlogl, R., et al., 2013, Structure Sensitivity in Oxidative Coupling of Methane Over MgO, Fritz-Haber-Institut der Max-Planck Society, 23rd North American Catalysis Society Meeting, O-W-Fre-12. (<u>https://nam.confex.com/nam/2013/webprogram/Paper8710.html</u>)

- 5. Hutchings, G.J., 2013, Alkane Activation by Selective Oxidation Using FeCuZSM-5, Catalysis Institute, Cardiff University School of Chemistry, 23rd North American Catalysis Society Meeting, KL-W-Fre-13. (https://nam.confex.com/nam/2013/webprogram/Paper9107.html)
- Chalupka, K.A., Rynkowski, J., Grams, J., et al., 2013, Catalytic Activity of NixAlBEA and NixSiBEA Zeolite Catalysts in Partial Oxidation of Methane: Influence of Zeolite Dealumination and Ni Incorporation, 23rd North American Catalysis Society Meeting, Lodz University of Technology, Institute of General and Ecological Chemistry, P-W-Wil-16. (<u>https://nam.confex.com/nam/2013/webprogram/Paper8940.html</u>)
- Srinivas, G., Mundschau, M.V., Martin, M., 2013, Syngas-to-Ethanol Using Homogeneous Catalysis, 23rd North American Catalysis Society Meeting. O-Th-Fre-5. (<u>https://nam.confex.com/nam/2013/webprogram/Paper9312.html</u>)
- 8. Hanna, D.G., Shylesh, S., Bell, A.T., 2013, Tandem Hydroformylation-Hydrogenation of Propene to Butanol Using Supported Catalysts, University of California, Berkeley, CA, 23rd North American Catalysis Society Meeting. (<u>https://nam.confex.com/nam/2013/webprogram/Paper7708.html</u>)

### References: Subtopic b:

- Nobrega, S.D., Fonseca, F.C., Gelin, P., et al., 2012, Gradual Internal Reforming of Ethanol in Solid Oxide Fuel Cells, <u>Energy Procedia</u>, <u>Volume 28</u>, p. 28–36. (<u>http://www.sciencedirect.com/science/article/pii/S1876610212013938</u>)
- Gorte, R.J., and Vohs, J.M., 2003, Novel SOFC Anodes for the Direct Electrochemical Oxidation of Hydrocarbons, Journal of Catalysis, Vol. 216, Issues 1–2, p. 477-486. (<u>http://repository.upenn.edu/cgi/viewcontent.cgi?article=1009&context=cbe\_papers</u>)

### References: Subtopic c:

- 1. U.S. Department of Energy, National Energy Technology Laboratory (NETL), Carbon Capture. (<u>http://www.netl.doe.gov/research/coal/carbon-capture</u>)
- U.S. Department of Energy, National Energy Technology Laboratory (NETL), 2013, DOE/NETL Advanced Carbon Dioxide Capture R&D Program: Technology Update. (<u>http://www.netl.doe.gov/research/coal/carbon-capture/capture-handbook</u>)

### References: Subtopic d:

 U.S. Department of Energy, National Energy Technology Laboratory (NETL), Supercritical CO<sub>2</sub> Power Cycles, Technology Development for Supercritical Carbon Dioxide (SCO2) Based Power Cycles. (<u>http://www.netl.doe.gov/research/coal/energy-systems/turbines/supercritical-co2-power-cycles</u>)

## **18. 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 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 large scale industrial and utility fossil energy power systems and natural gas recovery systems. These include R&D activities in carbon capture and storage, CO<sub>2</sub> utilization, coal and biomass utilization, advanced separation (CO<sub>2</sub>, H<sub>2</sub>, O<sub>2</sub>,REE), oil & gas, unconventional resources (oil shale, methane hydrates, etc.), gasification (IGCC, Coal and Biomass), algae to fuels, solid oxide fuel cells, turbines, sensors and controls for coal-fired power plants, and high-performance materials for power plants.

The only areas considered in this opportunity announcement include research and technology issues and opportunities for thermal desorption of contaminants in spouted beds, advanced shale gas recovery technologies for horizontal well completion optimization, carbon dioxide utilization, and low temperature sintering techniques for ceria barrier layers or YSZ electrolytes in solid oxide fuel cell (SOFC) applications. 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 <a href="http://www.nersc.gov/users/accounts/allocations/request-form/">http://www.nersc.gov/users/accounts/allocations/request-form/</a>.

Grant applications are sought in the following subtopics:

### a. Thermal Desorption using Spouted Beds

In a recent workshop [1] conducted by International Energy Agency Clean Coal Center (IEACCC) coal chemistry, control technologies and reduction strategies, legislation and policy, emission inventories and solid/liquid media containment and control were discussed. The speciation of mercury is attracting widespread interest because the emission, transport, deposition and behavior of toxic mercury species depend on its chemical form. Many novel techniques were discussed for mercury and other contaminant control. The Fossil Energy program at DOE is looking for such novel reactor systems and is specifically focusing on Spouted Beds [2] to provide an ideal reactor configuration for sequential extraction of mercury and other contaminants from coal. Studies [3] have shown that thermal desorption can be an appropriate technique for mercury speciation.

For Phase I of this proposed topic, it is expected that the selected recipient will investigate and report the effects of particle size distribution, mercury and other contaminant characteristics, and investigate design parameters (flow rates, feed location, heating rate) for a spouted bed design and configuration that will help in the removal of such contaminants (like mercury and other contaminants) from coal. The project will use the partial oxidation and thermal decomposition mechanisms provided in literature for mercury removal and illustrate the advantages of spouted bed systems for this and other thermal desorption applications. The study will emphasize the desorption characteristics as a function of solid particle characteristics and operating temperature.

The scope of the project can comprise design, fabrication, and testing of a small demonstrable unit with pulverized coal as feedstock. Research will include collecting various data and information to address any major technical gaps. If successful in Phase I the project has a chance to move to Phase II where substantially higher funding is given and it is expected that the program will conduct experimental studies on thermal desorption of mercury and other model compounds found in coal in a scaled up pilot plant spouted bed reactor and demonstrate the models that were developed and offer potential solution to attack this important problem.

Questions – Contact: Bhima Sastri, <u>bhima.sastri@hq.doe.gov</u>

### b. Advanced Shale Gas Recovery Technologies for Horizontal Well Completion Optimization

DOE is interested in developing novel technologies that can: (1) improve our ability to characterize hydraulic fractures, and further, (2) that can advance the use of natural gas as an alternative to water for high volume hydraulic fracturing. Advances in either these two areas could improve recovery of hydrocarbons in place in shale reservoir rocks.

<u>Area 1 -</u> In the case of the first topic area, DOE is interested in catalyzing the development of novel technologies that will improve our ability to understand much more precisely the dimensions (length, height, width), orientation (azimuth, dip) relative to the wellbore, and the conductivity and proppant distribution of created hydraulic fractures, either during or immediately after the hydraulic fracturing operation. Our ability to estimate all of these remains limited and some of the best techniques (e.g., microseismic fracture mapping) are expensive, time consuming, and to some degree dependent on the availability of monitoring wells (Cipolla, et al, 2000). DOE is currently funding several projects directly or indirectly related to this topic (e.g., NETL, 2015 a,b,c) but believes that there is still a need for more research in this area.

Specific subtopic technology interests include:

- 1. Cost effective tools or methods for measuring the dimensions and/or orientation of hydraulic fractures during or after the hydraulic fracturing process
- 2. Cost effective tools or methods for measuring the fluid conductivity of hydraulic fractures
- 3. Cost effective tools or methods for measuring proppant distribution within hydraulic fractures

Existing options like microseismic fracture mapping provide some idea of fracture length and orientation but do not accurately represent the propped fracture dimensions. Novel combinations of injectants and sensing tools that can be used to directly measure the dimensions and orientation of propped fractures, and potentially conductivity, are required. For example, there are currently two ongoing projects described on the NETL website. For example, NETL project DE-FE0024360 with Paulsson Inc. employs a micro-emitter injected along with proppant and a fiber-optic borehole seismic sensor array, and project DE-FE0024271 with UT Austin, employs a conductive proppant and a low frequency electromagnetic induction tool. We are looking for proposals that look to achieve similar results.

<u>Area 2</u> In addition, DOE is interested in proposals to develop and test technologies that will reduce the amount of water needed for hydraulic fracturing when completing natural gas wells or that will improve the apparent low (<30%) natural gas and liquids recovery efficiency currently associated with horizontal, hydraulically fractured wells producing from shale formations, through the use of natural gas as a fracturing fluid. Proposals should focus on addressing a number of important areas where cost effective

improvements may be possible. The objective is to increase the efficiency of resource recovery on a per well basis and reduce the volume of fresh water required to produce a unit volume of natural gas. Research areas of specific interest for dedicated research wells may include, but are not limited to:

- Quantitative assessments of the practical and economic limits and potential benefits (if any) of employing natural gas (not LPG) and water mixtures as a fracturing fluid to partially replace water in large volume multiple stage hydraulic fracturing treatments representative of those being applied in shale gas and shale oil plays today (2015, Millennium). Such analyses may be based on computer simulations that employ state-of-the-art commercial hydraulic fracturing models to characterize the potential volumes and rates of natural gas/water mixtures required to achieve well productivity similar to that when wells are fractured using water alone.
- Laboratory experiments that quantify the effect on relative permeability to gas in a producing wellbore when mixtures of water and natural gas (versus water only) are employed as fracturing fluids under conditions representative of major shale gas plays (e.g., Marcellus, Utica Shale).
- Other examples of analysis could aim to characterize the suitability of the rheology of such conventional fracturing fluid/natural gas mixtures for large volume hydraulic fracturing, and to prove the feasibility of employing natural gas as a partial alternative to water, as justification for a Phase II field experiment focused on testing the process.
- Proposals for research on fracturing techniques that are not focused on the use of natural gas as a fracturing fluid (e.g., liquid propellants or solid propellants) will be considered non-responsive.

All grant applications, for either of the above topical areas, must include a succinct discussion of the potential technical and economic advantages of the proposed technology, as compared to existing state-of-the-art systems.

Beyond-state-of-the-art research that can have (or lead to) "game-changing" impacts will be considered more responsive to this solicitation than research that proposes small, incremental advances.

Questions – Contact: Al Yost, <u>albert.yost@netl.doe.gov</u>

### c. CO<sub>2</sub> Utilization

To reduce risk and offset the cost of CCS, development of CO<sub>2</sub> utilization/conversion technologies processes to generate value-added products will be required. A larger and more diverse market is needed to facilitate deeper GHG reductions from CO<sub>2</sub> sales beyond what can be realized by Enhanced Oil Recovery (EOR) alone. For instance, a coal-fired power plant equipped with a CO<sub>2</sub> capture and purification unit could offer multiple gas streams with varying concentrations of CO<sub>2</sub> potentially suitable for CO<sub>2</sub> utilization/conversion to high value products, including: (1) flue gas exiting the desulfurization unit (prior to entering the downstream CO<sub>2</sub> capture and purification unit), (2) CO<sub>2</sub>-dilute flue gas being directed to the stack following bulk CO<sub>2</sub> removal, and (3) concentrated CO<sub>2</sub> exiting the CO<sub>2</sub> capture and purification unit that is ready for compression and storage.

Grant applications are sought for the development or enhancement of novel technologies that support DOE's goals of less than \$10 per tonne. It is expected that the revenue generated from these novel utilization processes may result in positive revenue that will reduce carbon emissions and the cost of associated carbon capture. The applicant must demonstrate a thorough understanding of the utilization/conversion process being proposed and its ability to integrate with coal-fired power plants. Of particular importance is a thorough discussion of the integration approach with the power plant,

hybridization of gas separation processes to increase CO<sub>2</sub> uptake and maintain optimal inlet CO<sub>2</sub> concentration, rate of CO<sub>2</sub> utilization and practical limits on how much flue gas could be processed from a single power plant, associated CO<sub>2</sub> emission reduction, process footprint, impact and ultimate fate of heavy metals and other flue gas impurities, novel dewatering concepts, knowledge gaps and key technical challenges, and process costs.

Preference will be given to applications that have the potential to be economically viable at large-scale based on the value of the products produced, considering the existing market for these products. Additionally, the proposal should include a preliminary, high-level life cycle analysis (LCA) to demonstrate that the proposed technology will not create more CO<sub>2</sub> than is utilized and/or show that the CO<sub>2</sub> emissions are less than the process that it would replace. Projects will be selected based on the strength of proposed concepts and approach, prior progress made by the applicant in developing the technology, potential for future and near-term commercialization, assessment of the technology's promise for substantive and cost effective CO<sub>2</sub> mitigation, and reasonableness of proposed cost of the technology.

DOE is currently supporting multiple small- and large-scale R&D projects to demonstrate the technical and economic feasibility of CCS. While advances have been made to reduce the cost of implementation, cost remains a primary concern. Recent studies support the approach that CO<sub>2</sub> utilization should focus on identifying technologies and opportunities that assist in reducing CO<sub>2</sub> capture costs as a means to accelerate industrial-scale implementation of geologic storage. Consequently, technologies that support this approach are of particular interest.

Questions – Contact: John Litynski, john.litynski@hq.doe.gov

d. Low Temperature Sintering Techniques for Ceria Barrier Layers or YSZ Electrolytes in SOFC Applications Barrier layers are a necessity in several SOFC designs to prevent the formation of ionically insulating phases at the electrolyte-barrier layer interface. Standard barrier layer material sets and sintering techniques impart a performance penalty due to their porous nature, which decreases ionic conductivity and allows for the formation of ionically insulating phases. Similarly, electrolytes typically require higher sintering temperatures (over 1200°C) to reach full density, which requires the use of relatively expensive furnaces.

Grant applications are sought for the research and development of methods and or materials that can produce high-density GDC barrier layers or high density electrolytes at temperatures below 1200°C. Approaches of interest include, but are not limited to, sintering aides or alternative sintering techniques that are better, faster, and less expensive than the current state of the art. A complete description of the material set or process required to achieve dense barrier layers or electrolytes should be provided to facilitate analysis of potential cost entitlements and implementation complexity. Applications must present a clear plan that outlines how dense barrier layers or electrolytes would be fabricated and implemented, and how they would perform.

Questions – Contact: Joseph Stoffa, Joseph.Stoffa@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.

### References: Subtopic a:

- 1. IEA Clean Coal Centre, 2015, 11th Annual IEACCC Mercury Emissions from Coal Workshop, Chennai, India November 16-20. (<u>http://mec11.coalconferences.org/ibis/MEC11/home</u>)
- Epstein, N., Grace, J.R., 2011, Spouted and Spout-Fluid Beds: Fundamentals and Applications, Cambridge University Press, p. 360. (<u>http://www.cambridge.org/us/academic/subjects/engineering/chemical-engineering/spouted-and-spout-fluid-beds-fundamentals-and-applications</u>)
- Rumayor, M., Diaz-Somoano, M., Lopez-Anton, M.A., and Martinez-Tarazona, M.R., 2015, Application of Thermal Desorption for the Identification of Mercury Species in Solids Derived from Coal Utilization, Chemosphere, Vol. 119, p. 459–465 (<u>http://www.sciencedirect.com/science/article/pii/S0045653514008601</u>)

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

The Biological and Environmental Research (BER) Program supports fundamental, peer-reviewed research on complex systems in climate change, subsurface biogeochemistry, genomics, systems biology, radiation biology, radiochemistry, and instrumentation. BER funds research at public and private research institutions and at DOE laboratories. BER also supports leading edge National Scientific User Facilities including the DOE Joint Genome Institute (JGI), the Environmental Molecular Science Laboratory (EMSL), the Atmospheric Radiation Measurement (ARM) Climate Research Facility and instrumentation for structural biology research at the DOE Synchrotron Light and Neutron sources.

BER has interests in the following areas:

(1) Biological Systems Science integrates discovery- and hypothesis-driven science with technology development on plant and microbial systems relevant to DOE bioenergy mission needs. Systems biology is the multidisciplinary study of complex interactions specifying the function of entire biological systems—from single cells to multicellular organisms—rather than the study of individual components. The Biological Systems Science subprogram focuses on utilizing systems biology approaches to define the functional principles that drive living systems, from microbes and microbial communities to plants and other whole organisms. Key questions that drive this research include: What information is encoded in the genome sequence? How is information exchanged between different sub-cellular constituents? What molecular interactions regulate the response of living systems and how can those interactions be understood dynamically and predictively? The approaches employed include genome sequencing, proteomics, metabolomics, structural biology, high resolution imaging and characterization, and integration of information into predictive computational models of biological systems that can be tested and validated.

The subprogram supports operation of a scientific user facility, the DOE Joint Genome Institute (JGI), and access to structural biology facilities at the DOE Synchrotron Light and Neutron Sources. Support is also provided for research at the interface of the biological and physical sciences and in radiochemistry and instrumentation to develop new methods for real-time, high-resolution imaging of dynamic biological processes.

(2) The Climate and Environmental Sciences subprogram focuses on a predictive, systems-level understanding of the fundamental science associated with climate change and DOE's environmental challenges—both key to supporting the DOE mission. The subprogram supports an integrated portfolio of research from molecular level to field-scale studies with emphasis on multidisciplinary experimentation and use of advanced computer models. The science and research capabilities enable DOE leadership in climate-relevant atmospheric-process research and modeling, including clouds, aerosols, and the terrestrial carbon cycle; large-scale climate change modeling; integrated analysis of climate change impacts; and advancing fundamental understanding of coupled physical, chemical, and biological processes controlling contaminant mobility in the environment. The subprogram supports three primary research activities and two national scientific user facilities. Atmospheric System Research seeks to resolve the two major areas of uncertainty in climate change model projections: the role of clouds and the effects of aerosols on the atmospheric radiation balance. Environmental System Science supports research that provides scientific understanding of the effects of climate change on terrestrial ecosystems, the role of terrestrial ecosystems in global carbon cycling, and the role of subsurface biogeochemistry in controlling the fate and transport of energy-relevant elements.

Climate and Earth System Modeling focuses on development, evaluation, and use of large scale climate change models to determine the impacts of climate change and mitigation options.

Two scientific user facilities the Atmospheric Radiation Measurement (ARM) Climate Research Facility and the Environmental Molecular Sciences Laboratory (EMSL) provide the broad scientific community with technical capabilities, scientific expertise, and unique information to facilitate science in areas integral to the BER mission and of importance to DOE.

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

# 19.TECHNOLOGIES FOR CHARACTERIZING AND MONITORING COMPLEX SUBSURFACE SYSTEMS

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

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 (e.g., pore to core to plot to watershed) scales. With increasing computational capability it is possible to simulate the coupled interactions of complex subsurface systems with high fidelity. The predictive skill of these advanced models is limited, however, by the accuracy of the parameters 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 fidelity measurements of the hydrobiogeochemical structure and functioning of the complex subsurface systems over the relevant spatial and temporal scales.

The focus of this topic is on the development of improved sensing systems for capturing the *in-situ* hydrobiogeochemical structure and functioning of complex subsurface systems because they serve as the substrate for natural, disturbed and managed terrestrial vegetation systems.

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://science.energy.gov/ber/research/cesd/terrestrial-ecosystem-science/. 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.

Grant applications are sought in the following subtopics:

a. Real-Time, In Situ Measurements of Hydrobiogeochemical and Microbial Processes in Complex Subsurface Systems

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 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, 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. <sup>2</sup>H, <sup>18</sup>O, CH<sub>4</sub>, CO<sub>2</sub>, 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, microbe or microbial association (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 also are 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 and microbiology community structure, (2) fiber optic, solid-state, chemical, or silicon micro-machined sensors; and (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. Grant applications that propose minor adaptations of readily available materials/hardware, and/or cannot demonstrate substantial improvements over the current state-of-the-art are not of interest and will be declined.

Questions – Contact David Lesmes, <u>david.lesmes@science.doe.gov</u>

### 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 David Lesmes, <u>david.lesmes@science.doe.gov</u>

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## **20.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 and precipitation processes, including aerosol formation, chemical evolution, and optical properties; initiation of cloud droplets, ice crystals, and precipitation; and feedbacks involving the terrestrialaerosol-cloud system (Reference 1). These data are necessary both for process understanding and for evaluation of numerical models that are used to assess the climate change impacts to global and regional systems. The Intergovernmental Panel on Climate Change (IPCC) Fifth Assessment Report (AR5) states that 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 low-weight and power instruments for measurement of planetary boundary layer height and cloud base.

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) Climate Research Facility is currently operating tethered balloon systems at its Oliktok Point site in Alaska (Reference 5) and is developing capabilities for mid-size UAS flights. 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) acquisition of high-resolution cloud particle images capable of distinguishing size and habit of ice particles as well as droplets in mixed-phase clouds, (2) a fast spectrometer for measurement of cloud condensation nuclei number concentrations over

supersaturation ranges of the order 0.02% - 1%, and (3) 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 (<u>http://www.skydocballoon.com/aerostats.html</u>) and the Navmar TigerShark UAS (<u>https://www.nasc.com/Tigershark.php</u>). 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, <u>rick.petty@science.doe.gov</u> (platform related) or Ashley Williamson, <u>ashley.williamson@science.doe.gov</u> (sensor related)

### b. Robust Field-Deployable Measurements of Aerosol Composition

Atmospheric aerosol particles may be caused by natural or anthropogenic sources and may form either from emissions of primary particulates or through formation of secondary particulates 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 the radiation budget or cloud formation, and ultimate climate effects. Long-term measurements of aerosol composition, in concert with measurement of other key atmospheric, aerosol, and cloud parameters, are critical to improving the understanding and numerical modeling of aerosol and cloud formation processes.

Major aerosol components of interest include (predominantly anthropogenic) secondary inorganic sulfate and nitrate compounds, (predominantly natural) mineral dust and sea spray, and carbonaceous material (of both natural and anthropogenic origin) which is typically a complex mix of oxidized organic material with a minor component of refractory "black carbon". The latter material is so named because it is highly optically absorbing and therefore the major aerosol component with a tendency toward atmospheric heating. 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 24 hr) 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 <u>suite</u> of instruments including mass spectral instruments (either single particle or short-time integrated) for near real-time data collection, <u>time-resolved collection</u> for later analysis, or short-term wet chemical collection with a Particle Into Liquid Sampler (<u>PILS</u>). In contrast to the daily sampling network strategy 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 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 technology, or to improve instruments using current measurement principles, in order to allow long-term, continuous measurements of key atmospheric aerosol components listed above [black carbon (BC), 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.
- 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.
  - o 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/m<sup>3</sup> 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, <u>ashley.williamson@science.doe.gov</u>

#### c. Compact, Low-power Ceilometer for Long-term Measurement Sites

The AmeriFlux network is a community of sites and scientists measuring ecosystem carbon, water, and energy fluxes, and committed to producing and sharing high quality eddy covariance data (http://ameriflux.lbl.gov/). There are more than 140 active AmeriFlux sites across the Americas, spanning nearly all major ecosystem types and climatic regimes on land. The sites are independently operated and are often located in remote locations; roughly 60% are not connected to line power and rely on solar, wind, and/or generator power. Instruments are mounted above the vegetative canopy on a tripod, scaffold, or tower. The latter may be walk-up or climbing structures. Instruments that are suitable for deployment at AmeriFlux sites are generally low power, capable of autonomous operation including remote configuration, light enough that two people can readily set up and take down the instrument from the flux tower or a mounting stand, and compact to reduce wind loading on the tower and to minimize interference with adjacent instrumentation.

The formation and life cycle of boundary layer clouds, which occur in nearly all environments, are influenced by surface processes that affect thermodynamic properties of the planetary boundary layer (PBL). Data collected at AmeriFlux field sites provide detailed information about the radiation balance and exchange of trace gases, heat, moisture, and momentum near the surface. They do not, however, collect information about the types of clouds present or macroscale cloud properties such as cloud-base height and cloud fraction. Ceilometers are laser-based instruments used to quantify cloud layers and heights, and they can also quantify PBL height.

Combining ceilometer data with existing instruments at AmeriFlux sites would provide the ability to accurately describe macroscale cloud properties and how they evolve with time, over a range of land use and ecosystem types. Such data could also be used to study the structure of the boundary layer in the precloud environment; constrain trace gas budgets in the PBL, for example shedding light on 'flushing' events in the canopy or near-surface and how they relate to growth and collapse of the PBL; and provide information about nocturnal boundary layers and nighttime mixing as they related to turbulent conditions, potentially filling in nighttime gaps of the eddy covariance technique when sufficient turbulence does not exist. Ceilometers, in conjunction with other instrument systems, have been used to investigate evolution of CO<sub>2</sub> fluxes in urban environments (Reference 6) and to develop relationships between cloud cover and solar radiation, and their impact on ecosystems (References 7-8).

Grant applications are sought to develop compact, low-power, and low-weight autonomously operated ceilometers suitable for deployment at remote AmeriFlux sites. The proposed systems should be capable of meeting the following minimum technical specifications:

<u>Power:</u> Maximum power of 100W. Systems requiring power less than 20 W that are suitable for deployment at AmeriFlux sites without grid power are desirable.

Weight: Maximum weight of 10kg.

<u>Size:</u> Maximum size of instrument (including any enclosure) less than 100 linear cm (length + width + height).

<u>Temperature range</u>: Systems capable of meeting data specifications at ambient air temperatures ranging from -40 °C to +50° C

Resolution: Height resolution of 30 m and temporal resolution 30s

<u>Sensitivity</u>: System must be capable of detecting cloud base heights between 100 m and 7 km above ground level. Sensitivity of height-resolved backscatter data must be sufficient to enable detection of planetary boundary layer depth during the daytime.

<u>Communication</u>: The system shall enable communications through one or more serial ports. Communication should be possible using a terminal or laptop computer with a serial interface and a terminal emulation program. The ceilometer shall be capable of receiving and responding to remote commands for instrument configuration.

<u>Window cleaning</u>: The system must include a means of cleaning the window that enables window cleaning to be controlled both automatically and by remote command.

- Safety standards: The instrument must be compliant with the following safety standards:
- Laser Eye Safety: Class 1M per IEC 60825-1
- (rated as safe for naked eye because site staff may work near or above the laser path.)
- Electrical: IEC 60950-1
- Electromagnetic: Class B per IEC 55022
- Environmental: ISO 10109-11
- Vibration: IEC 60068-2-6

Output data: The system must output the following data:

- Time
- Distance from lidar to center of each range gate
- Cloud base height
- Calibrated or uncalibrated attenuated backscatter
- Daytime PBL height
- Background light
- Status variables that indicate the health of the system
- Laser pulse energy
- Internal temperature
- Internal humidity
- Tilt angle

The ceilometer design should be suitable for housing inside an enclosure to provide adequate protection from weather and systems should be capable of being tower-mounted. The system must be capable of autonomous operation and must be able to smoothly power down the laser system when its internal

temperature exceeds its safe operating range, and automatically power it up when the system has cooled sufficiently. In cold weather, the system should "preheat" internal components to their normal operating temperature before the lidar transceiver is powered up. The system must include a tilt sensor that indicates the tilt of the outgoing laser beam with respect to zenith, and the mounting mechanism should enable the user to manually align the instrument to zero tilt. The ceilometer should have a modular design that allows for field replacement of components, including the laser and receiver. For tower-mounted systems, reduced sensitivity to vibration is desirable.

Questions – contact: Jared DeForest, <u>Jared.DeForest@science.doe.gov</u>

### 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: Ashley Williamson, <u>ashley.williamson@science.doe.gov</u>

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# 21.TECHNOLOGY TRANSFER OPPORTUNITIES: BIOLOGICAL AND ENVIRONMENTAL RESEARCH FROM BESC

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 8 of this document prior to submitting applications.

DOE's Office of Biological and Environmental Research (BER) Genomic Science Program supports DOE missiondriven fundamental research to identify the foundational principles that drive biological systems. Development of innovative approaches for sustainable bioenergy production will be accelerated by a systems biology understanding of non-food plants that can serve as dedicated cellulosic biomass feedstocks and microbes capable of deconstructing biomass into their sugar subunits and synthesizing next generation biofuels from cellulosic biomass. Genomic Science Program research also brings the -omics driven tools of modern systems biology to bear for analyzing interactions among organisms that form biological communities and between organisms and 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 commercialization utilizing one of the TTOs developed by the BESC program 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: Prem Srivastava, prem.srivastava@science.doe.gov

Grant applications are sought in the following subtopics developed by BESC:

a. Plants with Altered Pectin and Lignin Biosynthesis and with Improved Recalcitrance and Growth

Dr. Mohnen's group at The University of Georgia has identified a clade of genes that are associated with the control of the biosynthesis of both pectin and lignin (and possibly xylan). Mutations of these genes in certain plants (including switch grass and Populus) lead to considerable reduction of recalcitrance (v. wild type), as shown by means of bacterial degradation of modified biomass. Furthermore, Populus plants bearing some of these mutations have exhibited a considerable increase in height and stem diameter (v. wild type). Plants bearing these mutations may prove suitable for economically viable extraction and use of carbohydrates from plant cell wall, as recalcitrance is greatly reduced and rate of overall growth of modified plants increases. Tested in multiple plant species.

There is increasing interest in the use of biomass for biofuel production as an environmental friendly and socio-economically responsible fuel alternative. Bioenergy originates biomass generated by CO<sub>2</sub> fixation by land plants. Approximately 70% of plant biomass is estimated to be present in plant cell wall .As we are currently using only 2% of plant cell wall-based biomass, there is a great opportunity to use this valuable resource as a raw material for the production biofuels and commodity chemicals. The plant cell wall provides mechanical support to the plant and contributes to plant growth and development. Carbohydrates, proteins and phenolic (e.g., lignin) compounds are the major components in the plant cell wall with cellulose, hemicellulose and pectin comprising the major polysaccharides in the wall. Pectins, are enriched in the primary wall of dicot plants, are essential for plant growth, development, signaling, and cell adhesion and have diverse structural characteristics that greatly contribute to wall function. The goal of using bioenergy crops for bio-ethanol production in the United States is well established. However, cost effectiveness is one of the major limitations for this industry and intimately associated with biomass recalcitrance caused in part by lignin, pectin and xylan. The major barrier is the cost of the bacterial and fungal enzymes needed to degrade the plant cell wall. Therefore, an approach to find good candidate recalcitrance genes which can be modified to pro-duce genetically modified plant cell walls from which sugars can more easily be released, and thus, which would serve as raw materials for bio-ethanol industry, is key for greatly reducing the amount of enzymes, chemicals and/or energy demand used to circumvent biomass recalcitrance.

### Licensing Information:

The University of Georgia Contact: Gennaro Gama (GJG@uga.edu, (706)583-8088) TTO Tracking Number: Case 1542 Patent Status: International protection sought. Applications pending in the US, Israel, Canada, Australia and Brazil Type of License: Both exclusive and nonexclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-</u> bool.html&r=0&f=S&I=50&TERM1=Mohnen&FIELD1=IN&co1=AND&TERM2=Georgia&FIELD2=AS&d=PG01

### Website: <a href="http://research.uga.edu/gateway/licensing-opportunities/">http://research.uga.edu/gateway/licensing-opportunities/</a>

### b. Use of Extremophiles and their Enzymes for Biofuels and Biomaterial's Production

A collaboration between Drs. Michael W. Adams (UGA) and Robert Kelly (NCSU) led to the development of a portfolio of technologies that take advantage of characteristics of P. furiosus (a hyperthermophile) to metabolize CO<sub>2</sub> into chemical commodities. The portfolio includes isolated recombinant enzymes, as well as microbial constructs and methods of using the same.

Microbial conversion of  $CO_2$  into multiple commodity chemicals, with or without input of  $H_2$ . Such chemicals include, but are not limited to, 3-hydroxypropionic acid and succinic acid.

#### **Licensing Information:**

The University of Georgia Contact: Gennaro Gama (GJG@uga.edu, (706)583-8088) TTO Tracking Number: Cases 1563, 1576, 1889 Patent Status: US applications pending (exclude published appl # 20130102022) Type of License: Both exclusive and nonexclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-</u> <u>bool.html&r=0&f=S&l=50&TERM1=Adams&FIELD1=IN&co1=AND&TERM2=Georgia&FIELD2=AS&d=PG01</u> Website: http://research.uga.edu/gateway/licensing-opportunities/

#### c. Metabolic Engineering of Caldicellulosiruptor bescii for the Production of Biofuels and Bioproducts

University of Georgia researchers have invented a method, involving the use of C. bescii, to more efficiently decompose biomass. The Caldicellulosiruptor bacterium has unique properties for processing a type of lignocellulosic biomass. By genetically manipulating C. bescii through the introduction of key genes (thus altering the organism's metabolism) that allow the production of desired chemicals from biomass, the researchers have shown that ethanol can be more easily created. Specifically, the researchers have developed methods for genetic manipulation of members of this Caldicellulosiruptor genus, enabling them to produce ethanol and hydrogen from biomass.

Caldicellulosiruptor bescii, a thermophilic bacterium, has a high affinity for decomposing lignocellulosic biomass, which includes agricultural residues such as rice straw, switchgrass, as well as hard- and soft-woods. Lignocellulosic biomass consists of cellulose, hemicellulose, pectin and lignin. Caldicellulosiruptor are among the most thermophilic and cellulolytic bacteria, which enables them to degrade untreated biomass. This characteristic makes this organism especially appealing to biomass processing. However, its inability to produce compounds of economic interest require that the organism be modified in order to enable its use in industrial processes for the production of biofuels and other commodity chemicals.

### Licensing Information:

The University of Georgia Contact: Gennaro Gama (GJG@uga.edu, (706)583-8088) TTO Tracking Number: Case 1936 Patent Status: US Issued Patent # 9,309,542 Type of License: Both exclusive and nonexclusive USPTO Link: <u>http://patft.uspto.gov/netacgi/nph-</u> Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearchbool.html&r=1&f=G&l=50&co1=AND&d=PTXT&s1=9,309,542&OS=9,309,542&RS=9,309,542 Website: http://research.uga.edu/gateway/licensing-opportunities/

d. Transgenic Plants having Altered Expression of a Xylan Xylosyl Transferase and Methods of Using Same

Dr. Debra Mohnen's group at UGA has developed a method to genetically modify plants from the group comprised of Panicum, Zea, Oryza, Triticum, Hordeum, Sorghum, Avena, Secale, Fagopyrum, Digitara, and Chenopodiu, so as these plants exhibit increased glucose yield per gram of biomass, increased total sugar yield per gram biomass, decreased recalcitrance, increased saccharification efficiency, increased growth, or the combination these characteristics

#### Licensing Information:

The University of Georgia Contact: Gennaro Gama (GJG@uga.edu, (706)583-8088) TTO Tracking Number: Case 2336 Patent Status: US Provisional filed in October 2015 Type of License: Both exclusive and nonexclusive USPTO Link: N/A (provisionals are not published by the USPTO) Website: http://research.uga.edu/gateway/licensing-opportunities/

#### e. Genetic Regulation for Lignin Reduction and Flavonoid Enhancement in Sorghum Plants

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 (<u>caldwellit@ornl.gov</u>, (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: Exclusive USPTO Link: N/A Website: <u>https://www.ornl.gov/partnerships/genetic-regulation-lignin-reduction-and-flavonoidenhancement-plants</u>

f. Heat-stable Iron-dependent Alcohol Dehydrogenase for Aldehyde Detoxification in Lignocellulosic Hydrolysates

A heat-stable, NADPH-dependent alcohol dehydrogenase was cloned and overexpressed in E. coli. The enzyme displayed activity against a number of aldehydes including inhibitory compounds that are produced during the dilute acid pretreatment process for lignocellulosic biomass before fermentation to

biofuels. The enzyme reduced aldehydes to their corresponding alcohols, which are less toxic to microorganisms. The enzyme also has potential for use in metabolic engineering strategies for producing longer-chain alcohols from sugars using thermophilic, fermentative microorganisms.

## Licensing Information:

Oak Ridge National Laboratory Contact: Jennifer Caldwell (<u>caldwelljt@ornl.gov</u>, (865)574-4180) TTO Tracking Number: UTB ID 201202933 Patent Status: US Patent Application 15/060,078 filed on 3/3/2016 Type of License: Both exclusive and nonexclusive USPTO Link: Website: https://www.ornl.gov/sites/default/files/legacy\_files/File%20Library/Main%20Nav/ORNL/Partnerships/Av

ailable%20Technologies/ID-201202933 FC.pdf

## g. A Single Multi-functional Enzyme for Efficient Biomass Conversion

Enzymatic conversion of biomass to glucose and xylose is currently performed using mesophillic fugally derived enzymes mixtures from organisms such as T. reesi. These mixtures utilize several enzymes, such as glycoside hydrolase GH6 and GH7 cellulases; as well as GH 1 0/11 xylanases to perform sugar hydrolysis, these enzymes are widely used for the simultaneous saccharification and fermentation (SSF) of cellulose to ethanol and provide reasonable ethanol production rates at low to moderate enzyme loadings. An alternative approach is to utilize enzymes from hyperthermophilic bacterial organisms that contain no GH6/7 enzymes for either (SSF) or single step direct microbial conversion of biomass, these hyperthermophilic systems utilize a combination of GH9 and GH48 enzymes to hydrolyze cellulose and can operate at extremely high temperatures. Glycoside hydrolases from C. bescii include the multidomain (GH9/GH48) enzyme, CelA. CelA is able to function optimally at 75-850C. We have shown that in addition to efficiently hydrolyzing crystalline cellulose to glucose and cellobiose , this enzyme can also efficiently hydrolyze the xylan in natural plant cell walls to xylose.

## Licensing Information:

National Renewable Energy Laboratory (NREL) Contact: Eric Payne (<u>eric.payne@nrel.gov</u>, (303)275-3166) TTO Tracking Number: 12/28/2016 Patent Status: US patent 9249432 Type of License: Nonexclusive USPTO Link: <u>http://patft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-</u> <u>bool.html&r=1&f=G&l=50&co1=AND&d=PTXT&s1=9249432&OS=9249432&RS=9249432</u> Website:

# h. A New Version of Clostridium Thermocellum CbhA, in Which the Amino-acid Sequence is Modified in Such a way as to Result in Enhanced Catalytic Activity in the Saccharification of Cellulose

The amino-acid sequence of CbhA, an important cellulosomal enzyme from the cellulase system of Clostridium thermocellum, has been modified to produce a cellulase with more than twice the activity of the original enzyme. Replacement of the X1 (1)-X1 (2) segment of the sequence of CbhA with a putative 'linker'' sequence of amino-acids from the sequence of an enzyme produced by an organism from a different genus produces a cellulase capable of solubilizing a "target" level of 30% of the substrate

cellulose (Avicel PH1 01) in less than half the time required by the original, unmodified enzyme.

Licensing Information: National Renewable Energy Laboratory (NREL) Contact: Eric Payne (<u>eric.payne@nrel.gov</u>, (303)275-3166) TTO Tracking Number: 12/1/1933 Patent Status: 8993276 Type of License: Nonexclusive USPTO Link: Website:

# 22.TECHNOLOGY TRANSFER OPPORTUNITIES: BIOLOGICAL AND ENVIRONMENTAL RESEARCH FROM JBEI AND GLBRC

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 8 of this document prior to submitting applications.

DOE's Office of Biological and Environmental Research (BER) Genomic Science Program supports DOE missiondriven fundamental research to identify the foundational principles that drive biological systems. Development of innovative approaches for sustainable bioenergy production will be accelerated by a systems biology understanding of non-food plants that can serve as dedicated cellulosic biomass feedstocks and microbes capable of deconstructing biomass into their sugar subunits and synthesizing next generation biofuels from cellulosic biomass. Genomic Science Program research also brings the -omics driven tools of modern systems biology to bear for analyzing interactions among organisms that form biological communities and between organisms and 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 commercialization utilizing one of the TTOs developed by the JBEI and GLBRC programs 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: Prem Srivastava, prem.srivastava@science.doe.gov

Grant applications are sought in the following subtopics developed by JBEI and GLBRC:

#### a. Engineering Tolerance to Drought by Over Expression of a Grass Specific Protein

Researchers at the Joint BioEnergy Institute (JBEI) have used recombinant nucleic acid techniques to overexpress a gene — SAB18 — to increase plants' tolerance to both drought and flooding. SAB18, found in rice and other grass plants, is involved in carbohydrate and nucleotide metabolism and is responsible for a plant's natural tolerance to variations in water availability. Plants that are modified to over-express this gene have been shown to remain greener, taller, and more erect when subjected to extreme water conditions. When compared to natural plants under similar conditions, the viability and health of SAB18 modified rice plants increased substantially.

#### **Licensing Information:**

Lawrence Berkeley National Laboratory Contact: Peter Matlock (<u>pymatlock@lbl.gov</u>, (510)486-5803) TTO Tracking Number: 2014-108 Patent Status: US Patent Application Type of License: Exclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-</u> <u>adv.html&r=1&f=G&l=50&d=PG01&S1=20160068855.PGNR.&OS=DN/20160068855&RS=DN/20160068855</u> <u>5</u>

Website: http://ipo.lbl.gov/lbnl2014-108/

#### b. Microbial Production of Hydroxytyrosol and Tyrosol

JBEI researchers have developed a method for using a microbial host to synthesize the powerful antioxidant and dietary supplement hydroxytyrosol. The method could be modified to produce other desirable oxidized products of aromatic amino acids, such as L-DOPA, melatonin, serotonin, and various alkaloid natural products.

The scientists transformed a strain of E. coli to express a group of enzymes and cofactors that efficiently convert tyrosine to hydroxytyrosol, a process that includes selective oxidation of tyrosine to L-DOPA. They optimized various steps in this pathway to minimize the quantity of side products. In particular, they engineered the process to avoid over-oxidation of tyrosine, which would produce melanin and other impurities, and to exclude the production of tyrosol, a less potent antioxidant that needs to be removed when purifying hydroxytyrosol.

#### **Licensing Information:**

Lawrence Berkeley National Laboratory Contact: Peter Matlock (<u>pymatlock@lbl.gov</u>, (510)486-5803) TTO Tracking Number: 2939 Patent Status: US Patent Application Type of License: Exclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO2&Sect2=HITOFF&u=%2Fnetahtml%2FPTO%2Fsearch-</u> <u>adv.html&r=3&p=1&f=G&l=50&d=PG01&S1=%28hydroxytyrosol.CLM.+AND+Lee.IN.%29&OS=ACLM/hydro</u> <u>xytyrosol+AND+IN/Lee&RS=%28ACLM/hydroxytyrosol+AND+IN/Lee%29</u> Website: <u>http://ipo.lbl.gov/lbnl2939</u>

## c. Engineering Resistance and Root Growth in Plants

JBEI/UC Davis researchers have discovered a novel polypeptide (RraxX) capable of inducing root growth and stimulating the plant immune response.

Several methods of employing the polypeptide to stimulate growth and immunity are envisioned. For example, researchers have shown that direct application of the polypeptide or its synthetic derivatives can induce these responses.

## Licensing Information:

Lawrence Berkeley National Laboratory Contact: Peter Matlock (<u>pymatlock@lbl.gov</u>, (510)486-5803) TTO Tracking Number: 2016-030 Patent Status: PCT Application: PCT/US2015/036439 Type of License: Exclusive USPTO Link: <u>http://www.freepatentsonline.com/WO2015195921A2.html</u> Website:

#### d. Generation of Heritable Chimeric Plant Traits

Joint BioEnergy Institute (JBEI) have developed a technology to inactivate target genes in specific tissues such as in fiber cells. Small DNA damages are generated, in vivo, in target genes reducing or inactivating the function of these genes only in target cell types. This approach can be used to repress lignin biosynthesis or manipulate xylan biosynthesis to improve C6/C5 ratio and biomass quality – both approaches to achieving more economical biofuel production. Other uses of reduced-lignin and/or reduced-xylan plants include saccharification reaction to generate soluble sugars more efficiently; simplification of downstream processing for wood industry (paper, pulping, construction); improvement of the quality of wood for construction; or use as animal (ruminant) feed.

## Licensing Information:

Lawrence Berkeley National Laboratory Contact: Peter Matlock (<u>pymatlock@lbl.gov</u>, (510)486-5803) TTO Tracking Number: 2013-171 Patent Status: US Patent Application Type of License: Non-exclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO2&Sect2=HITOFF&u=%2Fnetahtml%2FPTO%2Fsearch-</u> <u>adv.html&r=1&f=G&l=50&d=PG01&p=1&S1=598599.APN.&OS=apN/598599&RS=APN/598599</u> Website: <u>http://ipo.lbl.gov/lbnl2013-171/</u> e. Discovery of a Hexose Transporter Variant in Sachharomyces Cerevisiae that Allows Growth on Xylose JBEI/LBNL researchers have developed a S. cerevisiae strain that is able to import and utilize xylose as a carbon source. S. cerevisiae is a dominant host microbe for industry applications for production of a large number of chemicals and commodities, including biofuels. In general, S. cerevisiae is cultivated solely on glucose, as native strains have a minor but negligible ability to metabolize xylose and lack native mechanisms to uptake xylose. Generating a yeast strain that utilizes xylose, especially in a glucose/ xylose mix, has been a topic of extensive research for several decades.

## Licensing Information:

Lawrence Berkeley National Laboratory Contact: Peter Matlock (<u>pymatlock@lbl.gov</u>, (510)486-5803) TTO Tracking Number: 2014-020 Patent Status: US Provisional Patent Application Type of License: Non-exclusive USPTO Link: Not yet published Website: To be posted

f. Engineered WRINKLED1 Transcription Factor with Increased Stability and Enhanced Oil Production WRINKLED1 is the primary transcription factor responsible for switching on oil production genes in a wide variety of plants. This technology is an improved version of WRINKLED1. Over-expression of this improved version leads to higher oil levels. MSU is looking for partners to advance this technology into food and feed crops, and into dedicated biofuel crops

## Licensing Information:

Michigan State University Contact: Tom Herlache, (<u>herlache@msu.edu</u>) TTO Tracking Number: TEC2015-0075 Patent Status: Provisional application filed 07/01/15, US 62/187,419. Type of License: Both exclusive and non-exclusive available USPTO Link: Website:

# g. A Method to Produce 3-Acetyl-1, 2-Diacyl-SN-Glycerols (ac-TAGs)

Michigan State University's inventions provide a source and production method for novel plant oils, acetyltriacylglycerols (ac-TAGs), with possible uses as biodiesel-like biofuel and/or as low-fat food ingredients. By combining an ac-TAG-related enzyme with a method for catalyzing large-scale synthesis of ac-TAGs, in a single crop, many benefits can be obtained. The inventions have lower viscosity and fewer calories per mole than TAGs. Pilot experiments by the inventors have achieved approximately a 60 mole percent accumulation of ac-TAGs in seed oil.

# Licensing Information:

Michigan State University Contact: Tom Herlache, (<u>herlache@msu.edu</u>) TTO Tracking Number: TEC2009-0108 Patent Status: U.S. 13/519,660 pending Type of License: Both exclusive and non-exclusive available USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u>

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bool.html&r=1&f=G&l=50&co1=AND&d=PG01&s1=%2213%2F519,660%22&OS=%2213/519,660%22&RS= %2213/519,660%22

Website: http://msut.technologypublisher.com/technology/5989

## h. 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 (<u>mstaudt@warf.org</u>, (608)265-3084) TTO Tracking Number: P100228US02 Patent Status: 8,178,331; 13/232327; 61/383185 Type of License: Exclusive USPTO Link: <u>http://patft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO1&Sect2=HITOFF&d=PALL&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.htm&r=1&f=G&l=</u> <u>50&s1=8,178,331.PN.&OS=PN/8,178,331&RS=PN/8,178,331</u> Website: <u>http://www.warf.org/documents/ipstatus/P100228US02.PDF</u>

## i. Genes for Xylose Fermentation, Enhanced Biofuel Production in Yeast

UW-Madison researchers have identified 10 genes in yeast that are involved in xylose fermentation. Efficient fermentation of biofuels and biorenewable chemicals from biomass-derived sugars would benefit from microbes that can utilize both glucose and xylose. These genes could be used to create an organism by modifying one that normally utilizes glucose to one that can ferment both xylose and glucose for enhanced biofuel production. These genes may be used in various combinations to produce useful industrial strains.

## Licensing Information:

University of Wisconsin – Madison Contact: Mark Staudt (<u>mstaudt@warf.org</u>, (608)265-3084) TTO Tracking Number: P100245US03 Patent Status: 8,795,996; 13/441381; 61/516650; 61/509849; 14/307128 Type of License: Exclusive USPTO Link: <u>http://patft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO1&Sect2=HITOFF&d=PALL&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.htm&r=1&f=G&l=</u> <u>50&s1=8795996.PN.&OS=PN/8795996&RS=PN/8795996</u> Website: <u>http://www.warf.org/documents/pubapps/P100245US03%20Published%20Application.PDF</u>

j. Cell-Free System for Combinatorial Discovery of Enzymes Capable of Transforming Biomass for Biofuels UW-Madison researchers have developed compositions and methods that expand the ability to make, express and identify target polypeptides, including enzymes capable of enhancing the deconstruction of biomass into fermentable sugars. This approach uses a cell-free system to express enzymes and other polypeptides in a combinatorial manner. Because the system is cell-free, the enzymes can be assayed without intermediate cloning steps or purification of the protein products. This system also is more reliable than conventional methods for analyzing biomass transformation because it does not utilize living systems, which could rapidly consume soluble sugars. This system could be used to efficiently screen enzyme combinations for effective deconstruction of biomass from different feedstocks and under different conditions.

## Licensing Information:

University of Wisconsin – Madison Contact: Jennifer Gottwald (<u>jennifer@warf.org</u>, (608)262-5941) TTO Tracking Number: P08301US02 Patent Status: 8,945,902; 12/792156; 61/183243 Type of License: Exclusive USPTO Link: <u>http://patft.uspto.gov/netacgi/nph-</u> Parser?Sect1=PTO1&Sect2=HITOFF&d=PALL&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.htm&r=1&f=G&l= 50&s1=8945902.PN.&OS=PN/8945902&RS=PN/8945902 Website: http://www.warf.org/documents/ipstatus/P08301US02.pdf

## k. 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 CeIE), 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. Multifunctional 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: 14/030290; 61/703063 Type of License: 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& I=50&s1=%2220140079683%22.PGNR.&OS=DN/20140079683&RS=DN/20140079683 Website: http://www.warf.org/technologies/clean-technology/biofuels-renewablefuels/summary/powerful-new-enzyme-for-transforming-biomass-p120371us02.cmsx

Production of Polyhydroxyalkanoates with a Defined Composition from an Unrelated Carbon Source UW–Madison researchers have developed recombinant E. coli capable of producing high yields of medium chain length polyhydroxyalkanoates from non-lipid, carbohydrate sources. The researchers previously designed and built a bacterial strain that produces high levels of C12 fatty acids (see WARF reference number P09329US02). This strain has been further modified by deleting various fad genes implicated in the breakdown of fatty acids. Also, the bacteria cells incorporate several genes taken from other species to increase conversion efficiency. These microbes could have applications in producing biorenewable PHA.

## Licensing Information:

University of Wisconsin – Madison Contact: Jennifer Gottwald (jennifer@warf.org, (608)262-5941) TTO Tracking Number: P120377US02 Patent Status: 13/833230; 61/699044 Type of License: Exclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO1&Sect2=HITOFF&d=PG01&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.html&r=1&f=G&I =50&s1=%2220140073022%22.PGNR.&OS=DN/20140073022&RS=DN/20140073022 Website: <u>http://www.warf.org/documents/pubapps/P120377US02%20Published%20Application.pdf</u></u>

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

UW–Madison researchers have genetically modified microorganisms to better tolerate organic acids like 3hydroxypropionic 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; 13/798835; 61/647001; 8,846,354; 14/200747; 8,846,329; 14/200686 Type of License: Exclusive USPTO Link: <u>http://patft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO1&Sect2=HITOFF&d=PALL&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.htm&r=1&f=G&l=</u> <u>50&s1=8715973.PN.&OS=PN/8715973&RS=PN/8715973</u> Website: http://www.warf.org/documents/ipstatus/P120017US02.PDF</u>

#### m. Fatty Acid-Producing Hosts

UW–Madison researchers have developed genetically modified E. coli that are capable of overproducing fatty acid precursors for medium- to long-chain hydrocarbons. The modified bacteria were transformed with exogenous nucleic acids to increase the production of acyl-ACP or acyl-CoA, reduce the catabolism of fatty acid products and intermediates, and/or reduce feedback inhibition at specific points in the biosynthetic pathway. The modified bacteria can be cultured in the presence of sugars to produce fatty acids. The fatty acid products formed during fermentation then can be separated from the fermentation media via a two-phase separation process or other method. The separated products can be used directly or as feedstock for subsequent reactions, including conversion to medium- and long-chain hydrocarbons. Production of medium- and long-chain hydrocarbons for use as biofuels or specialty chemicals

## Licensing Information:

University of Wisconsin – Madison Contact: Jennifer Gottwald (<u>jennifer@warf.org</u>, (608)262-5941) TTO Tracking Number: P09329US02 Patent Status: 8,617,856; 12/984343; 61/292918 Type of License: Exclusive USPTO Link: <u>http://patft.uspto.gov/netacgi/nph-</u> Parser?Sect1=PTO1&Sect2=HITOFF&d=PALL&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.htm&r=1&f=G&l=

## <u>50&s1=8617856.PN.&OS=PN/8617856&RS=PN/8617856</u> Website: <u>http://www.warf.org/documents/ipstatus/P120017US02.PDF</u>

#### n. Extending Juvenility in Grasses

UW–Madison researchers have developed methods for locking plants in a juvenile state by modifying genes related to maturation. The genes – GRMZM2G362718 or GRMZM2G096016 – have been analyzed by the researchers and shown to influence growth transition in corn. To alter plant development, these genes and their homologs could be knocked out or inhibited by small molecules or biologics. The process could involve additional genes known to affect juvenile to adult growth development. Plants altered in this trait could show higher yields and easier biomass processing.

#### Licensing Information:

University of Wisconsin-Madison Contact: Emily Bauer (ebauer@warf.org, (608)262-8638) TTO Tracking Number: P120179US02 Patent Status: 13/834114; 61/651540 Type of License: Exclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO1&Sect2=HITOFF&d=PG01&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.html&r=1&f=G&I =50&s1=%2220140013468%22.PGNR.&OS=DN/20140013468&RS=DN/20140013468 Website: <u>http://www.warf.org/technologies/summary/P120179US02.cmsx</u></u>

#### o. 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 (<u>ebauer@warf.org</u>, (608)262-8638) TTO Tracking Number: P130256US02 Patent Status: 14/296352; 61/831561 Type of License: Exclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO1&Sect2=HITOFF&d=PG01&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.html&r=1&f=G&l</u> <u>=50&s1=%2220140366213%22.PGNR.&OS=DN/20140366213&RS=DN/20140366213</u> Website: <u>http://www.warf.org/technologies/summary/P130256US02.cmsx</u>

p. Selective Catalytic Production of Linear Alpha Olefins from Lactones and Unsaturated Carboxylic Acids UW–Madison researchers have developed a method for producing linear Alpha olefins (LAOs) cheaply from biomass. In the process, an inexpensive solid acid catalyst is used in a reaction that converts the carboxylic acids and lactones present in the feedstock. The catalyst features Lewis acid catalytic sites and no precious metal components. This would allow LOAs (annual global demand 3.4 metric tons) to be produced from biomass rather than from petroleum.

## Licensing Information:

University of Wisconsin-Madison Contact: Mark Staudt (<u>mstaudt@warf.org</u>, (608)265-3084) TTO Tracking Number: P130275US01 Patent Status: 13/928811 Type of License: Nonexclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO1&Sect2=HITOFF&d=PG01&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.html&r=1&f=G&I =50&s1=%2220150005558%22.PGNR.&OS=DN/20150005558&RS=DN/20150005558 Website: <u>http://www.warf.org/technologies/summary/P130275US01.cmsx</u></u>

## q. 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; 61/928292 Type of License: Exclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO1&Sect2=HITOFF&d=PG01&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.html&r=1&f=G&l</u> =50&s1=%2220150197757%22.PGNR.&OS=DN/20150197757&RS=DN/20150197757 Website: <u>http://www.warf.org/technologies/clean-technology/biofuels-renewable-</u> fuels/summary/oxygen-responsive-bacterial-gene-switch-for-biofuel-production-and-morep130380us02.cmsx

## r. 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; 61/978585 Type of License: 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=%2220150307872%22.PGNR.&OS=DN/20150307872&RS=DN/20150307872 Website: http://www.warf.org/technologies/summary/P140199US02.cmsx

## s. 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; 62/037963; 62/134384 Type of License: Nonexclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> Parser?Sect1=PTO1&Sect2=HITOFF&d=PG01&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.html&r=1&f=G&I =50&s1=%2220160046952%22.PGNR.&OS=DN/20160046952&RS=DN/20160046952 Website: <u>http://www.warf.org/technologies/research-tools/gene-expression/summary/high-throughput-genome-editing-and-engineering-of-industrial-yeast-other-fungi-p140240us03.cmsx</u>

## t. Microorganisms and Methods for Producing Pyruvate, Ethanol, and Other Compounds

UW-Madison inventors have identified four different metabolic engineering routes to increase the production of pyruvate using modified E. coli strains. Guided by a genome-scale metabolic model of E. coli the inventors identified multiple gene deletion targets that couple growth rate with chemical production. The gene deletion targets were based upon pyruvate consumption pathways including the production of acids (e.g., lactate and acetate), minimization of acetyl-CoA formation and its subsequent use in the TCA cycle, and NADPH formation. These target pathways were used to produce a number of candidate strains in silico, a subset of which were generated and tested experimentally. These strains could provide an alternative, bio-based approach to produce pyruvate at high yields using renewable sources.

## Licensing Information:

University of Wisconsin-Madison Contact: Mark Staudt (<u>mstaudt@warf.org</u>, (608)265-3084) TTO Tracking Number: P140301US02 Patent Status: 14/848646; 62/047896 Type of License: Exclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> Parser?Sect1=PTO1&Sect2=HITOFF&d=PG01&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.html&r=1&f=G&I =50&s1=%2220160068871%22.PGNR.&OS=DN/20160068871&RS=DN/20160068871 Website: <u>http://www.warf.org/technologies/materials-chemicals/biochemicals/summary/modified-em-</u> e.-coli-em-for-enhanced-production-of-pyruvate-ethanol-p140301us02.cmsx

## u. 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; 62/018939 Type of License: Exclusive USPTO Link: <u>http://appft.uspto.gov/netacgi/nph-</u> Parser?Sect1=PTO1&Sect2=HITOFF&d=PG01&p=1&u=%2Fnetahtml%2FPTO%2Fsrchnum.html&r=1&f=G&I =50&s1=%2220150376659%22.PGNR.&OS=DN/20150376659&RS=DN/20150376659 Website: <u>http://www.warf.org/technologies/materials-chemicals/biochemicals/summary/bio-based-</u> production-of-non-straight-chain-and-oxygenated-fatty-acids-for-fuels-and-more-p140318us02.cmsx

# v. 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:

University of Wisconsin-Madison Contact: Jennifer Gottwald (<u>jennifer@warf.org</u>, (608)262-5941) TTO Tracking Number: P150101US01 Patent Status: 9,376,451; 14/588178 Type of License: Exclusive USPTO Link: <u>http://patft.uspto.gov/netacgi/nph-</u> <u>Parser?Sect1=PTO2&Sect2=HITOFF&p=1&u=%2Fnetahtml%2FPTO%2Fsearch-</u>

## bool.html&r=1&f=G&l=50&co1=AND&d=PTXT&s1=9376451.PN.&OS=PN/9376451&RS=PN/9376451 Website: http://www.warf.org/technologies/summary/P150101US01.cmsx

#### w. Transgenic Cyanobacteria: A Novel Direct Secretion of Glucose for the Production of Biofuels

A direct secretion of glucose by transgenic cyanobacteria creates an extremely efficient, cost effective feedstock for the production of ethanol. The compositions and methods of the present technology also include the use of the cyanobacteria-produced cellulose, which has a lower crystallinity than wild-type bacterial cellulose and allows for easier degradation to glucose for use in subsequent fermentation to ethanol. One distinct advantage of this technology is that it permits very large scale production of cellulose in areas that would otherwise not be available for cellulose production (e.g., areas with little or no rainfall) while at the same time producing cellulose with less toxic byproducts. The cellulose of the present technology has a lower crystallinity than wild-type bacterial cellulose and the lower crystallinity cellulose is degraded with less energy into glucose than wild-type cellulose and is further converted into ethanol.

#### **Licensing Information:**

UT Austin Contact: Mandana Ashouripashaki, (<u>mandana@otc.utexas.edu</u>, (512)475-7913) TTO Tracking Number: UT Tech ID: 5288 BRO Patent Status: 1 issued patent: 7803601, issued 9/28/2010 Type of License: Exclusive USPTO Link: http://portal.uspto.gov/pair/view/BrowsePdfServlet?objectId=GDUY5UOTPPOPPY5&lang=DINO; 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=2 0110003345.PGNR.&OS=DN/20110003345&RS=DN/20110003345 Website: http://www.otc.utexas.edu/ATdisplay.jsp?id=210

## **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.

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.

# 23.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 unprecedented speed and flexibility in collecting data from the new flash ADC based detectors. Experiments at such facilities are extremely complex, involving thousands of detector elements that produce raw experimental data at rates in excess of a GB/sec, resulting in the annual production of data sets of hundred Terabyte (100 TB) to Petabyte (PB) scale. Data sets of many 10s to 100s of TB are currently distributed to institutions worldwide for analysis, and with the increasing data generation rates seen at RHIC, PB scale datasets are anticipated. 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 should explicitly show relevance to the DOE nuclear physics program. In addition, applications should be informed by prior practice in nuclear physics applications, commercially available products, and emerging technologies. We note that a proposal that advocates incremental improvements or moderate levels of innovation may nonetheless have an enormous impact in the right context. Such proposals must of course make their case convincingly, as they may otherwise be considered non-responsive.

The subtopics below refer to innovations that will advance our nation's capability to perform nuclear physics R&D, 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 <a href="http://www.nersc.gov/users/accounts/allocations/request-form/">http://www.nersc.gov/users/accounts/allocations/request-form/</a>.

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, using web services or data grid infrastructure software (such as Globus, HTCondor, xrootd, or object stores), with the aim of achieving fast data processing and/or increased data availability across many compute facilities.

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, including but not

limited to automated data replication coupled with application-level knowledge of data usage, data transfers to Tier 2 and Tier 3 centers from multiple data provenance, to achieve the lowest wait-time or fastest data processing and maximal coordination (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-site data reduction, and repacking for remote analysis and data access); (3) new tools for co-scheduling compute and storage resources for data-intensive high performance computing tasks, such as user analyses in which repeated passes over large datasets are needed, requiring fast turnaround times; and (4) distributed authorization and identity management systems, enabling single sign-on access to data distributed across many sites.

Proposed infrastructure software solutions should consider and address the advantages of closely integrating relevant components of Grid middleware, such as are contained in the software stack of the Open Science Grid, as the foundation used by nuclear physics and other science communities. Applications that propose data distribution and processing projects are encouraged to determine the relevance of and possible future migration strategies into existing infrastructures, and to consider integrated solutions and designs with capacities that would seamlessly include Grid and Clouds computing resources, or help to transparently bridge between the two worlds of Clouds and Grids. For technical specifications in Large Scale Data Processing and Distribution contact Dr. Jerome Lauret at Brookhaven National Laboratory (jlauret@bnl.gov).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate for Software and Data Management: Frank E (Ted) Barnes, <u>Ted.Barnes@science.doe.gov</u>.

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

Modern nuclear physics data acquisition systems are becoming more heterogeneous and distributed. Event sizes are rapidly increasing as more detectors are used to better characterize scattering events and more information is extracted from detectors. This presents several new challenges in the readout, synchronization, and storage of the data as needs have emerged to address a constant evolution of modern experiment's requirements. 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, these information are 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 (VME, cPCI), custom interconnects, or serial connections (USB).

Future FRIB experiments anticipate event rates of a few per second to tens of thousands 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 new 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 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 work 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) determine a global trigger from information transmitted by the individual digitizer elements with minimal latency, (4) notify the digitizer elements of a successful trigger, in order to locally store the validated data; (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. The overall data transport should be capable of moving hundreds of megabytes per second from digitizers to storage. 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, particularly at FRIB. 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 physics experiments at facilities such as RHIC, (and later the possible next generation of experiments such as the Electron-Ion Collider (EIC) proposed at either RHIC or TJNAF) 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, control systems based on EPICS and archiver systems cannot provide the truly distributed and scalable infrastructures needed by remote control rooms. For example one might instead of the current monolithic architectures, consider a message queueing paradigm as a possible architecture for data and/or meta-data collection. This architecture may also benefit the software-driven data acquisition system described previously.

At TJNAF a major accelerator upgrade along with upgrades of the three existing experimental areas and a new fourth experimental area is close to completion. Data acquisitions systems are already in place to read out the new and upgraded detectors using technologies similar to those outlined in the previous section for FRIB. The next generation of detectors proposed for TJNAF will involve event and data rates that tax the capabilities of existing systems. Areas of interest are, using serial backplanes or point to point serial links to replace the traditional VME based backplanes, replacement of embedded Intel processors with FPGAs, streaming of time tagged data from ADCs and TDCs directly to short term storage where high performance computing systems implement the trigger and event building in software.

Applications are invited in the following areas; 1) the development of streaming data acquisition system and control systems: (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) data flow systems that are capable of responding to trigger accepts by reading data from the digitizers and making it available to interested clients, (e) scalable event builders that accept data from the data flow system and inject back to that system built 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; 2) soft core FPGA module(s) to implement the network protocol for Ethernet and/or Infiniband, able to drive existing and emerging commercial network chips, with sufficient buffering to support data aggregation using a commercial network switch, and with sufficient speed to drive up to 40 Gb/sec network links; 3) time distribution protocols and hardware to support fine-grained time tagging (with 1 nanosecond or better precision) of each network packet for later correlation and event or frame assembly, possibly integrated with FPGAs and possibly exploiting the commercial network for some aspects of tagging, 4) Data streaming (from up to 1 gigasample per second digitizers) and distribution hardware and software capable of routing time tagged data from several thousands of data sources to temporary storage where the data can be accessed in time order. For technical specifications in Softwaredriven Network Architectures contact Dr. Robert Varner at Oak Ridge National Laboratory (varnerrl@ornl.gov). For technical specifications in Software-driven Network Architectures related to RHIC contact Dr. Jerome Lauret at Brookhaven National Laboratory (jlauret@bnl.gov). For technical specifications in Software-driven Network Architectures related to FRIB contact Mr. Tom Rockwell (Rockwell@frib.msu.edu). For technical specifications in Software-driven Network Architectures related to TJNAF contact Dr. Graham Heyes (heyes@jlab.org)

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate for Software and Data Management: Frank E (Ted) Barnes, <u>Ted.Barnes@science.doe.gov</u>.

## 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 such as those planned for FRIB, data sets will be collected with each event having a large number of independent parameters/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, to carry out these tasks. 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 which provide computing resources 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 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, (3) the application of machine-learning techniques with standard frameworks (Google TensorFlow, Spark GraphX) to automate analysis tasks and provide intelligent diagnostics, (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. For more specifications on heterogeneous computing described above contact Dr. Mario Cromaz at Jefferson Lab (<u>mcromax@lbl.gov</u>).

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#### 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 is constrained by the effort required to port the software to the GPU environment. More capable cross compilation or source-to-source translation tools are needed that are able to convert very complicated templatized C++ code and into high performance codes for heterogenous architectures.

Utilizing High Performance Computing (HPC) and Leadership Computing Facilities (LCFs) is of growing relevance and importance to experimental NP as well. NP codes written or rewritten to have the concurrency needed to perform well on prevalent and emerging multi- and many-core architectures can potentially utilize HPC effectively. Experiments 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. Tools and technologies that can facilitate efficient use of HPCs and LCFs for the applications and data-intensive workflows characteristic of experimental NP are in the scope of this subtopic.

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#### e. Other

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

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# 24.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, durability, background suppression, programmability and functionality. Of particular interest are innovative readout electronics for use with the nuclear physics detectors described in Topic 26 (Nuclear Instrumentation, Detection Systems and Techniques).

This topic is related to Topic 26 (Nuclear Instrumentation...): to develop innovative readout electronics for use with the nuclear physics detectors. An important criterion is cost per channel of electronic devices and modules. Prior year Phase I resulted in 1-2 Phase I grant. NP is interested to be able to increase number of grants in this Topic by receiving stronger proposals in this topic.

All grant applications must explicitly show relevance to the DOE nuclear physics program. Additionally, applications must be informed by prior art in nuclear physics applications, commercially available products and emerging technologies. A proposal based on incremental improvements or little innovations, in the right context, can have an enormous impact or value. Such a proposal must be convincing, otherwise it will be considered as being non-responsive.

The subtopics below refer to innovations that will advance our nation's capability to perform nuclear physics R&D, 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.

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

## 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, position-sensitive detectors (e.g., germanium sensors with pixel sizes in the range of 0.4 mm<sup>2</sup> to 1 cm<sup>2</sup>) and from particle detectors (e.g., silicon pixel and strip detectors including drift versions, silicon photomultipliers (SiPMs), and gas detectors) used in nuclear physics experiments. Areas of specific interest include (1) low-noise preamplifiers, low-noise filters, peak and timing sensors, analog-to-digital and time-to-digital converters; (2) front-end ASICs capable of operating in cryogenic environment to allow for increased resolution, reduced power dissipation, and reduced number of feed-through lines in highly segmented germanium detectors and noble liquid Time Projection Chambers (TPCs); (3) front-end circuits for solid-state highly pixelated detectors, associated high-density interconnect technologies, circuits for processing and correcting charge sharing in real time; (4) integrable circuits for very high dynamic range, (5) integrable 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. These circuits should be low-power, low-cost, user friendly, and are capable of communicating with commercial auxiliary electronics.

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#### c. Advanced Devices and Systems

Grant applications are sought for improved or advanced devices and systems used in conjunction with the electronic circuits and systems described in subtopics a and b:

Areas of interest regarding systems include (1) bus systems, data links, event handlers, multiple processors, trigger logics, and fast buffered time and analog digitizers. For detectors that generate extremely high data volumes (e.g., >500 GB/s), (2) advanced high-bandwidth data links are of interest.

Grant applications also are sought for generalized software and hardware packages, with improved graphic and visualization capabilities, for the acquisition and analysis of nuclear physics research data.

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## d. 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. The innermost tracking detector of the STAR experiment at RHIC contains 356 million ( $21x21x50 \mu m$ ) APS pixels. Future high luminosity colliders such as the Electron Ion Collider (EIC) plan to operate at luminosities in the range  $10^{33}$ – $10^{35}$  cm<sup>-2</sup> s<sup>-1</sup> 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 thicker and is used as the active volume. A major advance would be to introduce an electric field into this drift 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, or even strip sensors. Options may include integrated CMOS detectors which combine initial signal processing and data sparsification on a standard CMOS wafer; superconducting large area pixel detectors; novel 2D- and 3D-pixel materials and geometry structure.

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#### e. 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 times to 10 times the density of standard inter-density connectors.

In addition, many next-generation detectors will have highly segmented electrode geometries with 5-5000 channels per square centimeter, covering areas up to several square meters. Conventional packaging and assembly technology cannot be used at these high densities. 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; (4) low-cost and low-mass methods for grounding and shielding; and (5) standards for interconnecting ASICs (which may have been developed by diverse groups in different organizations) into a single system for a given experiment – these standards should address the combination of different technologies, which utilize different voltage levels and signal types, with the goal of reusing the developed circuits in future experiments.

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 highest long term interest are high-

density high-functionality 3D circuits with direct bonding of high resistivity silicon detector layer of an appropriate thickness (50 to 500 microns) to a 3D stack of thin CMOS layers. 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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## f. Other

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

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# 25.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 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 <u>Relativistic Heavy Ion Collider (RHIC)</u>, with heavy ion beam energies up to 100 GeV/nucleon and polarized proton beam energies up to 255 GeV; technologies associated with RHIC luminosity upgrades; linear accelerator such as the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF) and the Argonne Tandem Linac Accelerator System 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) under construction at Michigan State University, and the development of a proposed future <u>electron-ion collider</u>. A major focus in all of the above areas is superconducting radio frequency (SRF) acceleration and its related technologies. Relevance of applications 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 prior 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.

The subtopics below refer to innovations that will advance our nation's capability to perform nuclear physics R&D, 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 <a href="http://www.nersc.gov/users/accounts/allocations/request-form/">http://www.nersc.gov/users/accounts/allocations/request-form/</a>.

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 radio frequency windows using alternative materials (e.g., sapphire), ceramics that have good dielectric properties such as a loss tangent better than 0.01% at 1 GHz yet exhibits a small dc conductivity to overcome charging by beams or field emission, RF power couplers, high power lowimpedance bellows and magnetostrictive or piezoelectric cavity-tuning mechanisms; (2) fast ferroelectric microwave components that control reactive power for fast tuning of cavities or fast control of input power coupling; (3) simple, low-cost mechanical techniques for damping length oscillations in accelerating structures, particularly for dressed superconducting radio frequency (SRF) cavities (SRF cavities equipped with He vessels and tuners), effective in the 10-300 Hz range at 2 and/or 4.5 K; (4) alternative cavity fabrication techniques to produce seamless SRF cavities of various geometries (including elliptical, quarter, half wave resonators and crab cavities). The resulting SRF accelerating structures should achieve Q<sub>0</sub>>3x10<sup>10</sup> at 2.0 K, and correspondingly lower Q's at higher temperatures such as 4.5 K; and (5) metal forming techniques with the potential for significant cost reductions by simplifying sub-assemblies e.g., dumbbells and beam tubes reducing the number of electron beam welds.

Grant applications are sought to develop advanced diagnostic techniques for SRF cavities/resonators, including new methods of temperature mapping, magnetic flux monitoring, optical inspection and second sound quench detections that will lead to better understanding of the cavity quality factors and quench limits.

Grant applications are sought to develop improved superconducting materials or processes applied to such material 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 and create high quality, NbN, Nb<sub>3</sub>Sn, or MgB<sub>2</sub> films with anti-diffusion dielectric overlayers. Demonstration of deposition should be on an actual RF cavity surface, e.g., elliptical, or another cavity surfaces, such as a quarter wave or crab geometry.

Finally, grant applications are sought to develop advanced techniques for surface processing of superconducting resonators, including methods for electropolishing, high temperature treatments, and laser or electron beam surface glazing of niobium for surface purification and annealing in vacuum. Methods which avoid use of hydrofluoric acid are desirable. Surface conditioning processes of interest should yield microscopically smooth ( $R_q$ < 10 nm / 10 $\mu$ m<sup>2</sup>), crystallographically clean bulk niobium surfaces; and/or reliably remove essentially all surface particulate contaminates (> 0.1  $\mu$ m) from interior surfaces of typical RF accelerating structures. Grant applications aimed at design solutions that enable integrated cavity processing with tight process quality control are highly sought. For questions related to items (1) through (6) in the first paragraph of this subtopic, contact Dr. Robert Rimmer at Thomas Jefferson National Accelerator Facility (rarimmer@ilab.org) or Dr. Ilan Ben-Zvi at Brookhaven National Laboratory (benzvi@bnl.gov). For all other specification questions, contact Dr. Charles Reece at Thomas Jefferson National Accelerator Facility (reece@ilab.org).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u>

#### b. Radio Frequency Power Sources

Grant applications are sought to develop designs and hardware for 5-20 kW continuous wave (cw) power sources at distinct frequencies in the range of 50-1500 MHz. Examples of candidate technologies include: solid-state devices, multi-cavity klystrons, tunable/phase stabilized magnetrons, Inductive-Output Tubes (IOTs), or hybrids of those technologies. Emphasis is on reduced power consumption, bandwidth, ease of manufacture, mitigating the risk of obsolescence, and enhanced reliability measures. Grant applications are also sought to develop computer software for the design or modeling of any of these devices; such software should be able to faithfully model the complex shapes with full self-consistency. Software that integrates multiple effects, such as electromagnetic and wall heating is of particular interest.

Grant applications also are sought for a microwave power device, klystron, IOT, tunable/phase stabilized magnetron or solid state amplifiers (especially class F devices) offering improved efficiency (>70%) while delivering up to 12.5 kW, 50 kW or 500 kW CW at 952.6 MHz. Similar requirements exist at 650 MHz. For further specifications on power sources, contact Dr. Robert Rimmer at the Thomas Jefferson National Accelerator Facility (TJNAF) (rarimmer@jlab.org), Dr. Ilan Ben-Zvi at Brookhaven National Laboratory (benzvi@bnl.gov), and Dan Morris at the Facility for Rare Isotope Beams (FRIB) (morrisd@nscl.msu.edu). For more details on technical specifications of BNL RF devices, contact Alex Zaltsman (zaltsman@bnl.gov).

Questions - contact Michelle Shinn, Michelle.Shinn@science.doe.gov

#### 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<sup>o</sup> or less of phase and 0.1% amplitude) and electron acceleration structures (0.1<sup>o</sup> of phase and 0.01% amplitude) 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) 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<sup>-4</sup>) superconducting RF cavities for acceleration and/or storage of relativistic heavy ions.

Grant applications are also sought to develop new concepts of stand-alone accelerator systems based on dressed SRF cavities (SRF cavities equipped with He vessels and tuners) that can provide total voltages of 1-5 MV in self-contained systems not requiring connections to central refrigeration and LN2 feeds. Such systems are seen to have applications as 'rebunchers' at larger accelerator facilities and as potential accelerators in industrial setting for material science and electronic chip manufacturing.

Grant applications also are sought to develop software for the design and modeling of the above systems. Desired modeling capabilities include (1) charged particle dynamics in complex shapes, including energy recovery analysis; (2) the incorporation of complex fine structures, such as higher order mode dampers; (3) the computation of particle- and field-induced heat loads on walls; and (4) the incorporation of experimentally measured 3-D charge and bunch distributions.

A high-integrated-voltage SRF cw crab crossing cavity is also of interest. Therefore, grant applications are sought for (1) designs, computer-modeling, and hardware development for an SRF crab crossing cavity

with 0.4 to 1.5 GHz frequency and 3 to 50 MV integrated voltage; and (2) beam dynamics simulations of an interaction region with crab crossing. The simulation tool should employ a graphical editor to enable data visualization and be designed for ease of use. For further specifications on fast frequency switching RF cavities, contact Dr. Dejan Trbojevic at Brookhaven National Laboratory (<u>trbojevic@bnl.gov</u>). For questions related to software design and modeling, contact Dr. Ilan Ben-Zvi at Brookhaven National Laboratory (<u>benzvi@bnl.gov</u>). For questions or further specifications on SRF crab cavities, contact Drs. Yaroslav Derbenev, Geoffrey Krafft or Yuhong Zhang at Thomas Jefferson National Accelerator Facility (<u>derbenev@jlab.org</u>, <u>krafft@jlab.org</u>, <u>yzhang@jlab.org</u>), or Dr. Ilan Ben-Zvi at Brookhaven National Laboratory (<u>benzvi@bnl.gov</u>).

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, emittance, or energy spread; (2) novel methods for in situ surface cleaning (scrubbing) of ultrahigh vacuum long narrow tubes and elliptical cavities to reduce secondary electron yield and outgassing; (3) novel, robust coatings to passivate conductance-limited beam pipe for UHV operation to reduce thermal and stimulated outgassing; (4) Techniques for energetic ion assisted in situ coating of long, small diameter, beam pipes with compacted thick crystalline copper film; and (5) techniques and devices for measuring RF resistivity of cryogenically cooled coated tubes.

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 5-50 MHz repetition rate; and (2) transporting and matching magnetized electron beams within a long (~30 m) superconducting solenoid. For further information on photocathodes please contact Carlos Hernandez-Garcia (chgarcia@jlab.org), John Smedley (smedley@bnl.gov), or Triveni Rao (triveni@bnl.gov). For additional information on accelerator design for: Multi-pass ERL's and Ion complex components for EIC contact Dr. Alex Bogacz (bogacz@jlab.org). For questions or further specifications on SRF deflecting cavities used as fast RF kickers, contact Drs. Yaroslav Derbenev, Geoffrey Krafft or Yuhong Zhang at Thomas Jefferson National Accelerator Facility (derbenev@jlab.org, krafft@jlab.org, yzhang@jlab.org), or Dr. Ilan Ben-Zvi at Brookhaven National Laboratory (benzvi@bnl.gov). For further questions to develop software for state-ofthe-art in the simulation of beam physics contact Dr. Ilan Ben-Zvi at Brookhaven National Laboratory (benzvi@bnl.gov) and Yves Roblin at Thomas Jefferson National Accelerator Facility (roblin@jlab.org). For further questions on items (3) and (4) "in situ coating", contact Dr. Ady Hershcovitch at Brookhaven National Laboratory (hershcovitch@bnl.gov).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u>

## 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, with longitudinal polarization greater than 80%; and a quantum efficiency > 10% at 780nm, (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, and (3) a cost-effective means to obtain and measure vacuum below 10<sup>-12</sup> Torr.

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 new beam polarimeters, particularly non-invasive devices; (3) absolute polarimeters for spin polarized <sup>3</sup>He beams with energies up to 160 GeV/nucleon (4) novel concepts for producing polarizing particles of interest to nuclear physics research, including electrons, positrons, protons, deuterons, and <sup>3</sup>He; and (5) sophisticated computer software for tracking the spin of polarized particles in storage rings and colliders. For further specifications on polarized electron sources and fast spin-flipping, contact Dr. Matthew Poelker at Thomas Jefferson National Accelerator Facility (poelker@jlab.org). For questions on non-invasive resonant polarimetry, contact Dr. Vasiliy Morozov at Thomas Jefferson National Accelerator Facility (morozov@jlab.org). For questions on polarized ion sources contact Dr. Anatoli Zelenski at Brookhaven National Laboratory (zelenski@bnl.gov).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u>

#### f. Rare Isotope Beam Production Technology

Grant applications are sought to develop (1) state of the art ion sources for radioactive beams, specifically high intensity Electron Cyclotron Resonance (ECR) Ion Sources. ECR ion sources are employed at several NP facilities to deliver intense, high charge state ions for efficient acceleration. Current and future NP rare isotope beam facilities will need an ECR ion source, often operating at 28 GHz or higher, that produces for a heavy ion beam such as uranium with a charge state ranging from Q=30+ to 40+ a current ranging from 0.5emA to 1emA. Extraction of the ion beam from an ECR ion source become critical for ion source operating at a frequency at or above 28 GHz as the total extracted current could amount to 15 to 20emA. The phase space must be compact to produce a high quality beam downstream and mitigate potential for particle losses. This is especially important with modern, high intensity SRF linacs, which are sensitive to damage from lost particles. Improved source performance also allows higher intensity on target and more reliable facility performance. ECR sources are also complex with dense plasma, complex confinement geometries, and long timescales. Grant applications are sought to improve the performance and understanding of ECR sources for delivery of higher current, improved source stability/drifts, improved collimation and selection of ion species emerging from the sources, and modeling of the sources to improve optimization. Novel modeling techniques and reduced models that retain essential physics are encouraged to keep simulation requirements modest. (2) techniques for secondary radioactive beam collection, charge equilibration, and cooling; and (3) development of radiation resistant thermal isolation systems for superconducting magnets. Support links connecting room temperature with the liquid helium structure have to support large magnetic forces, but at the same time have low thermal conductivities to limit heat input. Typically, all-metal links have ten to twenty times higher heat leaks than composite structures. Composites are, however, hundreds or thousands of times more sensitive to radiation damage than metals and so cannot be used in the high-radiation environment surrounding the production target or beam dump areas of high-power heavy ion accelerators. Given the high cost of cryogenic refrigeration, development of radiation resistant, high-performance support links is very desirable.

Grant applications are sought to develop cost-efficient production methods for thin wedge-shaped metal plates used for energy degraders: in-flight separation of rare-isotope beams at FRIB or similar facilities utilize thin, precision-shaped metal sheets to slow down beam particles. The "wedges" range in central thickness varies from about 0.5 mm to a few mm and can be up to 50 cm wide by 20 cm tall. The wedge

angles are on the order of 5 mrad but more sophisticated shapes may be necessary. Aluminum is typically used, but other low atomic number materials are not excluded (good heat conduction and thermomechanical properties are required). For optimum performance, these are custom shaped for every beam to control the energy degradation at a level of one part per thousand. This requires corresponding control over the shape, surface fluctuations, and density fluctuations. For further specifications on rare isotope beam technology contact the following: For special designs that are applicable for use in high radiation environments: Dr. Earle Burkhardt, FRIB/MSU (burkhardt@frib.msu.edu). For innovative approaches to the construction of large aperture magnets, interested parties should contact Dr. Wolfgang Mittig, NSCL/MSU (mittig@nscl.msu.edu). For high intensity ECR ion sources, contact: Drs. Guilliaume Machicone (machicoane@frib.msu.edu) at FRIB.

(Additional needs for high-radiation applications can be found in subtopic f "Technology for High Radiation Environments" of Topic 26, Nuclear Physics Instrumentation, Detection Systems and Techniques.)

Questions - contact Michelle Shinn, Michelle.Shinn@science.doe.gov

## g. Accelerator Control and Diagnostics

Grant applications are sought to develop (1) advanced beam diagnostics concepts and devices that provide high speed computer-compatible measurement and real-time monitoring and readout of particle beam intensity, position, emittance, polarization, luminosity, momentum profile, time of arrival, and energy (including such advanced methods as neural networks or expert systems such as those employing genetic algorithms, and techniques that are nondestructive to the beams being monitored); (2) beam diagnostic devices that have increased sensitivities through the use of superconducting components (for example, filters based on high T<sub>c</sub> superconducting technology or Superconducting Quantum Interference Devices); (3) measurement devices/systems for cw beam currents in the range 0.1 to 100  $\mu$ A, with very high precision (<10<sup>-4</sup>) and short integration times; (4) beam diagnostics for ion beams with intensities less than 10<sup>7</sup> nuclei/second (an especially challenging region is for intensities of 10<sup>2</sup> to 10<sup>5</sup> with beam energy from 25 keV to 1 MeV/u); (5) non-destructive beam diagnostics for stored proton/ion beams, such as at the RHIC, and/or for 100 mA class electron beams; (6) devices/systems that measure the emittance of intense (>100kW) cw ion beams, such as those expected at FRIB; (7) beam halo monitor systems for ion beams; (8) instrumentation for electron cloud effect diagnostics and suppression, and (9) new 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.

Grant applications are sought for the development of triggerable, high speed optical and/or IR cameras, with associated MByte-scale digital frame grabbers for investigating time dependent phenomena in accelerator beams. Image capture equipment needs to operate in a high-radiation environment and have a frame capture rate of up to 1 MHz. The imaging system needs to have memory capacity at the level of 1000 frames (10 GByte or higher total memory capacity). The cameras will be used for high-speed analysis of optical transition or optical diffraction radiation data.

Grant applications also are sought for "intelligent" software and hardware to facilitate the improved control and optimization of charged particle accelerators and associated components for nuclear physics research. Areas of interest include the development of (1) generic solutions to problems with respect to the initial choice of operation parameters and the optimization of selected beam parameters with automatic tuning; (2) systems for predicting insipient failure of accelerator components, through the

monitoring/cataloging/scanning of real-time or logged signals; and (3) devices that can perform direct 12-14 bit digitization of signals at 0.5-2 GHz and that have bandwidths of 100+ kHz.

Grant applications are sought to develop beam diagnostic instrumentation based on High Temperature Superconducting materials. Examples include low noise non-invasive beam monitors for current, position, and polarization of charged particle beams in accelerators. The instrumentation should be capable of measuring sub-nano amp beam properties with msec or better integration times.

Control System Studio (CS-Studio) is an Eclipse-based collection of tools to monitor and operate large scale control systems, such as the ones in the accelerator community. It is a product of the collaboration between the Facility for Rare Isotope Beams, the Spallation Neutron Source, and the National Synchrotron Light Source II. One of the primary concerns with CS-Studio remains its reliance on the Standard Widget Toolkit (SWT), used by the Eclipse Rich Client Platform which offers a look and feel similar to the running platform. Unfortunately this approach has also resulted in SWT having a rather limited widget set whose functionality and ease of use are significantly compromised by the need to be supported on all platforms. JavaFX represents a potential replacement for SWT in CS-Studio. As part of the JDK version 8, it comes with complex widgets and interactions. Grant applications are sought to develop (1) graphical editor framework to enable data visualization and creation of synoptic displays; and (2) 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 Graphical Editing Framework, while utilizing JavaFX and web-related technologies. For further specifications on triggerable, high speed frame grabber cameras or bunch length monitors contact Dr. Geoffrey Krafft at Thomas Jefferson National Accelerator Facility (krafft@jlab.org). For further specifications on beam diagnostics Mr. Kevin Jordan (jordan@jlab.org) or Dr. Geoffrey Krafft (krafft@jlab.org) at the Thomas Jefferson National Accelerator Facility. For further specifications on Control System Studio graphical editor framework and runtime environment contact Eric Berryman (berryman@frib.msu.edu) at the Facility for Rare Isotope Beams (FRIB). For further specifications and information on new beam diagnostics enabled by non-traditional bulk materials (item 9 in first paragraph) contact Dr. Zhehui (Jeff) Wang at the Los Alamos National Laboratory (zwang@lanl.gov)

Questions - contact Michelle Shinn, Michelle.Shinn@science.doe.gov

## h. Magnet Development for Proposed Future Electron-Ion Colliders (EIC)

A full utilization of the discovery potential of a next-generation electron-ion collider will require a fullacceptance detection 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 superconducting ( $\geq$  2 T pole-tip field) septum dipole with electronically adjustable field orientation (+/- 100 mrad); (2) radiation-resistant high-field ( $\geq$  9 T pole-tip field), large-aperture ( $\geq$  20 cm radius) quadrupole; and (3) radiation-resistant superconducting ( $\geq$  6 T poletip field) large-aperture ( $\geq$  20 cm radius) small-yoke-thickness ( $\leq$  14 cm OD-ID) quadrupole.

High-performance, low-cost, low-energy-consumption magnets and systems are of great importance for feasibility of future accelerator facilities. In particular, grant applications are sought for design, simulation and prototyping of such magnets and systems allowing for peak fields of greater than 3 T, field quality better than ~10<sup>-4</sup> within ~3 cm aperture radius, high ramp rate of greater than 1 T/s, lower power consumption than conventional room-temperature magnets, and significantly lower cost than

conventional cos-theta superconducting magnets. Of particular interest are superferric dipoles and/or quadrupoles, power supplies, cryogenic systems, manufacturing techniques, etc. applicable in future large-scale accelerator projects such as an electron-ion collider. Persons to contact: Dr. Dejan Trbojevic at Brookhaven National Laboratory -BNL (<u>dejan@bnl.gov</u>), and Dr. Vadim Ptitsyn – BNL (<u>vadimp@bnl.gov</u>), and Dr. Vasiliy Morozov, Thomas Jefferson National Accelerator Facility (<u>morozov@jlab.org</u>).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u>

i. Accelerator Systems Associated with the Capability to Deliver Heavy-Ion Beams to Multiple Users At present, ATLAS is the only U.S. national user facility for low-energy nuclear physics supported by the DOE. There is a concept to expand the scientific reach of ATLAS by providing different stable and/or radioactive beams simultaneously to 2 or 3 physics experiments. There is a motivation for the simultaneous production, acceleration and distribution of stable and radioactive ion beams in a superconducting linac. Particular interest is in switching devices for separation of ~8-25 MeV/u heavy ion beams. One of the options could be a pulsed magnet capable to operate with short (~0.25 ms) rise/fall time, ~1-2% duty factor and 30 Hz repetition rate. Contact: Drs. Peter Ostroumov or Brahim Mustapha at Argonne National Laboratory –ANL (ostroumov@phy.anl.gov) or (brahim@anl.gov).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u>

## j. 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, <u>Michelle.Shinn@science.doe.gov</u>

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## 26.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 and national 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 prior art in nuclear physics applications, commercially available products and emerging technologies. Generally, order-of-magnitude improvements are needed in performance or cost. 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.

The subtopics below refer to innovations that will advance our nation's capability to perform nuclear physics R&D, 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 <a href="http://www.nersc.gov/users/accounts/allocations/request-form/">http://www.nersc.gov/users/accounts/allocations/request-form/</a>.

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:

• Silicon Photomultipliers (SiPMs), in particular radiation-tolerant SiPMs, low radioactivity SiPMs, large area, low noise SiPMs or digital SiPMs with photon detection efficiency, especially in blue and

UV wavelengths, and noise significantly improved over current state of the art, with the goal of large arrays; and

• Photon detectors capable of working in a cryogenic environment such as in liquid helium, or other noble gas, or liquid ionization chambers;

## (2) Calorimetry

 New and innovative concepts in calorimetry for measuring the total electromagnetic and/or hadronic energies of high energy particles (typically in the range from ~ 10 MeV up to ~ 100 GeV). These could include high resolution scintillating crystals for lower energies (see Subtopic d below) and various types of sampling calorimetry at higher energies. Components of these calorimeter designs could include new absorber materials, plastic scintillators, wavelength shifting fibers, optical light guides and other light collecting schemes, and new methods for fabricating various calorimeter and readout components. Also of interest are more radiation hard materials that can survive high fluxes of gammas, electrons, charged particles and neutrons.

(3) 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 timeof-flight detectors;
- Large area Multigap Resistive Plate Chambers (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 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 handle a trigger at a high rate in noisy (very high rate, low-energy background) environments and that are also magnetic field tolerant;
- Affordable methods for the production of large volumes of high-purity xenon, argon and krypton gas (which would contribute to the development of transition radiation detectors);
- 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; and
- Detector technologies capable of measuring energies of alpha particles and protons with less than 5 keV resolution, thereby allowing spectroscopy experiments using light charged particles to be performed in the same way as spectroscopy experiments using gammas.

(4) Spectrometers and innovative magnet designs such as:

- Development of iron-free magnet systems with tilted crossed solenoid windings and active shielding for a broad variety of superconducting dipoles, which could be used in high-acceptance spectrometers; and
- Innovative designs for high-resolution particle separators and spectrometers for next-generation rare isotope beam and intense stable beam facilities. Developments of interest include both aircore and iron-dominated superconducting magnets that use either conventional low-temperature conductors or new medium to high-temperature conductors for magnetic spectrometers, fragment separators, and beam transport systems. Innovative designs such as elliptical aperture multipoles and other combined function magnets are of interest.

For development of iron-free magnet systems with tilted crossed solenoid windings listed above interested parties should contact Dr. Daniel Bazin, NSCL/MSU (<u>bazin@nscl.msu.edu</u>). For questions regarding calorimetry, please contact Dr. Craig Woody, Physics Department, Brookhaven National Lab (<u>woody@bnl.gov</u>).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate(s) for Instrumentation, Detection Systems and Technique: Elizabeth Bartosz, <u>Elizabeth.Bartosz@science.doe.gov</u>.

## b. Development of Novel Gas and Solid-State Detectors

Nuclear physics research has the need for devices to track charged particles, 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. The subtopic announcements are grouped into solid-state devices and novel gas detectors.

Grant applications are sought to develop novel solid-state gamma-ray detectors, including:

- Position-sensitive gamma-ray tracking devices for nuclear structure and astrophysics applications, as well as associated technology for these devices. High-resolution germanium (Ge) capable of determining the position (to within a few millimeters utilizing pulse shape analysis) and energy of individual interactions of gamma-rays (with energies up to several MeV), allowing for the reconstruction of the energy and path of individual gamma-rays using tracking techniques, are of particular interest.
- Gamma-ray detectors capable of making accurate measurements of high intensities (>10<sup>11</sup>/s count rate) with a precision of 1-2 %, as well as economical gamma-ray beam-profile monitors;
- Components of segmented bolometers with high-Z material (e.g., W, Ta, Pb) for gamma ray detection with segmentation, capable of handling 100 -1000 gamma rays per second; and
- Alternative materials, with resolution comparable to germanium, but with higher efficiency and room-temperature operation.

# Grant applications are sought to develop advances in the general field of solid-state devices for tracking of charged particles and neutrons, such as silicon drift, strip, and pixel detectors, along with 3D silicon devices. Approaches of interest include:

- Thicker (more than 1.5 mm) segmented silicon charged-particle and x-ray detectors and associated high density, high resolution electronics;
- Low mass active-pixel sensors with thickness  $\sim$  50  $\mu m$  and large area Si pixel and strip detectors with thickness < 200  $\mu m$ ; and
- Segmented solid state devices for neutron detection, with integrated electronics.

## Grant applications are sought in the general field of micropattern 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 (order of magnitude effects must be shown).
Innovations such as commercial and cost effective production of GEM foils or thicker GEM structures,
micro-pattern structures, such as fine meshes used in Micromegas and high resolution
multidimensional readout such as 2D readout planes are desired as are high density (>64 channels )
high bandwidth (>200 MB/s) micropattern gas detector ASIC readout with rate capabilities > 200 KHz.

Grant applications are sought for the advancement of more conventional gas tracking detector systems, including drift chambers, pad chambers, time expansion chambers, and time projection chambers such as:

- Gas-filled tracking detectors such as straw tubes (focusing on automated assembly and wiring techniques), drift tube, proportional, drift, and streamer detectors;
- Improved gases or gas additives that resist aging, improve detector resolution, decrease flammability and have a larger, more uniform drift velocity;
- Application of CCD cameras for optical readout in Time-Projection Chamber or other gaseous chamber detector technologies capable of tracking and measuring low momentum (<100 GeV/c) alpha particle, deuteron and proton with better than 10 keV resolution, thereby allowing tagged fixed-target experiments;
- New developments for fast, compact TPCs; and
- New developments in low-mass drift chambers for tracking of low-beta, heavily ionizing particles, particularly for use as vertex detectors for spectator protons.

Finally, grant applications are 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.

For questions related items above listed under general field of micropattern gas detectors contact Dr. Bernd Surrow (<u>surrow@temple.edu</u>). For questions related to advancement of more conventional gas tracking detector systems contact Dr. Wolfgang Mittig, NSCL/MSU (<u>mittig@nscl.msu.edu</u>). For item 2 listed above under development of detectors for rare isotope beams contact Dr. Marc Hausmann, FRIB/MSU (<u>Hausmann@frib.msu.edu</u>).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate(s) for Instrumentation, Detection Systems and Technique: Elizabeth Bartosz, <u>Elizabeth.Bartosz@science.doe.gov</u>.

## 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 neutrinoless double beta decay (NLDBD) and searches for new nuclear isotopes produced at radioactivebeam 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, 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;

- Novel materials with ultra-low trace contamination of radionuclides and solutions for the construction of ultra-low background detectors. This includes structural and vacuum-compatible materials, hermetic containers and cable feedthroughs;
- 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.

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate(s) for Instrumentation, Detection Systems and Technique: Elizabeth Bartosz, <u>Elizabeth.Bartosz@science.doe.gov</u>.

#### 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 scintillators (such as BGO, BaF2, LaBr 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. Many of these detectors 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 using timing and pulse shape information or other method; and
- Large-area, high optical quality Cherenkov materials (e.g., Aerogel).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate(s) for Instrumentation, Detection Systems and Technique: Elizabeth Bartosz, <u>Elizabeth.Bartosz@science.doe.gov</u>.

#### e. Specialized Targets for Nuclear Physics Research

Grant applications are sought to develop specialized targets, including:

- Polarized (with nuclear spins aligned) high-density gas or solid targets capable of withstanding high electron or proton beam currents beyond the current state of the art; polarized <sup>3</sup>He targets, especially novel high-pressure circulating gas concepts matching the next generation of high-luminosity electron and photon beam experiments;
- Very thin windows (<100 micrograms/cm<sup>2</sup> and/or 50% transmission of 500 eV X-rays) for gaseous detectors, for the measurement of low-energy ions; and
- 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.

Grant applications also 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.

## Finally, grant applications are sought to develop techniques for:

- Production of thin films (in the thickness range from a few μg/cm<sup>2</sup> to over 10 mg/cm<sup>2</sup>) for charge-state stripping in heavy-ion accelerators; and
- 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.

For questions on targets used in low-power nuclear physics experiments, contact John Greene (ANL) (<u>greene@anl.gov</u>). For questions on high-power targets for experiments at JLab, contact Dave Meekins (<u>meekins@jlab.org</u>). For questions related to technologies for high-power targets for FRIB contact Dr. Wolfgang Mittig, NSCL/MSU (<u>mittig@nscl.msu.edu</u>).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate(s) for Instrumentation, Detection Systems and Technique: Elizabeth Bartosz, <u>Elizabeth.Bartosz@science.doe.gov</u>.

#### f. Technology for High Radiation Environments

Next generation rare isotope beam facilities require new and improved techniques, instrumentations 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:

- Rotary vacuum and/or water seals for applications in a high-radiation environment: Vacuum rotary
  feedthroughs for high rotational speeds or vacuum compatible water rotary feedthroughs, which have
  a long lifetime under a high-radiation environment (order of months to years at 0.5-15 MGy/month),
  are highly desirable for the realization of rotating targets and beam dumps for rare isotope beam
  production and beam strippers in high-power heavy-ion accelerators.
- 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<sup>-4</sup> is highly desired.
- Improved models of radiation transport in beam production systems: The use of energetic and highpower 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.
- Fast neutron and photon dose-equivalent area monitors: Neutron and photon dose-equivalent area monitors that are fast and pulsed beam capable, have minimal total dead time, have dose response to high energy radiation (e.g. neutron energies > 1 GeV), and can meet high safety standard requirements (e.g. IEC 61511) would be beneficial at high power research accelerator facilities like FRIB or medical

accelerator facilities where full beam loss accidents can have significant dose consequences. Response times in the range of 0.3 seconds or faster are desirable.

For rotary vacuum seals contact Dr. Frederique Pellemoine, FRIB/MSU (<u>pellemoi@frib.msu.edu</u>). For radiation resistant magnetic field probes contact Dr. Georg Bollen, FRIB/MSU (<u>bollen@frib.msu.edu</u>). For models of radiation transport in beam production systems and for fast neutron and photon dose-equivalent area monitors contact Dr. Mikhail Kostin, FRIB/MSU (<u>kostin@frib.msu.edu</u>).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate(s) for Instrumentation, Detection Systems and Technique: Elizabeth Bartosz, <u>Elizabeth.Bartosz@science.doe.gov</u>.

#### 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

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate(s) for Instrumentation, Detection Systems and Technique: Elizabeth Bartosz, <u>Elizabeth.Bartosz@science.doe.gov</u>.

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- 10. NP SBIR/STTR Topic Associate(s) for Electronics and Circuits: Manouchehr Farkhondeh: <u>Manouchehr.Farkhondeh@science.doe.gov</u>
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## 27.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 to research in chemistry, physics, energy, environmental sciences, and 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. and of which there exists insufficient domestic commercial production capability; some exceptions include some special nuclear materials and molybdenum-99, for which the National Nuclear Security Administration has responsibility. The benefit of a viable research and development program includes an increased portfolio of isotope products, more cost-effective and efficient production/processing technologies, a more reliable supply of isotope year-round and reduced dependence on foreign supplies. Additional guidance for research isotope priorities is provided in the Nuclear Science Advisory Committee Isotopes (NSACI) report published in 2015

(<u>http://science.energy.gov/~/media/np/nsac/pdf/docs/2015/2015\_NSACI\_Report\_to\_NSAC\_Final.pdf</u>). The NSACI reports serve to guide production plans and research activities supported by the Isotope Program.

All entities submitting proposals to SBIR/STTR Isotope Science and Technology topic must recognize the moral and legal obligation 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 perform nuclear physics R&D, 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.

Grant applications are sought in the following subtopics:

#### a. Novel or Improved Production Techniques for Radioisotopes or Stable Isotopes

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 research or applied usage communities (i.e.

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 supply of isotopes complementing the existing portfolio produced and distributed by the Isotope Program.

The 2015 NSAC-I report provides exemplary guidance. In the medical community, production of radionuclides capable of functioning as diagnostic/therapeutic (theranostic) pairs or single isotopes combining both traits (e.g., <sup>64</sup>Cu/<sup>67</sup>Cu, <sup>44</sup>Sc/<sup>47</sup>Sc, or <sup>186</sup>Re) are of particular interest, as are novel or indemand 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 development of high quality, robust targets is required to utilize the high-current high-power-density available from advanced accelerators; of particular concern is the design and fabrication of encapsulated salt targets and liquid metal targets. These targets could be subjected to energies greater than 50 MeV at beam currents of 100  $\mu$ A to 750  $\mu$ A. 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 inhot-cell target fabrication technologies to facilitate the recycling of precious and 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.

Additionally, proposals are sought for new technologies to produce large quantities of enriched isotopes. Enriched stable isotopes are used in radioisotope production targets and are important in fundamental nuclear physics experiments and medical applications. Development of process technologies aimed at optimizing the recovery and recycling of enriched stable isotopes is of interest. Isotopes of interest for nuclear physics measurements include kilogram to ton quantities of <sup>76</sup>Ge, <sup>82</sup>Se, <sup>130</sup>Te, <sup>129</sup>Xe, and <sup>136</sup>Xe. Novel methods are also sought for separation of stable isotopes that are needed in small quantities, as listed in the NSAC-I report.

Proposals are also sought for the development of electromagnetic isotope separation techniques for radioactive isotopes, including development of highly-efficient ionization methods, recovery and recycling techniques for target material that is not ionized, and collection methods for the separated isotope of interest. Of particular interest is isotope separation of actinides that can be used for radioisotope production via neutron capture reactions and the development of isotope separation techniques for medically-important radioisotopes that are currently only available with low specific activity.

New production methods for mg quantities of transuranic elements such as <sup>249</sup>Cf, <sup>251</sup>Cf, and <sup>249</sup>Bk, and ng quantities of <sup>254</sup>Es, and <sup>257</sup>Fm are of interest to the heavy element research community for chemistry research, rare particle and rare decay experiments, and heavy element creation in nuclear physics

research. Guidance for research isotope priorities is provided in the 2015 NSACI report (<u>http://science.energy.gov/~/media/np/nsac/pdf/docs/2015/2015 NSACI Report to NSAC Final.pdf</u>). For further specifications on items in subtopic a contact Dr. Meiring Nortier at LANL (<u>meiring@lanl.gov</u>), Dr. Leonard Mausner at BNL (<u>Imausner@bnl.gov</u>) or Dr. Kevin Hart at ORNL (<u>hartkj@ornl.gov</u>).

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate for Isotope Science and Technology: Ethan Balkin, <u>Ethan.Balkin@science.doe.gov</u>.

#### 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 separation 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 in order to reduce 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.

Applications are sought for innovative developments and advances in separation technologies to reduce processing time, to minimize radiation exposure to personnel, to improve separation efficiencies, to automate separation systems, to minimize waste streams, and to develop advanced materials for high-purity radiochemical separations. In particular, the DOE Isotope Program seeks breakthroughs in lanthanide and actinide separations. Incremental improvements are also encouraged, such as (1) in 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.

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 <sup>211</sup>At, <sup>225</sup>Ra, <sup>225</sup>Ac, and <sup>227</sup>Ac from contaminant metals, including thorium, radium, lead, lanthanides, and/or bismuth; b) improve ion-exchange column materials needed for generating <sup>212</sup>Pb from <sup>224</sup>Ra, <sup>213</sup>Bi from <sup>225</sup>Ac and/or <sup>225</sup>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 improving treatment efficacy and safety. Among those listed, advanced methods for the preparation of high purity <sup>225</sup>Ra and <sup>225</sup>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. For further specifications on items in subtopic b contact Dr. Saed Mirzadeh (mirzadehs@ornl.gov) at ORNL, Dr. Leonard Mausner (Imausner@bnl.gov) at BNL, Dr. Jonathan Engle jwengle@lanl.gov at LANL, or Matt O'Hara (Matthew.OHara@pnnl.gov) at PNNL.

Questions – contact Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate for Isotope Science and Technology: Ethan Balkin, <u>Ethan.Balkin@science.doe.gov</u>.

#### 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 Michelle Shinn, <u>Michelle.Shinn@science.doe.gov</u> or the NP SBIR/STTR Topic Associate for Isotope Science and Technology: Ethan Balkin, <u>Ethan.Balkin@science.doe.gov</u>.

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