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PROGRAM AREA OVERVIEW OFFICE OF ELECTRIC TRANSMISSION AND DISTRIBUTION

http://www.electricity.doe.gov/

The mission of the Office of Electric Transmission and Distribution is to lead a national effort to modernize and expand America's electricity delivery system in order to ensure a more reliable and robust electricity supply. A modernized grid will significantly improve the Nation's electric reliability, efficiency, and affordability, and contribute to economic and national security. The risk of multi-regional blackouts (such as the August 2003 blackout) will be reduced through better visualization of the electric grid, advanced cable design, energy storage, superconductivity, use of distributed energy resources and microgrids, as well as other technologies supported by the Office. Effective application of all these technologies requires development of less expensive, more reliable sensors and power electronics.

1. ADVANCED POWER ELECTRONICS FOR ENERGY STORAGE, TRANSMISSION, AND DISTRIBUTION APPLICATIONS

Power electronic conversion systems (PCS) constitute major cost elements and reliability issues in most distributed generation and energy storage systems. As these systems move to higher power levels, it is desirable to improve the functionality and manufacturability of the power conversion systems. Several paths to improvement are possible. Moving from silicon to silicon-carbide based devices has the potential to increase power rating and switching frequency while replacing electrolytic capacitors with other components offers the potential of significantly increasing the reliability of these devices.

a. Wide Band Gap Power Converter Application—Wide Band Gap (WBG) devices, such as Silicon Carbide (SiC), have gained a lot of interest recently in the power electronic conversion world. WBG devices offer higher operating temperatures, higher blocking voltages, lower switching losses translating to increased efficiencies, and higher frequency of operation compared to silicon based components. SiC-based Schottky diodes and field effect transistors and other three terminal devices are currently available in the marketplace. Advances are sought in utilizing currently available WBG devices in power conversion system design to improve performance and manufacturability. This project will produce the design of an advanced PCS using WBG devices. Potential follow-on projects could be the demonstration of a 100kW to 500kW power converter showing increased performance, cost reduction, better thermal management design, and decreased footprint compared to comparable Silicon based systems.

b. Improving Capacitor Lifetime in Power Electronic Converters—Electrolytic capacitors are extensively used in power converters today. They have been known to have the shortest lifetime of any element, active or passive, used in the power converters. Capacitor failure is a significant problem for power electronics resulting in high maintenance and replacement costs. Pulsed power conditioning capacitors (film capacitors) with high reliability, lower dissipation, and larger voltage transient characteristics are required for high reliability power electronics. Advances in polymeric film capacitors are of particular interest. This project seeks to incorporate advanced capacitor components in the design of power electronic converters with the goal of demonstrating increased reliability at reasonable (preferably lower) cost. It is also desirable to improve the manufacturability of these devices as well as the performance. The initial phase of the project will focus on the design of high reliability systems incorporating advanced capacitor elements with possible follow-on fabrication and testing of the concepts produced.

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2. SENSORS FOR REAL-TIME MONITORING OF TRANSMISSION AND DISTRIBUTION LINES

The "National Transmission Grid Study" discusses the use of advanced technologies to enhance performance of the nation's electricity delivery system. Today's system benefits from the countless technological innovations that have lowered costs and increased reliability. However, many more innovations are not being utilized because their pathway to market is blocked by uncertainties. This topic seeks to develop low cost sensors for the real-time monitoring of transmission and distribution lines. To assure that these technologies can obtain commercial viability, grant applications should also address the manufacturing of proposed components, so that

costs can be reduced without sacrificing product reliability or function. Grant applications are sought in the following subtopic:

a. Low-Cost Sensors for Real-Time Monitoring of Transmission and Distribution Lines—Extracting maximum performance from overhead transmission line conductors or underground cables requires knowledge of the existing conditions at all sections of the line. For example, consider the case of an overhead conductor – the wind speed, ambient air temperature, and solar insolation can vary from span to span and dramatically impact line capacity. In establishing loading limits, system operators typically assume worst-case conditions; therefore, reduced line loading must be accepted, even when actual conditions do not merit such reductions. Because real-time sensors and monitoring systems are relatively expensive, few transmission lines or underground cables utilize dynamic ratings based upon existing conditions. The installation of low-cost, reliable, robust sensors to monitor conditions in real-time could release additional capacity, and improve the reliability and economic efficiency of the nation's transmission and distribution corridors.

Grant applications are sought to develop and implement low-cost sensors for the real-time monitoring of system conditions. Measurement parameters could include conductor temperatures, voltages, current amplitudes and waveforms, and power flows, as well as inclination in the case of overhead line monitoring. Sensors should be capable of easy installation in a non-invasive manner and be able to communicate data with minimal additional cost or hardware. Grant applications must address: (1) how the particular conditions to be monitored will enable more efficient operation (i.e. closer to actual safety limits), while still maintaining system reliability; (2) issues of sensor locations and spacing, scalability of a network of sensors, measurement uncertainties, data resolution, means of communication, and power requirements for long-term monitoring; and (3) manufacturing issues, to assure that the sensors can be produced at low cost.

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PROGRAM AREA OVERVIEW OFFICE OF BIOLOGICAL AND ENVIRONMENTAL RESEARCH

http://www.er.doe.gov/ober/ober_top.html

The Biological and Environmental Research (BER) Program supports fundamental, peer-reviewed research in climate change, environmental remediation, genomics, systems biology, radiation biology, and medical sciences. BER funds research at public and private research institutions and at DOE laboratories. BER also supports leading edge research facilities used by public and private sector scientists across a range of disciplines: structural biology, DNA sequencing, functional genomics, climate science, the global carbon cycle, and environmental molecular science.

BER has a particular interest in the following areas:

(1) Climate Change research aimed at the development of advanced climate models to describe and predict the roles of oceans, the atmosphere, ice and land masses on climate over time and research to understand how carbon dioxide moves through the environment, ways to increase its removal from the atmosphere, and its impacts on the Earth's climate and ecosystems.

(2) Environmental Remediation research aimed at the development of advanced treatment options for nuclear waste, thereby extending the frontiers of biological and chemical methods for remediation, including the use of Earth's own microbe-based clean-up strategies; this research will yield science-based strategies to reduce the costs, risks, and time for cleanup of DOE sites contaminated from years of weapons research.

(3) Medical Sciences research aimed at the development of advanced imaging and other medical technologies including highly sensitive radiotracer detectors, radiopharmaceuticals, and new technologies such as an artificial retina that will give vision to the blind.

(4) Life Sciences research aimed at the development of innovative solutions along unconventional paths to solve challenges in energy and the environment. Research is focused on understanding nature's remarkable array of multi-protein molecular machines and the intricate workings of complex microbial communities; and on enabling us to use and even redesign these microbial machines and communities to produce clean energy, remove carbon dioxide from the atmosphere, and cleanup the environment. This program also supports research to understand the biological effects of low doses of radiation.

3. ATMOSPHERIC MEASUREMENT TECHNOLOGY

World-wide energy production is modifying the chemical composition of the atmosphere and is linked with environmental degradation and human health problems. The radiative transfer properties of the atmosphere may be changing as well. Various technological developments are needed for high accuracy and/or long term monitoring of these changes to support a strategy of sustainable and pollution-free energy development for the future.

Grant applications must propose Phase I bench tests of critical technologies. ("Critical technologies" refer to components, materials, equipment, or processes that overcome significant limitations to current capabilities, with respect to the subtopics that follow.) For example, grant applications proposing only computer modeling without physical testing will be considered non-responsive. Grant applications also should describe the purpose and benefits of any proposed teaming arrangements with government laboratories or universities in the technical approach or work plan. Applications submitted to any of the subtopics should 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 are sought only in the following subtopics:**

a. Measurements of the Chemical Composition of Carbonaceous Aerosols-There is a need to develop improved measurement methods to characterize the bulk and the size-resolved chemical composition of ambient aerosols in real time, particularly carbonaceous aerosols. Improved measurements would facilitate the identification of the origin of aerosols, i.e. primary versus secondary and fossil fuel versus biogenic. Also, they would help to elucidate how aerosol particles are processed in the atmosphere by chemical reactions and by clouds, and how their hygroscopic properties change as they age. This information is important because relatively little is known about organic and absorbing particles, which are abundant in many locations in the atmosphere. In particular, there is a need for instruments suitable for real-time measurements of the composition of particles at the molecular level. Although recent advances have led to the development of new instruments such as particle mass spectrometers and single particle analyzers, these instruments still have important limitations in their ability to quantify black carbon vs. organic carbon, provide speciation of refractory and volatile organic compounds, and calibrate both organic and inorganic components. Therefore, grant applications are sought to improve these instruments, or develop new technology, in order to provide one or more of the following attributes related to the measurement of the chemical composition of carbonaceous aerosols: (1) quantifiable results over a wide range of compounds – a problem for laser ablation aerosol mass spectrometer methods; (2) measurements over a range of volatility so that dust, carbon, and salt are detectable – a problem for thermal decomposition aerosol mass spectrometers; (3) speciation of individual organics, including those containing oxygen, nitrogen, and sulfur; (4) identification of elemental carbon and other carbonaceous material, so that the makeup of the absorbing fraction is known; (5) measurements with high time resolution, an inherent problem with filter techniques; (6) identification of source markers, such as isotopic abundances in aerosols; and (7) the ability to probe the chemical composition of aerosol surfaces.

b. Instrumentation for Characterizing Atmospheric Aerosols—Improved instrumentation and techniques are required to understand other characteristics of atmospheric aerosols. This subtopic deals with three of them:

(1) Aerosol precursors. Improvements in gas phase chemistry are needed to further understand the evolution of aerosols in clouds. For example, gas phase measurements of H_2SO_4 , a major aerosol precursor, have revealed a wealth of new information in the last decade. To make further progress, grant applications are sought to develop instruments that can make fast measurements of NH_3 , ion clusters, and gas phase organics, substances that might either condense or dissolve into preexisting aerosols or cloud droplets.

(2) Aerosol absorption. The aerosol absorption coefficient, together with the aerosol scattering coefficient, determines the single-scattering albedo. This key aerosol property and the factors that contribute to it are critical for determining heating rates and climate forcing by aerosols. Therefore, grant applications are sought to develop reliable instruments for the *in situ* measurement of the single-scattering albedo for particles containing black and organic carbon, dust, and minerals. The measurements must cover the solar wavelengths (UV, visible, and near infrared), must not alter aerosol properties, and must address the influence of relative humidity.

(3) Aerosol size distributions. Knowledge of the particle size distribution is essential for describing both direct and indirect radiative forcing by aerosols. However, current techniques for determining these distributions are often ambiguous because of the assumption that the particles are spherical. In particular, the optical techniques most often used in the 0.5-10 μ m size range have inherent problems. Therefore, grant applications are sought for techniques to determine the size distribution of ambient aerosols, in the 0.5-10 μ m size range, that are not based on optical properties. The techniques must address the influence of relative humidity and must be integrated with the simultaneous measurements of such properties as mass, area (extinction) and number.

c. Oxygen A-band Spectrometer for Photon Pathlength Measurements—The high-resolution spectrometry of strongly absorbing atmospheric bands is capable of providing information about the distribution of scatterers and absorbers in the atmosphere. This information cannot be obtained by other passive optical remote sensing techniques. The Oxygen A-band (around 764 nm wavelength, in the near infra-red) is a particularly useful domain for remote sensing, with useful applications both in stand-alone instruments and in combination with millimeter-band cloud-sensing radar. Low-resolution A-band sensing has been used in downward looking platforms (satellite or high-altitude aircraft) to sense surface pressure and cloud-top heights. High-resolution A-band instruments were considered as part of the Picasso-CENA (now Calypso) and Cloudsat instrument packages and are being considered for future missions such as the Orbiting Carbon Observatory (OBO).

The highest performance achieved to date with an A-band instrument provides spectral coverage of at least the entire P-branch of the A-band, spectral resolution of 0.5 wavenumber or better, wavelength stability better than 1/20 of full-width at half-maximum (FWHM), and a far out-of-band (OOB) rejection ratio better than 10^{-4} . However, for practical purposes, this level of performance could be relaxed – a lower resolution of 5-10 wavenumbers would be sufficient to obtain two useful parameters, the mean and variance of the photon path length. Grant applications are sought to develop innovative optical detector methods to lower the cost of such moderate performance A-band instruments, in order to permit them to be more widely deployed. For this class of instruments, the OOB rejection ratio could be modestly lower, the wavelength stability must be comparable, and the stability of responsivity must be better, compared to the performance levels described above.

d. Measurement of the Size Distribution of Water Drops in Clouds—Existing *in situ* optical instruments, commonly used on research aircraft and at the surface, for measuring the drop size distribution of water clouds suffer inherent limitations. Because the measurement technology of these instruments (e.g., forward scattering and phase Doppler probes) is based on the light scattering properties of individual drops, the sample volume must be very small to prevent the coincidence of two or more drops from influencing the measurement. However, in clouds with low drop concentrations, these very small sample volumes make it difficult to obtain statistically significant drop samples when the drops are greater than approximately 50 µm in diameter. Yet, clouds with low drop concentrations and with drops greater than 50 µm are scientifically very important,

because this is the regime in which drizzle drops (i.e., drops with diameters from 50 to 200 μ m) are formed. The formation of drizzle can lead to a rapid modification of the cloud drop size distribution, which in turn has a strong influence on a cloud's radiative properties, especially for marine and arctic stratus clouds. (For example, the formation of drizzle often leads to a rapid increase in effective drop radius and a corresponding decrease in number concentration, thereby decreasing the reflectance of a cloud.) Because stratus clouds cover a large portion of the earth, this process has a strong impact on the global radiative budget. Grant applications are sought to develop new instrument technology that is capable of providing statistically significant measurements of the size distribution of water drops with diameters from 3 to 200 μ m in clouds that have a total drop concentration on the order of 10 to 100 per cubic centimeter. The new instrumentation should be capable of operation on research aircraft, tethered balloons, and on the ground without degradation in performance. The Phase I project should demonstrate the feasibility of the technology in the laboratory. In Phase II, an operational sensor should be built and tested on a research aircraft, on a tethered balloon, and on the ground. Potential commercial applications of the new sensor could extend to measurements of industrial and agricultural sprays.

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4. MEDICAL SCIENCES

The Department of Energy (DOE) Medical Sciences program covers a broad range of energy-related technologies including nuclear medicine and advanced imaging instrumentation. DOE is interested in innovative research involving medical technologies to facilitate and advance the current state of diagnosis and treatment of human disorders.

Principles of physics, chemistry, and engineering are being employed to advance fundamental concepts dealing with human health, to utilize the study of molecular interactions for a better understanding of organ function, and to develop innovative biologics, materials, processes, implants, devices, and informatics systems for the prevention, diagnosis, and treatment of disease and for improving human health. The DOE Advanced Medical Instrumentation program seeks to capitalize on the unique physical sciences and engineering capabilities at the DOE's national laboratories to develop new technologies that will have a significant impact on human health.

With respect to nuclear medicine, current areas of research include the development of: (1) radiopharmaceuticals as radiotracers to study *in vivo* chemistry, metabolism, cell communication, and gene expression in normal and disease states, and as therapeutic agents; and (2) new radionuclide imaging systems. **Grant applications are sought only in the following subtopics:**

a. Development of Novel Probes for Biomedical Applications—Grant applications are sought to develop improved and new probes (fluorescent, electron dense, vibrational tags, etc.) with optimum physico-chemical properties for visualization, tracking, assembly, and disassembly of the multiprotein complexes that execute cellular functions and govern both cell form and components. These multifunctional probes would measure structure, including post-translational modification, and would function in real time. Novel probes are also needed to enable rapid visualization and quantification of intracellular processes with high spatial resolution. Probes should be selective, non-perturbative, resistant to degradation, and have unique spectroscopic signatures. Grant applications must present unambiguous experimental systems to validate probe performance and demonstrate that the research will ultimately result in new sensors for medical applications. Several DOE national laboratories have developed considerable expertise in this research area and are available for possible collaboration.

b. Radiopharmaceutical Development for Radiotracer Diagnosis and Targeted Molecular Therapy— Grant applications are sought to develop: (1) radiolabeled compounds that could have applications as radiotracers for radionuclide imaging technologies such as positron emission tomography and single photon emission computed tomography; (2) improved and simplified production of radiolabeled compounds through the use of mini-accelerator technology or automated radiochemical analysis/synthesis techniques; and (3) radiopharmaceuticals for targeted molecular therapy. Of particular interest are radiochemical, synthetic, and combinatorial molecular engineering approaches. All efforts should ultimately result in a product for nuclear medicine use.

c. Advanced Imaging Technologies—Grant applications are sought for new, sensitive, high resolution instrumentation for radionuclide imaging. The instrumentation should advance the application of radiotracer methodologies for imaging molecular biological functions including cell communication and gene expression *in vivo*. Areas of interest include the development of: (1) new detector materials and detector arrays for both positron emission and single photon emission computed tomography; (2) software for rapid image data processing and image reconstruction; and (3) methods of integrating *in vitro* and *in vivo* instrumentation technologies for real time molecular imaging of biological function and for new drug development and utilization.

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5. GENOMICS: GENOMES TO LIFE AND RELATED BIOTECHNOLOGIES

The Department of Energy (DOE) supports research to acquire a fundamental understanding of biological and environmental processes. This includes the display of genomes as DNA sequences; the functional characterization of gene products, especially from DOE-relevant microbes; structural biology user stations at synchrotron sources and neutron sources; computational genomics; and the development of integrating information systems. This topic is focused on the goals of the Genomes to Life (GTL) program, namely, to develop a detailed understanding of the molecular machines of DOE-relevant microbes and their networking in living cells and microbial communities. Microbes with capabilities that can further several DOE programmatic missions are being used as the current subjects for these studies. The knowledge thus gained would enable both the public and private sectors to apply genome knowledge to the production of energy, promote environmental applications such as bioremediation and carbon sequestration, promote cleaner industrial processes using biotechnology, and enable increasingly effective computational models of the microbial cell. For some of the subtopics below, capabilities already exist in a few laboratories, but commercial involvement will be needed before the technology can be exported to the broader research community. **Grant applications are sought only in the following subtopics:**

a. Genome Scale Reagent Sets—There is an increasing availability of genomes as sequenced chromosomes with their constituent genes. These genes number in the thousands for bacteria and in the 10-100 thousand range for higher organisms. Each gene may give rise to numerous distinct mRNAs and proteins, through processes of alternative RNA splicing and post-translational modifications. Micro-arraying methodologies are enabling highly parallelized interrogations of these huge macromolecule collections. However, production and management systems are required to assure the availability of the numerous analytical reagents that are needed in small quantities. Grant applications are sought for: (1) systems that will produce thousands of affinity reagents (oligo-nucleotides, synthetic genes, antibodies, and other affinity reagents) in pico-molar quantities; (2) miniaturized delivery systems for such reagent sets; and (3) reagent sets for quantitation of RNA splicing.

b. Proteomics—A number of proteomics tasks are being pursued to achieve the goals of the GTL program. These tasks include high throughput production and purification of proteins, correlation of proteins with the genes encoding their primary structure, identification of protein isoforms encoded by the same gene, identification of memberships in functional complexes of proteins, and identification of the variations of proteome constituents under change to useful physiological states. However, a number of obstacles are preventing the accomplishment of these tasks. For example, several host-vector systems are available for the production of proteins encoded in a hyper-expressed source gene; yet, for some source genes, the proteins fail to fold into physiologically effective three-dimensional conformations (entrapment in insoluble inclusion bodies is one cause of such failures). Another difficulty is that proteins targeted to membranes are problematic. Lastly, the lack of affinity reagents that bind to proteins in their native conformations adversely impacts structure, protein association, and function analyses. Therefore, grant applications are sought for the improved recovery and analysis of effective proteins. Areas of interest include: (1) the production of solubilized proteins in active confirmations with or without post-translational modifications; (2) the development of synthetic membranes or nano-structures enabling analyses of membrane proteins; (3) and the development of improved affinity reagents.

c. Instrumentation for Single Macromolecule Analysis and Control—Over the last decade, research laboratories have made substantial progress in developing instrumentation for the interrogation and manipulation of single macromolecules. Techniques include the use of optical-laser tweezers, atomic force microscopy, and single molecule fluorescence microscopy. Although the effectiveness of these techniques has improved steadily and the instrumentation is now robust, most of these single-molecule biophysics instruments are locally built. The lack of commercial support has severely hindered the export of these technologies to the broader user community. Grant applications are sought to expand the commercialization of techniques, instrumentation, and software systems so as to enable the broader usage of single macromolecule analysis methods.

d. Informatics—The development of an effective computational model of the cell not only would contribute to the GTL program but also would have numerous applications, including the preliminary processing of genome scale data sets being generated by experimental groups. Grant applications are sought to improve one or more of the component software packages that have already been developed by laboratory groups, in order to enhance user friendliness and thereby support their broad export to the biologist community. Grant applications also are sought to develop novel software in support of cellular modeling tasks. Of particular interest are approaches related to: (1) systems biology, (2) the processing of proteomics and metabolomics data sets, (3) improved integration and or querying of heterogenous data sets, and (4) the automated development of cellular metabolic models from data sets on newly studied microbes.

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6. MEASUREMENT/MONITORING AND CHARACTERIZATION TECHNOLOGIES FOR THE SUBSURFACE ENVIRONMENT

The characterization and monitoring of soils, subsurface sediments, and ground water are important elements of Department of Energy (DOE) research efforts. Objectives include determining the fate and transport of contaminants generated from past weapons production activities and from current energy production activities, assessing and controlling processes to remediate contaminants, and long-term monitoring of sites. Grant applications submitted to this topic must detail why and how proposed *in situ* fieldable technologies will substantially improve the state-of-the-art and must include bench tests to demonstrate the technology. Projected dates for likely operational deployment must be clearly stated. New or advanced technologies that operate

under field conditions with mixed/multiple contaminants and that can be deployed in 2-3 years will receive selection priority. Claims of commercial potential for proposed technologies must be supported by information such as endorsements from relevant industrial sectors, market analysis, or identification of commercial spin-offs. Grant applications that propose incremental improvements or enhancements to existing technologies are not of interest and will be declined, as will enhancements to predictive models.

For some of the following subtopics, collaboration with government laboratories or universities may speed the development of the measurement or monitoring technology. For example, the Environmental Molecular Sciences Laboratory (EMSL), a DOE scientific user facility located at the Hanford Site in Richland, WA, can provide analytical instrumentation and capabilities with direct application to sensor development and testing. Potential applicants are invited to review the Web site for the Interfacial Chemistry and Engineering group (http://www.emsl.pnl.gov/homes/ice/) and the Interfacial and Nanoscale Science Facility (http://www.emsl.pnl.gov/capabs/insf.shtml) at the EMSL. 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 only in the following subtopics:

a. Mapping Hydrogeologic Processes in the Shallow Subsurface—Accurate information about the distribution of parameters that control the shallow flow of water (vadose zone to water table), such as hydraulic conductivity, water content, and lithology are prerequisites to predict the flow and transport of contaminants. Natural heterogeneity and the large spatial variability of hydraulic conductivity are predominant factors that affect the subsurface flow. Geophysical data collected from the ground surface and between boreholes hold much promise for providing high-resolution information about the distribution of subsurface properties and associated uncertainties. In this subtopic, the emphasis is on describing water flow associated with contaminant transport processes within the complex, shallow subsurface.

Grant applications are sought to develop high-resolution geophysical sensors to: (1) detect hydrogeologic or geophysical processes that control the transport and dispersion of contaminants in the subsurface, or (2) measure mass-transfer processes and rates within and among individual flow paths in the subsurface. Small diameter applications (e.g., cone penetrometer technology (CPT) – a direct push technology for subsurface access) are of particular interest. Conventional logging tools for such applications typically provide information over relatively short distances (few cm); therefore, a technology that can provide images from tens of meters from the hole (such as the single well, crosswell, and vertical seismic profiling methods developed for larger boreholes) are desired. The following issues should be addressed and tested: coupling, resonance, and power radiation.

While geophysical characterization methods are improving and yielding higher-resolution data, they have not routinely been used to describe flow and transport processes or for guiding remediation activities. Therefore, grant applications also are sought to develop user-friendly software packages to facilitate the use of high resolution geophysical measurements for interpreting the hydrogeologic parameters. Proposed approaches must allow site personnel to utilize the dense, non-invasive information obtainable from geophysical methods for improved subsurface characterization and monitoring.

b. Real-Time, *In Situ* Biogeochemistry Measurements in Soils, Subsurface Sediments, Biofilms, or Groundwater—There is a need for sensitive, accurate, and real-time monitoring of biogeochemical processes and their interactions with microorganisms in contaminated soils, sediments, biofilms, or ground water environments (hereafter referred to as the subsurface). The use of highly sensitive monitoring devices in the subsurface (*in situ*) would allow for low-cost field deployment in remote locations and an enhanced ability to monitor processes at finer levels of resolution. For this subtopic, the following radionuclides and metals are of interest: americium, cesium, chromium, cobalt, mercury, plutonium, strontium, technetium, and uranium. Grant applications that address other contaminants will be declined.

Grant applications are sought to develop sensors and systems to detect biogeochemical processes that control the transport or transformation of contaminants (namely, the aforementioned metals and radionuclides) in the subsurface. Grant applications must provide convincing documentation (experimental data, calculations, etc.) to show that the sensing method is both highly sensitive (i.e., low detection limit) and highly selective to the target analyte (i.e., immune to anticipated physical/chemical/biological interferences). Approaches that leave significant doubt regarding sensor functionality in realistic multi-component samples will be excluded from consideration.

Grant applications also are sought for integrated sensing and controller/signal processing systems for autonomous or unattended applications of the above measurement needs. Innovative integration of components (such as micro-machined pumps, valves, and micro-sensors) into a complete sensor package with field applications in the subsurface will be considered responsive to this subtopic. Approaches of interest could include fiber optic, solid-state, chemical, or silicon micro-machined sensors; or biosensors (devices employing biological molecules or systems in the sensing elements) that can be used in the field. Biosensing systems may incorporate, but are not limited to, whole cell biosensors (i.e., chemiluminescent or bioluminescent systems), enzyme or immunology-linked detectors), lipid characterization systems, or DNA/RNA probe technology with amplification and hybridization. As substantial progress has been made in fiber optics and chemical sensing technology in the last decade, grant applications that propose minor adaptations of readily available materials/hardware, and/or can not demonstrate substantial improvements over the current state-of-the-art, are not of interest and will be declined.

c. Sensor Technology for Monitoring Tank or Landfill Waste—Grant applications are sought for the longterm and continuous monitoring of gases or liquids that are contained within, or could be released from, DOE tanks or DOE landfills containing mixtures of contaminants. Sensors would be used to detect and/or quantify contaminants, or their degradation products, in off-gases, effluents, or other samples. Sensors could also be used *in situ* to monitor changes in waste chemistry during storage. Contaminants of interest include a number of metals and radionuclides (americium, cesium, chromium, cobalt, mercury, plutonium, strontium, technetium, and uranium); anions such as nitrate; chelators; extractants such as tributyl phosphate; and gases such as ammonia, hydrogen, carbon dioxide, and methane. Relevant wastes are expected to contain more than one type of contaminant; therefore, the sensor technology must be both sensitive and specific for targeted contaminant(s). Development of robust sensors, capable of use with high-level waste, is encouraged. Moreover, sensors suitable for use with other waste types (such as low-level, mixed or solid wastes) and sites (DOE landfills or slit trenches) are desirable.

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7. BIOLOGICAL SOLUTIONS AND TECHNOLOGIES FOR REDUCING ATMOSPHERIC CARBON DIOXIDE

The burning of fossil fuels adds carbon to the atmosphere, principally in the form of carbon dioxide, and the potential environmental impacts have made carbon management an international concern. There is increasing national and international interest in enhancing natural mechanisms to slow the rate of atmospheric CO_2

increase, or in developing new approaches to mitigate the current atmospheric rise in CO_2 levels. The U.S. Climate Change Technology Program [reference 9] calls for the development of biological approaches to remove CO_2 from the atmosphere in addition to energy production strategies that reduce or eliminate CO_2 emissions. A DOE report on carbon sequestration science and technology [6] describes research needs and technology requirements for sequestering carbon by aquatic and terrestrial systems, including a discussion of advanced biological processes and chemical approaches.

This topic focuses on biological mechanisms that offer the potential to slow the rate of atmospheric CO_2 increase, convert carbon into relatively stable organic or inorganic forms, or increase hydrogen production as a potential "clean energy" source. For example, some terrestrial and aquatic plants might be studied for CO_2 conversion to biomass; others to transform carbon into long-lived (refractory) organic compounds, thereby sequestering the CO_2 and slowing the rate of atmospheric increase. Research is solicited to identify and quantify mechanisms for CO_2 transformation at rates that will lead to the long term fixation and/or sequestration of large quantities of carbon (i.e., where fractions of giga tonnes or more of carbon per year transformed or fixed is considered significant) when applied to either natural (e.g., unmanaged terrestrial ecosystems) or managed aquatic systems.

Microbes also can make a significant contribution to the cycling of elements that are critical for life (including carbon, nitrogen, sulfur, hydrogen, and oxygen) as well as to the unwanted release of gases to the atmosphere responsible for the "greenhouse effect." Some terrestrial microbes, found both in the subsurface and on the surface, have the potential to dramatically impact carbon sequestration, either directly or through their effects on plants. Other microbes can also produce hydrogen. Therefore, this topic also is concerned with the use of microbes for sequestering atmospheric CO_2 or for producing hydrogen.

Grant applications must provide for a systematic evaluation of proposed biological mechanisms for either carbon sequestration or hydrogen production systems. Estimates of the amount of CO₂ transformed or hydrogen produced must be provided, and any assumptions concerning quantities and conditions for carbon fixation and sequestration or for hydrogen production must be clearly defined. Feasibility tests (analytical, bench, or field) performed in Phase I must demonstrate that the proposed approach, when scaled up, could theoretically result in a meaningful rate reduction in atmospheric CO₂ concentration, significant amounts of carbon sequestration or hydrogen production. Phase I should identify processes and mechanisms, and provide preliminary data on prospective rates and quantities of enhanced carbon transformation and sequestration or hydrogen production, with more comprehensive and peer-reviewed data sets developed in Phase II. Grant applications proposing only computer modeling without improvements in physical mechanisms or the enhancement of field approaches will not be considered.

The facilities and expertise of the DOE Consortium for Research on Carbon Sequestration in Terrestrial Ecosystems (CSITE - <u>http://csite.esd.ornl.gov/</u>) can be made available to potential SBIR applicants to this topic. The CSITE is a consortium based at Oak Ridge National Laboratory (ORNL), Pacific Northwest National Laboratory (PNNL), and Argonne National Laboratory (ANL). The co-directors are Robin Graham (ORNL/email: <u>grahamrl@ornl.gov</u>) and Blaine Metting (PNNL/email: <u>fb_metting@pnl.gov</u>). Applications of Biotechnology to Mitigation of Greenhouse Warming: Proceedings of the St. Michaels II Workshop, April 2003, available at: <u>http://www.battelle.org/bclscrpt/Bookstore/booktemplate.cfm?ISBN=1-57477-141-8%20</u>. Scientists at Texas A&M University, Colorado State University, the University of Washington, North Carolina State University, and the Joanneum Research Institute in Austria can also provide support to potential applicants. The DOE also supports carbon sequestration research at the National Energy Technology Laboratory (NETL). **Grant applications are sought only in the following subtopics:**

a. Sequestration of Carbon by Plant-Soil and Aquatic Systems—Virtually all plant species effectively capture CO_2 from the atmosphere and produce organic compounds, which sustain productivity of the Earth's ecosystems. Some of the fixed carbon is sequestered in soils or sediments and in wood products of terrestrial

ecosystems. For example, woody species sequester carbon as lignocellulose, which is a stored product for the lifetime of the tree, and the below-ground productivity of many ecosystems is transformed into organic soil matter with intrinsically long residence times. Aquatic plants produce peat or organic-rich sediments. Grant applications are sought to identify and quantify the biological pathways and mechanisms leading to increased quantities of carbon sequestration by plant, soil (including soil microorganisms), and sediment components of terrestrial and aquatic ecosystems. Areas of particular interest include: (1) research on plant metabolic pathways or mechanisms that allow increased CO₂ fixation rates, achieved through conventional molecular or traditional genetic means, and leading to overall productivity increases; (2) novel technologies for managing vegetation and soils (such as cost-effective nutrient management, forest regeneration, ecosystem modification, and aquatic cultures) to enhance carbon uptake and retention, thereby significantly increasing CO₂ fixation and Carbon (C) storage; (3) techniques for increasing the fraction of recalcitrant organic compounds produced during natural microbial conversion of plant biomass in soils, resulting in increased long-term C-storage; and (4) measurement techniques that allow for the validation of technologies developed to enhance net long-term C sequestration in man-made and natural environments.

Grant applications should provide information about rates and quantities of carbon fixation or the enhancement of sequestration that the proposed technology can reasonably achieve. For terrestrial systems, proposed approaches should exhibit a capability to increase, or to measure increases of, carbon fixation or sequestration by at least 1 tonne per hectare per year. For rapidly C-fixing aquatic biosystems, the desired rate of consumption would be at least 5 grams of carbon (expressed on an atom basis) per gram cell dry weight per hour at ambient temperature (e.g., 15°C) conditions. Phase I must demonstrate the basic feasibility and efficacy of proposed sequestration mechanisms, with larger field-scale applications designed and tested in Phase II.

b. Microbe-Based Carbon Sequestration in Harsh Environments—Microbes exist in essentially every conceivable environment on Earth. In particular, the remarkable diversity and capabilities of microbes offer the possibility of developing novel microbe-based solutions for carbon sequestration in harsh environments (in contrast to the environments assumed in the previous subtopic). Therefore, grant applications are sought to demonstrate and quantify terrestrial, photosynthetic, microbe-based strategies to increase the carbon sequestration potential in harsh environments, such as deserts or brackish water. Field studies are not necessarily expected and should not be proposed without appropriate NEPA approval.

c. Microbe-Based Hydrogen Production—Biotechnology offers the promise of capitalizing on the natural capabilities found in the microbial world to produce new fuels, leading to a reduction in green house gas emissions. In particular, many microbes have the ability to produce hydrogen under particular conditions. Therefore, grant applications are sought to demonstrate and quantify: (1) microbe based hydrogen production reactors, or (2) high-throughput assays for assessing and quantifying the production of microbe-based hydrogen in experimental reactors.

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8. CARBON CYCLE MEASUREMENTS OF THE ATMOSPHERE AND THE BIOSPHERE

Eighty-five percent of our Nation's energy results from the burning of fossil fuels from vast reservoirs of coal, oil, and natural gas. These processes add carbon to the atmosphere, principally in the form of carbon dioxide (CO_2) . It is important to understand the fate of this excess CO_2 in the global carbon cycle in order to assess the terrestrial ecosystem response, the sensitivity of climate, and the potential for sequestration in natural carbon sinks of lands and oceans. Therefore, improved measurement approaches are needed to quantify carbon changes in components of the global carbon cycle, particularly the terrestrial biosphere, in order to improve understanding and assess the potential for future carbon sequestration.

A DOE working paper on carbon sequestration science and technology describes research needs and technology requirements for sequestering carbon by ocean and terrestrial systems (see Reference 1). This document calls for substantially improved technology for measuring carbon transformation of the atmosphere and biosphere. The document also describes advanced sensor technology and measurement approaches that are needed for detecting changes of carbon quantities of terrestrial (including biotic, microbial, and soil components) and oceanic systems, and for evaluating relationships between these carbon cycle components and the atmosphere.

Grant applications submitted to this topic should demonstrate performance characteristics of proposed measurement systems, and show a capability for deployment at field scales ranging from experimental plot size (meters to hectares of land – with comparable dimensions for marine systems) to nominal dimensions of ecosystems (hectares to square kilometers). Research to develop miniaturized sensors to determine atmospheric CO_2 concentration is also encouraged. In addition, Phase I projects must perform feasibility and/or field tests of

proposed measurement systems to assure a high degree of reliability and robustness. Combinations of stationary remote and *in situ* approaches will be considered, and priority will be given to ideas/approaches for verifying biosphere carbon changes and for estimating carbon sequestration. Measurements using aircraft or balloon platforms must be explicitly linked to real-time ground-based measurements. Proposals based on satellite remote sensing platforms are beyond the scope of this topic. **Grant applications are sought only in the following subtopics:**

a. Sensors and Techniques for Measuring Terrestrial Carbon Sinks and Sources-Measurement technology is required to quantify carbon sequestration by natural vegetation and ecosystems (i.e., carbon sinks) as well as CO₂ emissions to the atmosphere from natural or industrial sources. Grant applications are sought to develop sensors and unique measurement techniques (and associated system technology, if appropriate) to detect and quantify annual net carbon changes of terrestrial vegetation for large areas, or to measure and verify the magnitude of CO_2 emissions from various sources. For the measurement of CO_2 sinks, the sensor systems or new technology must be applicable for forests, grasslands, shrub lands, agricultural lands, and/or wetlands, and have the capability of producing spatially resolved aggregate estimates of terrestrial carbon changes to an accuracy of 10 to 25 g/m²/yr (or approximately 0.25 tonnes of carbon per hectare per year), with less than 25 percent uncertainty. For measuring emissions, the apparatus must be located at a point remote from the actual site of CO₂ release and provide accuracy estimates for CO₂ concentrations of approximately 0.5 ppm or less. Mechanical sensors must be durable in the full range of normal environmental conditions and exposures, including exposure to dust, rain, snow, heat, extreme cold, and fog. Operation in unattended, remote locations for weeks at a time, without degradation of the measurement, is also required; however, daily telecommunication with the system for monitoring performance and detecting potential operational problems would be desirable.

Proposed approaches, including both mechanical sensors and non-mechanical technology should consist of new, innovative methodologies that are significant advances over conventional scientific approaches used to measure CO_2 , carbon, and related compounds. Specifically, the measurement systems should be different from, or substantially augment, existing methods for eddy flux (covariance), routine monitoring of atmospheric CO_2 concentrations, or estimating carbon quantities of land and/or ocean constituents of the carbon cycle. Grant applications proposing *in situ* or in-stream measurement of flue gas emissions will be declined, as will applications that offer only incremental or marginal improvements over existing measurement systems.

b. Novel Measurements of Organic Carbon and its Isotopes in Terrestrial and Atmospheric

Media—Improved measurement technology is needed to better characterize processes involving carbon transformations of soil, vegetation, and associated ecosystem components and exchanges with the atmosphere. Grant applications are sought for measurements of carbon content in the atmosphere, vegetation, soil, and associated environmental media. This includes high resolution measurements of soil carbon/organic matter and other solid substrates, as well as the carbon content of biological tissues in various components (e.g., phytomass, detritus) of terrestrial ecosystems, as noted in item #1 below. Improved measurement technology for atmospheric CO_2 are noted in items #2 and #3 below.

(1) For determining carbon content of biota and soil, grant applications are sought that demonstrate measurements for estimating changes of carbon quantities and/or fluxes involving major components of ecosystems, with an accuracy on the order of 10 grams per square meter or less. Quantification of spatially resolved aggregate estimates of terrestrial carbon changes should have an accuracy of 10 to 25 g/m²/yr (or approximately 0.25 tonnes of carbon per hectare per year), with less than 25 percent uncertainty.

(2) Grant applications also are sought to design and demonstrate a new CO_2 analyzer with the following characteristics: (i) ability to determine the mole fraction of CO_2 in dry ambient air to a relative precision of 1 part in 3000 or better in one minute or less; (ii) low gas use (30 cc/min or less) to minimize problems due to water vapor and to minimize consumption of reference gases, if employed; (iii) robust enough for unattended

field deployment for periods of half a year or longer; (iv) cost less than \$5000 when manufactured in quantity; and (v) not sensitive to motion.

(3) For applications to develop monitoring-type instruments for measuring atmospheric CO_2 , lightweight (approximately 100 grams) sensors are needed that are capable of measuring fluctuations of CO_2 in air of the order of plus or minus 1 ppm in a background of 370 ppm. The devices must be suitable for launch on balloonsondes or similar such platforms, and therefore must be insensitive to large changes in ambient temperature and pressure. They must be able to operate on low power (e.g., 9v battery), and have a response time of less than 30 seconds.

Grant applications also are sought to develop new technology platforms that can be used to measure fluxes and/or concentrations of important trace gas constituents in the atmosphere, such as isotopes of carbon, methane, CO, etc. Special attention should be provided to design elements that ensure long-term and robust field deployment.

Lastly, grant applications are sought for unique, rapid, and cost-effective methods for measuring the natural carbon isotopic composition of plant, soil, and atmospheric materials. The idea is to use isotope technology to identify sources and sinks of carbon materials, and to use carbon isotopes to distinguish relative carbon exchanges between terrestrial or aquatic media and the atmosphere. New isotope approaches and technology should demonstrate a quantitative capability for both estimating and distinguishing the carbon flux among atmosphere, biosphere, and soil components of natural and manipulated carbon cycles.

The following requirements apply to isotope measurements based on discrete CO₂ sampling. New instrument development must have the capability of resolving a biospheric isotopic CO₂ signal (either $^{13}C/^{13}C$ or $^{18}O/^{16}O$) of 20 ppm CO₂ when mixed with ambient air CO₂, or produce 0.2 per mil measurement resolution. For continuous measurement of these isotopes in air (e.g., for a 1-hr period), resolution of 3 per mil or better is acceptable for detecting a biological signal in air in the absence of instrument drift.

In general, new technology for measuring terrestrial biota and soil must be accomplished by *in situ* and/or noninvasive means and/or remote sensing of organic carbon forms across a range of temporal scales (from seconds to days) and spatial scales (from millimeters to kilometers), depending on the system properties being observed. Instruments must be portable and deployable in remote locations, and must not adversely impact the site of deployment. The term "remote sensing" means that the observation method is physically separated from the object of interest. Research that develops unique surface-based observations and uses them for the calibration/interpretation of other remotely derived data is of interest; however, except for the potential application of CO_2 sensors via balloonsonde, other methods of remote sensing data acquisition by airborne or satellite platforms will not be considered.

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PROGRAM AREA OVERVIEW --OFFICE OF FOSSIL ENERGY

http://www.fe.doe.gov/

Fossil energy plays a key role in our Nation's prosperity, and it is important that we secure an adequate energy supply from our coal, natural gas, and oil resources. However, national complacency, derived from low-cost imported oil, has allowed petroleum imports to increase to alarming levels. We need not go far back in history

to find out how uncertainty in petroleum supply can affect our Nation's economic growth. Nonetheless, our near term power generation, heating, and transportation needs still require the utilization of these hydrocarbonbased fuels. As the economy expands, demand for hydrocarbons will increase accordingly. Therefore, the Office of Fossil Energy seeks to develop advanced fossil energy technologies that are environmentally sound and economically competitive.

Technological innovation is required to take advantage of the United States' large supply of coal and natural gas reserves. Coal's major drawback is that it contains sulfur, nitrogen, and trace heavy metals, precursors of pollutants that could have deleterious effects on the environment. Natural gas is also produced with a wide variety of pollutant-forming compounds, which preclude some applications such as fuel cells and advanced gas turbines. For both coal and natural gas, further improvements are needed to develop advanced, low cost, high-efficiency processes for the production of clean energy. In addition, it is prudent to consider ways to reduce carbon dioxide and other greenhouse gases that are generated by the combustion of fossil fuels, to investigate impacts on water resources. Advanced technology development in materials to assure compatibility with advances in power systems, will be needed for these challenges – as well as innovations in fuel cells, measurements, sensors, monitors, and controls – to be commercially competitive.

Improvements are also needed in our ability to recover both oil and natural gas. About two-thirds of our national petroleum reserve is "unrecoverable"; i.e., it cannot be extracted economically by conventional means. This unused resource could play a major role in supplementing the national petroleum supply if efficient approaches were developed for improved extraction. Natural gas production and utilization could also be increased through improved characterization of reserves and through better infrastructure.

This solicitation seeks the participation of small businesses in addressing problems related to utilization of coal and natural gas to produce power, and to the recovery of oil and natural gas. Many of the topic offerings indirectly support the DOE initiative of FutureGen, a platform to demonstrate hydrogen production and carbon sequestration. The objectives of FutureGen are to produce hydrogen at \$4/MMBtu, sequester 100% of the carbon-dioxide, and produce electricity with zero emissions at less than a 10% increase in cost.

9. CAPTURE, SEQUESTRATION, AND UTILIZATION OF CARBON

The world is becoming increasingly concerned about the greenhouse effect, and CO_2 emission is a significant contributor to it. Hence, the capture and permanent sequestration of CO_2 has become a major world wide goal. In the United States, the capture and sequestration of CO_2 is expected to be an important element of any strategy implemented to reduce the emission of this greenhouse gas to the atmosphere. **Grant applications are sought only in the following subtopics:**

a. Advanced Technologies for Monitoring, Mitigation, and Verification— Monitoring, mitigation, and verification (MM&V) is defined as the capability to measure the amount of CO_2 stored at a specific sequestration site, monitor the site for leaks or other deterioration of storage integrity over time, and verify that the CO_2 is stored in a way that is permanent and not harmful to the host ecosystem. MM&V can be divided into three broad categories – subsurface, soils, and above-ground – each having its own set of needs.

Subsurface MM&V involves tracking the fate of CO₂ within the geologic formations underlying the earth and identifying possible migration to the surface. This category also includes developments to mitigate leakage, should it occur. For subsurface MM&V, grant applications are sought for technologies/approaches for monitoring and verifying subsurface sequestration options. Approaches of interest include surface-to-borehole seismic, micro-seismic, cross-well electromagnetic, electrical resistance tomography, CO₂ tracers, surface leak detection, and mineralization concepts for leakage mitigation.

Soils MM&V involves tracking carbon uptake and storage in the first several feet of topsoil and identifying potential leakage pathways into the atmosphere from the underlying geologic formation. For soils MM&V, grant applications are sought for low cost technologies that are capable of measuring carbon at one-tenth of the cost and time required to analyze samples using current methods. Systems must have a minimum detection limit of 0.1 percent carbon in soil, with an accuracy and precision of measurement of $\pm 10\%$. The soil carbon must be measured at a minimum within the top 30 cm, with measurement at 100 cm below the surface desired. The system can either take *in situ* measurements or incorporate soil sampling (soil core) techniques for later analysis. Soil sampling devices that are capable of measuring other soil properties (such as bulk density and the concentrations of soil nutrients -- e.g., phosphorus, nitrates-nitrogen, potassium, magnesium, calcium, and iron) along with the carbon will be considered to have an advantage. Because the measurement of soil bulk density may be required to determine the mass of carbon in a sample, approaches that also can improve existing methods for measuring the bulk density of soil are of interest. In field or in-situ measurement technologies are needed to reduce the cost and time of measurement to one-tenth of current methods. For bulk density measurements, the minimum detection limit should be $0.1g/cm^3$, with accuracy and precision of $\pm 10\%$.

Above-ground MM&V refers to terrestrial sequestration and involves the quantification of above-ground carbon stored in vegetation. For above-ground MM&V, grant applications are sought to develop new technologies for measuring the carbon stored in above ground vegetation on carbon sequestration projects, as well as to verify the permanence of the carbon storage. The technology must be able to reduce the costs of measuring above ground carbon stored in biomass by a factor of 10, compared to the cost of current field methods. Technologies that use remote sensing are of particular interest because they offer the most immediate potential. For trees, current methods use the diameter at breast height for estimating the amount of biomass, and subsequently the amount of carbon. New remote sensing applications may need to use other relationships such as crown diameter and height of the vegetation to estimate carbon content. Because many sequestration projects also offer the potential for forest products, technologies that are capable of providing quantitative estimates of the forest products that exist in a particular location have an advantage over those that only measure carbon storage.

b. Advanced Separation and Capture Techniques for CO_2 —Significant research and development is currently being pursued for new technologies to separate and capture CO_2 from both fuel and flue gas streams. This subtopic seeks separation/capture technologies for fuel and flue gas streams, gasification processes, and oxycombustion.

Aqueous amine absorption is the state-of-the-art technology for post-combustion CO_2 capture from flue gas. However, amine absorption has a number of drawbacks, including significant capital and operating costs. Therefore, grant applications are sought to develop alternative technologies that can substantially lower the cost of CO_2 separation from the flue gas. Among the candidate technologies, some data has already been developed for membrane separations and solid adsorbents (reference 4); therefore, these technologies are of interest along with technologies that optimize amine absorption processes. Grant applications should demonstrate familiarity with both current commercial technologies and ongoing research, discuss how the presence of minor flue gas components would affect the proposed technology, and account for the effect of flue gas conditions such as flow rate and temperature.

In a gasification processes, a carbonaceous fuel is thermally decomposed in the absence of oxygen to form a hydrogen-rich "synthesis gas" that can be converted to electrical energy through a variety of means (e.g., combustion turbine, electrochemical cell, or combined cycle). The state-of-the-art for CO_2 capture from synthesis gas is a process involving a liquid glycol solvent. The glycol is highly effective and can be used to capture both CO_2 and H_2S . However, the CO_2 is released at near atmospheric pressure and requires compression from 14-20 psi up to 2,000 psi, resulting in considerable increases in cost. Therefore, grant applications are sought to develop new technologies that can more cost effectively capture CO_2 from synthesis gas. Research areas of interest include physical sorbents, membranes, and other separation processes.

With oxycombustion, the fuel is burned in oxygen rather than air, resulting in a highly pure CO_2 exhaust that requires no separation. Unfortunately, no commercial oxygen combustion power plants are currently in operation, due mainly to the high cost of oxygen. Another barrier to oxygen combustion is energy loss due to the large quantity of CO_2 exhaust that must be recycled to the oxygen boiler to maintain combustion temperatures at a level that is compatible with boiler materials. Grant applications are sought to develop technologies to overcome these barriers to oxycombustion. Research areas of interest include oxygen transport membranes, circulating fluidized bed designs without recycle, and chemical looping.

c. Non-Carbon Dioxide (Non-CO₂) Greenhouse Gas Reduction—Until recently, efforts to understand and reduce the level of greenhouse gases have focused on carbon dioxide sequestration, more efficient use of carbon fuels, and lower carbon-content fuels. Recent publications by Hansen, et al., have shed new light on the importance of non-CO₂ contribution to greenhouse effects. Therefore, grant applications are sought to develop technology that could significantly reduce the escape to the atmosphere of two of these non-CO₂ gases: methane (CH₄) and nitrous oxide (N₂O). Areas of interest include the reduction of these emissions from oil and gas exploration and production, coal mines, landfills, refineries, rice cultivation, enteric fermentation, fertilizer utilization, manure, residue burning, biomass production and use, and other sources.

d. Breakthrough Technologies—Over the past two years the DOE's Sequestration Program has been working with the National Research Council/National Academy of Sciences in an effort to bolster the high-risk/high reward portion of the research portfolio. Accordingly, "Breakthrough Concepts" R&D is focused on the pursuit of revolutionary and transformational sequestration approaches with the potential for low cost, permanence, and large global capacity. Grant applications are sought for concepts/technologies that have the potential to provide "leap frog" performance and cost improvements compared to existing technologies. Areas of interest include: (1) the development of new chemical or biochemical processes that utilize captured CO_2 from power plants or coal gasification plants as a feedstock to produce value-added products – these processes should have the potential to utilize up to 100 million metric tons of CO_2 as a feedstock and be economically viable without parasitic energy losses; (2) CO_2 conversion (via photosynthesis processes, biological processes, or mineralization processes, etc.) to either useful products, as discussed above, or stable solids that enhance geologic sequestration; (3) chemical looping, where oxygen for combustion is delivered to the fuel via a redox agent rather than by direct air or gaseous oxygen; and (4) novel soil amendments that increase the rate at which carbon can be returned to soil.

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10. COAL GASIFICATION TECHNOLOGIES

Coal gasification offers a versatile and clean way to convert the energy content of coal into electricity, hydrogen, other high quality transportation fuels, and high-value chemicals to meet specific market needs. Most importantly, in a time of electricity and fuel price spikes, flexible gasification systems can provide a capability to operate on low-cost, widely-available feedstocks. Gasification may be one of the best ways to produce clean-burning hydrogen for tomorrow's automobiles and power-generating fuel cells. Hydrogen and other coal gases can also be used to fuel power-generating turbines or as the chemical "building blocks" for a wide range of commercial products. The Office of Fossil Energy is working on coal gasifier technology advances that enhance efficiency, environmental performance, and reliability. **Grant applications are sought only for the following subtopics:**

a. Technologies to Produce High-Value Added Products from Coal Gasification—The positive economic impact of technologies that produce high value-added products and/or materials from the coal gasification process and its byproducts would expedite the development of coal gasification. For this subtopic, grant applications are sought for novel technologies to convert coal gasification byproduct(s) into a value-added material. Of particular interest are innovative technologies that maximize the value of byproducts from inferior coal gasification feedstocks, such as high-sulfur coal, or a mixture containing at least 75% coal along with biomass and/or municipal/industrial waste. Approaches should include laboratory-scale experimentation aimed at defining the critical processes applicable to the creation of value-added materials. Grant applications should describe how the value-added material will be used and identify likely end users or markets. In addition, downstream plans for commercializing the value-added material/product should be addressed, along with how the remaining non-value-added byproducts will be handled in an environmentally-friendly manner.

b. Improved Methods for Cleanup of Multiple Contaminants—Grant applications are sought for cleaning/conditioning of the synthesis gas produced from the gasification of carbonaceous fuels in advanced power systems, hydrogen production, and chemical/liquid fuel production, at significantly reduced capital and operating cost. Proposed technologies may be conceptual or experimental, but must have the potential to remove multiple syngas contaminants to near zero limits, due both to environmental considerations and to prevent fouling of downstream equipment and/or catalysts. Contaminants of interest are Hg, As, Se, Cd, NH₃, and Cl. Process conditions of interest include temperatures from 400°F to 700°F and pressures from 300 to 1000 psi.

Of particular interest are multi-contaminant control concepts that result in a significant reduction in the number of unit operations and processes. All approaches must be economically attractive and minimize loss of, but preferably increase, overall system efficiency.

c. Novel Concepts in Air Separation (Non-Cryogenic)—Oxygen is the third largest commodity chemical in the U.S., with an annual market over \$2B. However, the high cost of oxygen has been a barrier to the widespread application of oxygen-enriched combustion and oxygen-blown gasification in coal-fired power plants. Grant applications are sought to develop new concepts for the non-cryogenic separation of oxygen from

air at temperatures ranging from ambient to 900°C. Some approaches of interest include the development of: (1) novel membrane compositions including, but not limited to, inorganic, ceramic, or porous materials or a combination thereof – approaches may include first producing oxygen-rich air, followed by cost-effective separation of the oxygen to commercial purity by a different technique; (2) oxidation-reduction approaches using appropriate oxygen carriers, including new approaches for enhancing the intrinsic oxygen storage capacity of candidate carriers; (3) catalytic porous substrates for depositing thin-films of oxygen conductors, in order to improve oxygen separation flux; and (4) advanced oxygen storage materials that are mechanically stable through thermal and pressure cycles, in order to improve the performance of the chemical looping technique. Grant applications must describe the potential economic advantage of the proposed technology over conventional cryogenic air separation processes.

d. Novel Gasifier Concepts—Current commercial gasification systems, based on concepts developed many years ago, use steam gasification at high temperature and elevated pressure to produce a mixture of hydrogen and carbon monoxide. Unfortunately, many problems remain. The high temperatures cause significant materials problems. The elevated pressure makes solids feeding difficult: lock hoppers are expensive and often problematic. The need to use water slurry feed systems to smoothly carry the coal into the gasifier results in efficiency losses, but is a common feed mechanism because its reliability is critical for profitable gasifier operation (a problem exacerbated with low ranked coal because of its high water content). Overall, these processes are mechanically complex, leading to high capital costs, long construction times, and significant downtime for repairs. To make matters worse, the syngas from current commercial gasification systems is contaminated with trace metals and small amounts of such gases as hydrogen cyanide, hydrogen chloride, nitrogen, sulfur, and even carbon dioxide. To address these problems, grant applications are sought to develop: (1) gasifier feed systems. Grant applications also are sought to develop gasifiers that produce syngas with high hydrogen or methane content; such fuels would help meet the needs of the hydrogen economy and will be more directly compatible with fuel cells.

Finally, grant applications are sought to develop small gasifiers with less than 100 MWe equivalent capacity, or to improve the economics of existing small scale gasifiers. Smaller gasifiers can be used to meet the needs of distributed generation and allow the use of opportunity fuels that exist in smaller quantities in some locations. Designs for small scale systems must address the loss of economy-of-scale advantages and consider the overall economics for these small scale power and/or poly-generation applications.

For this solicitation, gasifiers must use coal for at least 75% of their fuel input. Grant applications submitted under this subtopic should include carefully crafted laboratory-scale experimentation aimed at defining the critical processes that control the proposed gasification concept. Applications must describe how successful development will result in lower cost and more efficient gasifier operation, compared to conventional systems.

- Gasification Technologies, U.S. Department of Energy (DOE), National Energy Technology Laboratory Web site. (<u>http://www.netl.doe.gov/coalpower/</u>. In the circle at the center of the page, select "Gasification Technologies.")
- 2. *Gasification Technology R&D*, U.S. DOE Office of Fossil Energy Web site. (http://fossil.energy.gov/programs/powersystems/gasification/)
- 3. *Carbon Capture* Research, U.S. Department of Energy, Office of Fossil Energy Web site. (<u>http://fossil.energy.gov/programs/sequestration/capture/</u>)

- "FutureGen A Sequestration and Hydrogen Research Initiative," U.S. Department of Energy, Office of Fossil Energy, February 2003. (<u>http://fossil.energy.gov/programs/powersystems/futuregen/futuregen_factsheet.pdf</u>)
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- Browning, G. J., et al., "The Effects of Heterogeneous Slag Character on Viscosity and Slag Flow in IGCC Gasifiers," *International Flame Research Foundation Combustion Journal*, Communication No. 199901, December 1999. (ISSN: 1562-479X) (Full text available at: <u>http://www.journal.ifrf.net/199901browning.html</u>.

11. ENVIRONMENTAL TECHNOLOGY AND SUPPORT FOR EXISTING FOSSIL ENERGY FACILITIES

The use of coal in energy utilization and conversion systems suffers from a number of considerations with respect to the fuel itself. Coal is a solid fuel containing components that are precursors of environmental pollutants or materials that are potentially damaging to downstream components. Further, coal contains mineral matter that is converted into ash, which can lead to suspended particulates in air, erosion of or deposition in downstream components, and problems of solid waste disposal. This topic seeks to mitigate the environmental disadvantages of coal utilization, including its potential impact on water quality and availability, through improvements in various aspects of the coal utilization cycle. The research is expected to provide high-quality scientific information on present and emerging environmental issues for use in regulatory and policy decisionmaking. Environmental considerations and the concomitant need for low-cost compliance options are the primary drivers of the current research program.

In addition, this topic addresses two other requirements for coal power systems: (1) the use and disposition of by-products from coal combustion and gasification, and (2) the further development of micro-sensors that can withstand the harsh conditions of advanced power generation systems. **Grant applications are solicited only in the following subtopics:**

a. Continuous Measurements of Mass Concentration and Chemical Composition of Primary PM 2.5 Emitted from Coal-Fired Utility Boilers—Continuous (or near-continuous) emission monitors (CEMs) for primary PM 2.5 (particulate matter with an aerodynamic diameter less than 2.5 µm) mass and composition would be more desirable than filter-based methods. However, due to continuing concerns over the complexity, high cost, and uncertain field reliability of these monitors, they have not been readily adopted by the utility industry. Furthermore, currently-available CEMs for PM 2.5 mass are expected to perform even less reliably in the cooler, moister conditions characteristic of flue gas released from wet flue gas desulfurization (FGD) systems. Technology for continuously measuring the chemical composition of primary PM 2.5 emissions from exhaust stacks is even less well-developed; none of the prototype instruments designed for this purpose have been applied to coal-fired utility boilers. Therefore, grant applications are sought to identify novel concepts and technologies for measuring, in near-real-time, the mass concentrations and chemical composition of primary PM 2.5 emitted from coal-fired utility boilers with and without wet FGD systems. Proposed concepts and technologies must demonstrate the promise of being more reliable and more cost-effective than currentlyavailable CEMs for PM 2.5 mass and composition measurements. It also should be noted that experimental dilution sampling devices and plume aging chambers have already been developed to simulate the changes in PM 2.5 mass and composition that may occur within the boiler exhaust plume. Therefore, proposed concepts and technologies may be designed for use with or without the use of such devices; however, grant applications that further refine or develop sampling protocols for dilution samplers or plume aging chambers are not of interest, nor are grant applications that seek to further refine or develop existing PM 2.5 CEMs.

b. Water Usage in Electric Power Production—Power generated from fossil fuels is dependent on water. On average, approximately 21 gallons of water are required for each kWh of power produced. Thermoelectric power production uses approximately 195 billions of gallons of water per day. In power generation, the largest single use of water is for cooling the low-pressure steam from the turbine. Under the Clean Water Act, section 316(b), the EPA has developed new regulations to reduce this cooling usage of water and improve cooling water intake structures. Research opportunities exist for reducing or eliminating the need to use water for cooling purposes. Air has been considered as an alternative, but air-cooled systems (sometimes referred to as dry systems) can have associated capital-cost and energy-inefficiency penalties, particularly in retrofit applications. Non-potable water is another option for cooling purposes, but there may be negative impacts on existing cooling towers. Other water-related issues associated with power plants involve their wastewater streams, including cooling tower blow-down water and flue gas desulphurization wastewater; these waste streams are often large volume, low concentration waters that are expensive to treat on a per-contaminant basis. Therefore, grant applications are sought to identify novel concepts and technologies to reduce both the amount of water used in coal power generation and the potential impact on water quality. Grant applications must be directed toward one of the following areas of interest: (1) reducing the amount of water used in power generation, (2) water quality improvements in power generation, (3) improvements in wet or dry cooling towers, (4) novel, low-cost treatment technology to allow for the use of wastewater as process water in power plants, or (5) novel, low-cost treatment technologies for power plant wastewater.

c. High Volume Utilization of Coal Combustion By-Products—More than half of the electricity generated in the U.S. is produced by coal-fired facilities. In January of 2004, the EPA published draft regulations to control mercury emissions from coal-fired electric utilities. One of the proposed technologies to control mercury involves the addition of activated carbon to the flue gas. The activated carbon would be collected with the fly ash via electrostatic precipitators or fabric filters. Currently, fly ash is considered a non-hazardous material for disposal; however, the increased levels of mercury, from the addition of activated carbon to the fly ash could change this status. Preliminary research suggests that the addition of activated carbon to the fly ash could make the fly ash unmarketable or increase the cost of disposal. Simultaneously, the EPA published another draft regulation, it is anticipated that more units will be equipped with flue gas desulfurization (FGD) technology. In fact, FGD production in the U.S. may increase by an order of magnitude to almost 200 million tons, thus exceeding the production of all other coal combustion products.

In the wake of these regulations, grant applications are sought to: (1) develop novel high volume utilization technologies for fly ash that contains very high concentrations of either unburned or activated carbon from mercury control technologies, and (2) develop high volume utilization technologies of flue gas desulfurization materials in novel applications (excluding wallboard production).

d. Engineering Needs for Micro Sensors in Coal-Based Power Systems—The DOE, along with other government agencies and sensor developers, have put forth a significant effort to develop micro-electric-mechanical-systems-based and other types of micro-sensors for measuring physical parameters (pressure, temperature, strain, etc.) and detecting gases in coal-based power systems. Research and development has focused on sensors for high temperature (300-1000 °C), harsh environments (strongly reducing or oxidizing conditions, particulates, etc.) The micro-gas-sensor development has focused on common fossil fuel exhaust species (e.g., O₂, CO₂, H₂, CO, NO, NO₂, SO₂, etc.) Many of these types of prototype sensors are progressing to the point where long term or large scale testing is necessary to assess their commercial viability. Much of the effort has been expended on how to best package and protect the micro-sensors from harsh environments while allowing the sensor to be exposed to the gas stream in a quasi *in situ* approach. Therefore, grant applications are sought to develop a standard, engineered testing package, with an integrated protective housing, for applying micro-sensors in high temperature harsh environments. Interested applicants should focus on one type of fossil fuel power system, including coal-fired boiler systems and coal gasification systems, so that the design

meets the specifications and requirements of that system, which may include temperature ranges and fluctuations between 300 and 1000 °C, pressures up to 350 psig, and high concentrations of particulates. Packaging designs must consider proper selection of high temperature materials, appropriate size, ease of installation through standard process ports or couplings, ease in accessing or replacing the micro- sensors, adequate gas conditioning and particulate removal, high temperature electronics, provision for power input, provision for signal output, and provision for temperature and pressure control.

Descriptions of the coal-based power systems can be found at <u>www.netl.doe.gov</u> and descriptions of a select number of ongoing micro-sensor projects that could be potential candidates for testing are also listed on National Energy Technology Laboratory's (NETL) website.

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<u>http://www.netl.doe.gov/cctc/resources/library/bibliography/misc/bibm_cwbu.html</u>. Scroll halfway down page to citation, "C. J. Moretti...".)

- 8. Choudhry, V. and Hadley, S., "Utilization of Lightweight Materials Made from Coal Gasification Slag," *Advanced Coal-Fired Power Systems '96 Review Meeting, Morgantown, WV, July 16-18, 1996.* (Available in PDF at: <u>http://www.netl.doe.gov/cctc/resources/library/bibliography/misc/bibm_cwbu.html</u>. Citation is two thirds of the way down page.)
- Hassett, D. J., "Current Practices and Issues for Placement of Coal Combustion By-Products in Mine Settings," presented at the Western Region Ash Group 2nd Annual Coal Combustion Products (CCPs) Forum: CCP Utilization in Mining Applications, Scottsdale, AZ, August 17, 1999. (Full text of paper available via: <u>http://www.undeerc.org/carrc/firstsearch/abstract.asp?abstractid=180</u>)

Subtopic d: Engineering Needs for Micro Sensors in Coal-Based Power Systems

10. The 2002 NETL Sensor and Control Program Portfolio Review and Roadmapping Workshop, [Pittsburgh, PA, October 13-14-2002]: Workshop Proceedings. (Full text available at: http://www.netl.doe.gov/publications/reports/2002/ISCS%20Workshop%20Proceedings.pdf)

12. OIL, TAR SANDS, AND OIL SHALE TECHNOLOGIES

The DOE seeks innovative methods and concepts that will contribute to more efficient and economic processes for the recovery and utilization of oil, tar sands, and oil shale. Much of the known reserves of oil in the U.S. cannot be recovered by conventional means, and advanced technologies will be required for extraction. With respect to oil, new technology approaches are needed for drilling and refining. For tar sands and oil shale, new technology is needed to cleanly extract and treat the organic material. **Grant applications are sought only in the following subtopics:**

a. Lost Circulation Material in Drilling—When drilling for oil and gas, it often happens that the drill pipe gets stuck in the borehole; millions of dollars a year are expensed due to stuck pipe. A common reason for a stuck drill pipe is a condition called "lost circulation," which occurs when the pressure in the borehole exceeds the rock formation pressure. Usually these formations are very porous, and at the moment of lost circulation, drilling fluid is forced into the rock. In extreme circumstances, hundreds of barrels of drilling fluid can be forced into the rock, which can often cause permanent fractures. In addition to the pipe sticking to the borehole wall, the adverse effects of lost circulation include the creation of a fractured weak rock zone that constantly causes drilling problems, the loss of expensive drilling fluid, and borehole cave-ins. Another dangerous effect is that, due to the loss of hydrostatic pressure in the borehole, a high pressure zone may cause flow into the borehole, resulting in a "kick" or "blowout." Although numerous commercial products, circulated into the borehole through the drill pipe, exist to plug the porous lost circulation zones, grant applications are sought to develop new or improved methods of plugging lost circulation rock formations because methods and techniques are insufficient to properly perform the job.

b. Small Bore "Microhole" Drilling—"Microhole" technologies, which use portable drilling rigs with a smaller footprint and lower environmental impact, are being developed to benefit the small driller. Some specific advantages of microhole drilling are: (1) equipment is smaller (microdrilling systems could occupy a space roughly 1/20th that of a typical rig) and weighs less (less than one tenth as much) than conventional systems, reducing equipment costs (by up to 90 percent) and manpower to operate equipment; (2) materials required for drilling and well completion are reduced; (3) the use of coiled tubing saves time and money because it requires fewer trips in and out of the wellbore, compared to conventional drilling techniques; (4) volumes of drilling fluids and cuttings can be reduced by one-fifth, reducing disposal costs; and (5) drill rigs

and associated equipment have smaller footprints, reducing environmental impact and making the system particularly advantageous when operating in environmentally sensitive areas. When holes this small are used for exploration – for example, to locate the best prospects for producing natural gas from coal beds – it may be possible to reduce drilling costs by a third or more. When used for field development, microholes may be less than half as expensive as conventional wells. Grant applications are sought to develop innovative production and completion equipment, based on microhole technologies, in drilled wells that use coiled tubing. Of particular interest are approaches that provide for a high penetration rate for downhole drilling systems suitable for coiled tubing.

c. Oil Refining Capacity—Refinery capacity is an increasing concern for the U.S., and recent gasoline prices have brought this issue into focus for the consumer. In introducing his energy policy, President Bush noted that the refining industry is operating at capacity:

"We are not just short of oil, we're short of the refineries that turn oil into fuel. So while the rest of our economy is functioning at 82 percent of capacity, our refineries are gasping at 96 percent capacity. A single accident, a single shutdown can send prices of gasoline and heating oil spiraling all over the country. The major reason for dramatic increase in gasoline prices today is the lack of refining capacity."

Because of the historical low return on investment, most of the research in refining has focused on problem solving and trouble-shooting. Relatively little research has addressed new refining technology, especially with regard to the heavy, sour crude oil found in the Western Hemisphere, which requires more intensive processing. It is important that our refineries be able to use the heavy oil from these secure sources. This subtopic focuses on innovative approaches to petroleum conversion processes that could lead to a step-change in refining, rather than the process optimization that is now being done by industry. Only those projects that would lead to a step-change in the ability to refine heavy crude oil will be considered.

Refineries are increasingly being forced to start with poorer quality, heavier crudes due to decreasing volumes of higher quality, light crudes. The U.S. has 105 billion barrels of heavy oil; yet, only about 4 billion barrels have been produced. There are also extensive reserves of heavy oil in the rest of the hemisphere. Being able to easily process heavy crude oil or the higher boiling cuts of the less heavy crudes would give refineries more flexibility in their choice of feedstock. Therefore, grant applications are sought for innovative chemical or physical refining processes that could enhance the use of domestic and Western Hemisphere heavy, sour crude oil.

Another issue with oil refining is that EPA regulations are requiring lower sulfur levels in both gasoline and diesel. Although desulfurization processes/catalysts are available, they result in a lower octane product. Because octane levels are critical to gasoline performance, it would be highly beneficial to have a process to remove sulfur without reducing octane. Therefore, grant applications are sought for new processes/catalysts that would economically remove sulfur from gasoline without octane loss.

d. Tar Sands and Oil Shale Development—The U.S. has a huge resource in tar/oil sands, 40 - 76 billion barrels. However, these sands must be rigorously treated for conversion into an upgraded crude oil before they can be used by refineries to produce gasoline and diesel fuels. While conventional crude oil flows naturally or is pumped from the ground, oil sands must be mined or recovered *in situ*. Oil sands recovery processes include extraction and separation systems to remove the bitumen from sand and water. The resulting bitumen and syncrude produced is high in naphthenic acids, chlorides, and nitrogen levels. These constituents pose problems in both corrosion control and catalyst poisoning which can limit their acceptability in a refinery. Grant applications are sought to develop:

(1) A cost-effective, environmentally benign separation process to extract bitumen from oil sands (with very low fines carryover) and leave clean sand that rapidly dewaters or dries to a solid mass, permitting the rapid revegetation of mined areas in months rather than decades. If a water-based bitumen extraction system is used, it should have low organics carryover and should not flocculate the clays. If an organic-based system is used, it should rapidly coagulate and drain without excessive volatiles that would exceed air quality standards for the area. In addition, the organic bitumen phase (with or without an organic diluent) should have minimal fines carryover for water washing (desalting) and further processing/upgrading to liquid fuels or asphalt.

(2) A process to remove chlorides and/or nitrogen from either the oil sand bitumen or the refined syncrude.

(3) An economical process to remove and treat the naphthenic acids in the water generated by the extraction or upgrading of bitumen.

The U.S. also has billions of barrels of oil shale (the "shale" is usually a relatively hard rock). In 2004, U.S. DOE published two summaries of The Strategic Significance of America's Oil Shale Resource, Vol. I, Assessment of Strategic Issues, and Vol. II, Oil Shale Resource Technology and Economics." These two volumes summarize the world's oil shale industry and challenges. Grant applications are sought to develop:

(1) Cost-effective, environmentally low-impact separation processes to extract kerogen, the organic material in oil shale, with high yield. Any process should have very low fines carryover into the organic phase and should leave clean "spent shale" that rapidly dewaters, thus permitting rapid re-vegetation of mined areas (in months rather than decades). Also, the system should not leave hot molten spent shale for surface disposal. If an organic/gaseous-based surface extraction system (super-critical extraction) is used, the organic phase must be free of fines, and the processed shale/sands must rapidly consolidate and have low organics carryover. Also, if the extraction system yields a fines-free organic phase, the processed shale/sands must rapidly consolidate with a low organics carryover.

(2) Processes to upgrade the kerogen phase (with or without a diluent) for transport to processing/upgrading. The organic product must have minimum fines carryover for pipeline transport.

(3) Cost-effective, environmentally benign processing/upgrading technology for conversion of kerogen or diluted kerogen to marketable transportation fuels that are fungible with petroleum based transportation fuels. The processing/upgrading can be in combination with the extraction step, wherein separate streams are recovered from the extraction and transported individually for further processing/upgrading and conversion to marketable transportation fuels. Also, the processing/upgrading should use the entire kerogen stream and extract select components before processing/refining into marketable transportation fuels.

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- "Strict Environmental Regulations Compel Petroleum Refiners to Opt for Sophisticated Catalytic Processes," Frost & Sullivan, July 7, 2004. (Full text available at: <u>http://www.frost.com/prod/servlet/press-release.pag?docid=20230869</u>)
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13. NATURAL GAS AND HYDROGEN SEPARATION TECHNOLOGIES

The DOE seeks innovative methods and concepts that will contribute to more efficient and economic processes for the recovery, delivery, and utilization of natural gas. Much of the known reserves of natural gas in the U.S. cannot be recovered by conventional means, and advanced technologies will be required for extraction. The utilization of natural gas can be further enhanced by new technology for storage and delivery. In addition, because of the adoption of hydrogen as fuel in many advanced applications, this topic addresses the extraction (or production) of hydrogen from natural gas. **Grant applications are sought only in the following subtopics:**

a. Natural Gas Sustainability—To prolong the sustainability of the natural gas supply over the longer-term, dramatic increases in production from deep (>20,000 ft.) reservoirs will be required. Toward this end, Deep Trek, a program addressing technical issues associated with deep drilling, is working to provide fundamental advances in high-temperature, high-pressure materials and electronics that will enable the construction of durable deep drilling and completion tools. With respect to drilling fluids, completion fluids, and cements, grant applications are sought for: (1) advanced technologies for well control and hole stability with little or no damage to target formation or pass through formations; (2) new concept-changing, non-damaging drilling fluids (smart fluids); and (3) novel cements that can economically replace Portland. Grant applications also are sought for: (4) advanced unconventional completion techniques, materials, and fluids for high temperature, high pressure deep tight gas formations; (5) materials and metallurgy tubulars and tools, especially suited to handle caustic (H₂S, CO₂, etc.) gas resources; (6) advanced motors and drilling systems; and (6) rechargeable batteries and high temperature capacitors. All technology developments must be capable of operation in high temperature (>225°C), high pressure (>20,000 psi) environments.

b. Natural Gas and Liquefied Natural Gas (LNG) Storage—The current distributed electricity generation model in the U.S. is designed to provide emergency and stand-by power to minimize the impact of electricity outages. This service is dominated by diesel generating equipment because of the need for on-site fuel storage. Penetration into this market by mini-turbine and fuel cell systems, which not only could provide emergency/stand-by service but also could contribute to base loads and peak needs, will require safe and efficient means of storing natural gas. On-site natural gas storage would provide protection against electric utility outages and supplement the natural gas arriving via the servicing pipeline during periods of peak demand or at times of low pipeline pressure or availability. Therefore, grant applications are sought to develop and evaluate technology for safe and efficient small-scale, on-site storage of natural gas or LNG for distributed electricity generation. Partnering with industry is encouraged. Applicants are encouraged to review related information on the National Energy Technology Laboratory (NETL) Website at http://www.netl.doe.gov/scng/index.html.

c. Natural Gas Delivery Reliability—Maintaining the integrity and reliability of the natural gas distribution and transmission systems across the U.S. is essential to ensure the availability of clean, affordable energy for homes, businesses, and industries. Natural gas consumption in the U.S. is projected to reach or exceed 31 trillion cubic feet (TCF) per year by 2025, increasing from 22 TCF per year in 1997, and this increase will require not only that the existing natural gas infrastructure be maintained but also that it be expanded. LNG imports are expected to play an increasing role in meeting the Nation's demand for natural gas. DOE's NETL, through the Strategic Center for Natural Gas (SCNG), implements a program, Delivery Reliability for Natural Gas, to provide research and development for maintaining and enhancing the integrity and reliability of the Nation's gas transmission and distribution network. Grant applications are sought to develop: (1) advanced non-metallic pipeline materials (although some metallic constituents would be acceptable), capable of containing higher pressures (above 300 psi) and suitable for fabrication into pipes from 6 to 20 inches in diameter; (2) sensors that can be incorporated into or onto the pipe and can detect unauthorized right-of-way intrusion prior to pipeline damage; (3) improved technologies or tools for repair of damaged pipe – both metallic (i.e., steel) and non-metallic (i.e., polyethylene) – that are suitable for small openings, meaning "keyhole" or "micro-excavation" technologies; or (4) devices to rapidly, accurately, and inexpensively characterize the composition of pipeline gas to determine gas quality.

Applicants are encouraged to review the document "Pathways for Enhanced Integrity, Reliability and Deliverability" (available on the NETL website at <u>http://www.netl.doe.gov/scng/publications/t&d/naturalg.pdf</u>) and the update to that document "Roadmap Update for Natural Gas Infrastructure Reliability" (at <u>http://www.netl.doe.gov/publications/proceedings/02/naturalgas/driscoll.pdf</u>), which summarizes a NETL-sponsored road mapping session to identify priority research needs for the natural gas pipeline infrastructure.

d. Conversion of Natural Gas to Hydrogen—U.S. demand for hydrogen is now about 9 million tons per year [reference 6] and is anticipated to greatly expand as the Nation moves toward a hydrogen economy. Currently, the principal uses of hydrogen include petroleum refining and manufacture of nitrogen fertilizers. As a primary hydrogen source, many refineries rely on the hydrogen that is a byproduct from naphtha catalytic reformers. Supplemental hydrogen, as well as hydrogen used in fertilizer and petrochemical manufacturing, is produced primarily from the catalytic steam reforming of natural gas. Natural gas, which has a favorable hydrogen to carbon ratio (4:1) compared to coal (0.7:1) or biomass (1:1), is the most affordable near term resource for producing large amounts of hydrogen. Current commercial technology, steam methane reforming, produces hydrogen from methane at a cost of \$5.54/MM Btu, with a feed natural gas price of \$3.15/MM Btu. This figure does not include the costs of carbon sequestration, which is the major driving force toward a hydrogen production must be reduced.

Current DOE and industry funded research is developing technology that will simplify the production of hydrogen from natural gas by combining two steps – air separation to produce oxygen and partial oxidation of natural gas to produce synthesis gas – into one, leading to lower costs and increased efficiencies. Also, membranes to separate hydrogen from hot synthesis gas are being developed. The goal is to reduce the cost of hydrogen production from natural gas by 25% over the next ten years. This is a considerable task, since, over a period of decades, the petroleum and chemical industries have optimized the current technology on an operating and capital cost basis.

Grant applications are sought to develop new, non-microbial, technologies for the production of hydrogen from natural gas. Cost effectiveness, compared to currently available hydrogen production technologies [references 7 and 8] must be demonstrated. The process must produce hydrogen at lower cost (both capital and operating) and higher efficiency than steam reforming technology. Hydrogen production processes that also enable the separation of carbon (as carbon dioxide or elemental carbon) are of particular interest. Other areas of interest include catalysis (syngas and/or water-gas shift), separation processes, and reactor systems.

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14. SOLID OXIDE FUEL CELL (SOFC) AND MATERIAL RESEARCH

The goal of the DOE-sponsored Solid State Energy Conversion Alliance (SECA) is to develop commerciallyviable (\$400/kW) 3 to 10 kW Solid Oxide Fuel Cell (SOFC) systems by year 2010. SOFC power generation systems are attractive alternatives to current technologies in diverse stationary, mobile, and military applications. SOFC systems are very efficient, from 40 to 60 percent in small systems and up to 85 percent in larger co-generation applications. The electrochemical conversion in a SOFC takes place at a lower temperature (650 to 850°C) than combustion-based technologies, resulting in decreased emissions – particularly nitrogen oxides, sulfur oxides, and particulate matter. These systems all offer fuel flexibility as they are compatible with conventional fuels such as hydrogen, coal, natural gas, gasoline, or diesel. Despite these advantages, advances in balance of plant (BOP) component design must be developed before the SECA program goal can be realized. This topic seeks to develop these key support technologies for SOFC systems.

Grant applications are sought only in the following subtopics:

a. High-Temperature Anode Gas Recycle Blowers—SOFC systems that incorporate some recycling of the anode exhaust gas, which is mixed with incoming fresh fuel prior to entering the pre-reformer, have a higher efficiency and offer the potential for lower overall system cost. Grant applications are sought for the design and development of motor-driven blowers for the recycle of SOFC anode exhaust gas, with cost, manufacturability, and reliability being critical factors for meeting the SECA Program goal. The blower inlet gas temperature may vary from 600 to 850°C and the inlet pressure is atmospheric. The pressure rise requirements is 4 to10 inches of H₂O and the flow requirement is 100 standard liters per minute (slpm), which is nominally composed of 46 slpm H₂O, 27 slpm CO₂, 20 slpm H₂, and 7 slpm CO. Overall efficiency should meet or exceed 40% under the aforementioned operating conditions. The unit should be capable of variable speed control with a flow turndown ratio of 5 to 2. The blower unit must have a design life of 40,000 hours, with a 100% duty cycle and 10,000 hour maintenance interval. The unit must be able to tolerate at least 30 thermal cycles, between operating and room temperatures, over its design life. The unit cost, based upon a production volume of 50,000 units per year, should be estimated and is considered a higher priority than efficiency.

b. Low-Cost High-Temperature Heat Exchangers for SOFC Systems—The high-temperature heat exchangers used in SOFC are attracting increasing attention because of their adverse impact on overall SOFC system cost. The operating temperatures of these heat exchangers depend upon the fuel cell application, and range from 25 to 800°C on the sink side and from 300 to 1000°C on the source side, which is usually the fuel cell stack effluent. Grant applications are sought to develop novel, low-cost, high-temperature heat exchanger designs that address the cost issues and technical performance requirements for two distinct applications of SOFC systems: (1) where the sink side is an air preheater; and (2) where the sink side is a natural gas fuel preheater.

Where the sink side is an air preheater, the heat exchanger requires a very low differential pressure drop (<4-10 inches of water column on the air side; 3-5 inches on stack side), high effectiveness (approaching 90%), and long life (10,000 hour maintenance interval/40,000 hour lifetime). Although material sets such as high nickel alloys (i.e., 600 series Inconels) are currently being used, they are very expensive and prone to long term high temperature creep and sulfidation attack.

In the application where the natural gas fuel preheater is on the sink side, the concern is that the fuel stream contains up to 50 ppm of sulfur and small amounts of SO_2 in the stack effluent. Currently, shell and tube or plate fin exchangers are being used for this application. However, ceramic materials would be considered a candidate, provided that the thermal shock/ramp rate can be adequately addressed.

c. 1 to 5 kW Diesel Reformer—SOFC systems should have a strong early market in Class 8 diesel trucks in the form of auxiliary power units (APUs), which allow for on-board power while the vehicle engine is off. In the near term, the choice of fuels for these applications will focus on diesel liquid fuels because of their availability, low cost, and existing distribution networks. However, commercially-available hydrocarbon-based liquid fuels such as diesel must be reformed in order to achieve the desired gas compositions (consisting of hydrogen, carbon monoxide, and moderate levels of methane (< 10 mole %)), required for acceptable SOFC electrochemical performance. Therefore, grant applications are sought to develop innovative, low-cost, compact, and reliable reforming technologies to meet this requirement, including integrated plasma-assisted partial oxidation, catalytic partial oxidation (CPOX) or autothermal (ATR) diesel reformers. Designs must explicitly address and include the diesel injection system, mixing chamber, reactor vessel, and catalyst bed. Additional design requirements include: (1) operation within the temperature range 600 to 1000 °C; (2) turndown capability maximized and limited to not less than 4 to 1; (3) pressure drops below 1 psi, throughout the device; (4) minimal water usage; and (5) maximum carbon suppression. Also, practical APU SOFC system applications require fast start-up, processed fuel reformate availability to accommodate power demand

transients, and the ability to accommodate part-load operation – all with minimal hydrocarbon (preferably methane) slip.

Catalyst-based reformers, which mostly operate in the temperature range 700 to 900°C, carry their own set of issues. In an ATR or CPOX reactor, where the fuel is sprayed into preheated steam and/or air, the fuel must be mixed as a vapor before entering the catalyst. Great care must be taken when exposing the diesel fuel to the catalyst surface, in order to avoid cracking and pyrolysis reactions that can lead to carbon deposition. (The high vaporization temperature of the heavy hydrocarbon compounds present in diesel fuel favors pyrolysis and carbon deposition in the preheat zones of the reactor.) Preventing this carbon formation, as well as autothermal ignition, requires that the local steam-to-carbon (S:C) and oxygen-to-carbon (O:C) ratios be maintained within a given range. Failure to uniformly mix the fuel with the air and/or steam prior to entering the reactor can result in hot spots, carbon fouling of the reactor, and deactivation of fuel reforming catalysts via localized carbon deposition. Finally, the diesel reformer catalyst itself must be able to handle up to 50 ppmv of sulfur in the fuel without sulfur poisoning and provide stable, long-term operation (> 5,000 hours) before maintenance is required.

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15. MATERIALS RESEARCH

New materials ideas and concepts are required to significantly improve performance and reduce the costs of existing fossil systems or to enable the development of new systems and capabilities. The Fossil Energy Materials Program conducts research and development on high-performance materials for longer-term fossil energy applications, including gas separations and storage. The program is concerned with operation in the hostile conditions created when fossil fuels are converted to energy. These conditions include high temperatures, elevated pressures, corrosive environments (reducing conditions, gaseous alkali), and surface coating or fouling. **Grant applications are sought only in the following subtopics:**

a. High Temperature Electrolysis, Hydrogen Separation, and Storage Materials—Applications of high temperature electrolysis range from small natural gas systems to hydrogen units for automotive fueling stations to large electrolyzers for use in conjunction with nuclear power. The development of high temperature electrolysis systems could be efficiently accomplished using traditional solid oxide fuel cell (SOFC) architectures. Although some differences, such as electrode materials, do exist between SOFCs and high temperature electrolyzers, the development is expected to be synergistic. One area of concern in all of these systems is the sealing of the hydrogen collection area. Grant applications are sought to develop and

demonstrate a high temperature electrolysis system based on solid-oxide fuel cell technology and architecture. The work should proceed from concept demonstration to small system demonstration. Technology development projects also will be considered.

Hydrogen separation membranes are critical supporting technologies for next generation power systems. Two types of membranes are being investigated for the recovery of hydrogen from coal gasification streams: membranes which are selective for hydrogen and membranes which are selective for carbon dioxide. Grant applications are sought to further the development of either or both types of these membranes for commercial hydrogen production.

For hydrogen membranes, approaches should have the potential to meet or exceed the targets outlined in the table below. Because the proposed membrane type may differ from that used to develop this target table, the hydrogen separation membrane system should aim for: (1) a high flux rate; (2) low cost; (3) improved durability; (4) low parasitic power requirements; and (5) low membrane fabrication costs.

Characteristics	Units	Status	Target
Flux Rate	scf/hr-ft2	60	200
Cost	\$/ft ²	150-200	<100
Durability	Hrs	<1,000	100,000
Operating Temp	оC	300-600	300-600
Parasitic Power	kWh/	3.2	<2.8
	1,000 scf		

HYDROGEN-PERMEABLE MEMBRANE SEPARATION TARGETS

 CO_2 -selective membranes are another way to concentrate the hydrogen on the high-pressure side of the separation device. A novel material that appears to have the potential to accomplish this type of separation consists of carbon nanotubes. CO_2 is adsorbed on nanotubes in special configurations, allowing separation from H_2 . However, other separation systems may provide cost-effective means of leaving hydrogen on the high-pressure side of the system. Grant applications are sought to develop systems that will separate carbon dioxide from the exit stream of a water-gas shift reactor. Proposed approaches must demonstrate that the hydrogen left on the high-pressure side of the separation system can be produced in large quantities and at high purity. Also, proposed approaches should include simulations, experiments to measure isosteric heats of adsorption, and the characterization of binding sites and energies.

Another critical need is the development of materials for hydrogen storage as a necessary precursor to the eventual implementation of the hydrogen economy. There are several advantages to using hydrogen over carbon fuels for transportation applications. First, the chemical energy per unit mass of hydrogen is higher than that for liquid hydrocarbons. Secondly, the combustion of hydrogen with oxygen or the electrochemical reaction of hydrogen with oxygen in a fuel cell eliminates carbon emissions. Therefore, grant applications are sought to develop materials that provide high hydrogen storage density and stability at commercially relevant conditions of temperature and pressure. The materials currently being investigated for hydrogen storage include metal organic frameworks; alloys and intermetallics; sodium and lithium alanates; nanocubes; carbon nanotubes; and other emerging materials. These materials should have the potential for achieving DOE's long-term hydrogen storage goal of 3 kWh/kg (9 wt %) at a cost of \$2/kWh. The materials to be investigated must be amenable to realistic processing conditions and to the likelihood of large-scale manufacturing. For practical transportation applications, the hydrogen storage material must function in the temperature range of 0-100°C and pressure range of 1-10 bar.

b. Nanotechnology for Coatings in Coal-Fired Environments—In fossil energy power generation applications, where sulfur and water vapor can cause severe oxidation problems, typical examples of surface damage include: (1) accelerated high-temperature fire-side corrosion associated with the presence of molten alkali-containing salts: (2) accelerated medium-temperature fire-side corrosion associated with the presence of a low oxygen activity environment and sulfur; and (3) steam-side oxidation of tubing, piping, and valves in fossil fuel-fired boilers. In order to achieve higher operating temperatures, the corrosion resistance of Fe- and Nibased alloys must be improved. Grant applications are sought to develop nanotechnology approaches to protective coatings and coating techniques for the Fe- and Ni-based alloys, and for nickel-based superalloys as well. At least one ferritic and one austenitic alloy should be selected as substrate materials for study. The coatings must provide superior corrosion resistance in oxidizing, sulfidizing, carburizing, and water-containing environments, and should show adhesion on the substrate (the tube outsides) as well as slide- and anti-stickproperties on the surface at the same time. The protective coatings and coating techniques should be optimally designed as part of the overall power generation system, should be maintainable, and should be capable of nonintrusive evaluation to determine remaining life. To this end, model coatings should be fabricated for corrosion testing and diffusion studies, in order to provide sufficient data to evaluate lifetime performance in applicable environments.

c. Novel Coating Processes and Materials Sets for Turbine Blades—Both current gas turbines and those being designed for coal-based synthesis gas operation will greatly benefit from improved manufacturing processes to coat turbine blades, coupled with new material sets that can withstand higher firing temperatures. Grant applications are sought to develop novel, low cost blade coating processes and new material sets that improve thermal barrier coating (TBC) structures and turbine blade robustness, thereby allowing higher temperatures in natural gas and synthesis gas environments. TBC systems aimed at enhancing the effective operating temperature of cooled super alloys by as much as 165°C are needed. Coating systems with diminished thermal conductivity have evident appeal and are of interest; however, such approaches must address how to avert uncertainties in their life expectancy, in order to avoid compromising the survivability of the underlying component. While recognizing the need for coatings with improved base capabilities, the overarching issue for advanced gas turbines is prime reliance; namely, the coating should be an integral part of the overall design, rather than an add-on feature. If the operating envelope is to be pushed significantly beyond its current limit, both alloys and ceramics will have to depend on the capabilities, durability, and reliability of the coatings to achieve the requisite performance.

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PROGRAM AREA OVERVIEW OFFICE OF BASIC ENERGY SCIENCES

http://www.sc.doe.gov/bes

The Basic Energy Sciences (BES) program supports fundamental research in the natural sciences leading to new and improved energy technologies. The program's purpose is to create new scientific knowledge by supporting basic, peer-reviewed research in areas of materials sciences, chemical sciences, geosciences, plant and microbial biosciences, and engineering sciences that are relevant to energy resources, production, conversion, and efficiency. 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 national user facilities to serve researchers at universities, national laboratories, and industrial laboratories, thus enabling the acquisition of new knowledge that cannot be obtained in any other way. The scientific facilities include synchrotron radiation light sources, high-flux neutron sources, electron-beam microcharacterization centers, nanoscale science research centers, and specialized facilities such as the Combustion Research Facility. These national resources are available free of charge to all researchers based on the quality and importance of proposed nonpropriety 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, mitigation of the adverse impacts of energy production and use, and future fusion 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.

16. ADVANCED FOSSIL FUELS RESEARCH

For the foreseeable future, the energy needed to sustain economic growth will continue to come largely from fossil fuels. In supplying this energy need, however, the Nation must address growing global and regional environmental concerns, supply issues, and energy prices. Maintaining low-cost energy in the face of growing demand, diminishing supply, and increasing environmental pressure requires new technologies and diversified energy supplies. These technologies must allow the Nation to use all of its indigenous resources more wisely, cleanly, and efficiently. These resources include inherently clean natural gas and the Nation's most abundant and lowest cost resource, coal. **Grant applications are sought only in the following subtopics:**

a. Hydrogen Fuels and Technologies—Clean forms of energy are needed to support sustainable global economic growth while mitigating greenhouse gas emissions and impacts on air quality. Hydrogen systems can provide viable, sustainable options for meeting energy requirements in all energy sectors – transportation, buildings, utilities and industry. However, hydrogen energy systems still face a number of technical and economic barriers that must be overcome for hydrogen to become a competitive energy carrier. Advances must be made in hydrogen production, storage, transport, and utilization technologies and in the integration of these components into complete energy systems.

Domestic coal can be a major source of hydrogen. Long-term research will improve technology that will lower the cost to produce hydrogen from coal, and also enable sequestration of carbon. An important component of

hydrogen production from coal syngas is the water-gas shift process. Therefore, grant applications are sought for improved catalysts that will enable water-gas shift chemistry at lower temperatures or with faster kinetics or that are impurity tolerant, thereby lowering the cost of producing hydrogen from coal syngas. These catalysts not only would be potentially useful for providing hydrogen from hydrocarbons for stationary and vehicular fuel cells, but also would be a welcome improvement to other hydrogen production processes and other chemical transformations.

b. Biogeochemical Carbon Sequestration/Conversion—Carbon sequestration is a relatively new approach to the stabilization of greenhouse gas concentration (i.e., new compared to the other two pathways – improving the efficiency of energy use and reducing the carbon content of fuels). Current approaches include the conversion of carbon dioxide to benign, stable compounds for long-term storage or to value added products for reuse. Grant applications are sought to develop practical methods to: (1) grossly accelerate the natural bioconversion of carbon dioxide to methane in geologic reservoirs by employing methanogen microorganisms as catalysts, as well as other geochemical reactants, (2) apply similar processes to the capture of carbon dioxide at large point sources, and (3) efficiently employ microorganisms and/or biomimetic catalysts to convert carbon dioxide in flue gas to intermediates that can be subsequently reacted to calcium/magnesium carbonates for terminal sequestration.

c. Instrumentation for Surface Science Investigations of Electrochemically Active Solid Oxide

Materials—In the electrode boundary regions of Solid Oxide Fuel Cells (SOFCs) charge transfer takes place at electrochemically active oxide surfaces, as neutral gas phase atoms become part of the ionic solid. The electrode oxides are structurally defective, both atomically and electronically, in ways that are not yet fully characterized. Current surface science investigations are limited by the environmental constraints of high temperature (≥ -600 C) and oxidizing gas concentrations (~ 2 kPa pO₂) that affect the mobility and defect density of the active surfaces. Traditional surface science tools (for example, photo-electron spectroscopy and low energy electron diffraction) employ high vacuum systems to inhibit the gas absorption of the excitation source (electrons, UV light, etc.) and allow for the spectroscopic detection of the emitted response. New tools such as scanning tunneling microscopy (STM) have been successfully employed at high temperatures, but usually in high vacuum environments to prevent oxidation of the STM components and allow effective thermal shielding of critical parts. Synchrotron-radiation-based x-ray techniques may allow for *in situ* X-ray Photo-emission Spectroscopy (with total electron yield detection), x-ray absorption spectroscopy, and grazing incidence x-ray diffraction, but these techniques will require specialized sample manipulation and signal detection schemes.

Therefore, grant applications are sought to develop surface science analytical instruments capable of investigating solid oxide materials under appropriate chemical and thermal boundary conditions (high T, high pO_2). For the SOFC materials, parameters of interest include the concentration and mobility of surface vacancies, the electronic structure of mixed ionic/electronic conducting surface states, the valence and oxygen coordination of surface cations, and the distribution and nature of electrochemically active atomic surface defects. All of these physical parameters should be investigated as a function of the electrochemical potential (which, at one extreme, is simply modified by changing the partial pressure of gas phase oxygen). Approaches must demonstrate the relevance of the new instrument to high-temperature solid-oxide electrochemistry, and must include examples of typical experiments that would be enabled by the new instrument.

d. A More Economic Method for Making Liquid Fuels from Coal by Hydrogenation—An added source of distillate fuels is needed as world demand grows and sources of petroleum diminish. Coal could be a potential source, and could provide energy for a long time, if the cost of converting coal to liquid fuels cold be substantially reduced. Current processes, which involve the direct high-temperature hydrogenation of coal, are not competitive. Therefore, grant applications are sought to define process chemistries and/or reactor designs that can provide a slate of transportation fuel products from coal, at a cost that is competitive with currently

used fuels. Possible approaches include improvements to two liquefaction processes, already under development:

(1) A new technology for the hydrogenation of hydrocarbons, which could lead to the required cost reduction, has been published. It is based on the treatment of HCOOH (formic acid) over a noble metal catalyst at 450 C. Under these process conditions, this HCOOH has the character of a supercritical solvent, which is known to be a superior solvent for coal derived organics. (Note that the feed to such a reactor would likely be the product of a first liquefaction stage, so that the coal-derived organics are mostly in solution.) The process was shown to saturate selected olefinic and ring compounds at the relatively mild conditions of 1200-3000 psi and 80-200 C; however, the required noble metal catalysts that are required have not yet been shown to be sulfur tolerant. A significant task would be identifying or developing an economic source or process to provide the formic acid feed.

(2) The DOE has developed a process that largely uses bubble column reactors. Although workable, there are significant weaknesses in the process design of the slurry-phase. For example, the reactants in the reactor are nearly fully mixed, leading to over-reaction that tends to result in undesirable conversion to tars and over-consumption of hydrogen through conversion to gaseous hydrocarbons. (By comparison, a plug flow reactor would permit more complete reaction.) At the same time, the dispersion of the hydrogen gas phase and its mixing intensity are poor, slowing its contact with the incompletely reacted coal and partially reacted liquids.

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Subtopic a: Hydrogen Fuels and Technologies

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- 2. Basic Research Needs for the Hydrogen Economy: Report on the Basic Energy Sciences Workshop on Hydrogen Production, Storage and Use, [Rockville, MD], May 13-15, 2003, U.S. Department of Energy Office of Science, February 2004. (Full text available at: <u>http://www.sc.doe.gov/bes/hydrogen.pdf</u>)
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Subtopic b: Biogeochemical Carbon Sequestration/Conversion

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17. TECHNOLOGIES RELATED TO ENERGY STORAGE FOR ELECTRIC AND HYBRID VEHICLES

The commercial use of electric and hybrid electric vehicle technologies, including fuel cell vehicles, has been limited by a variety of technical barriers. In conjunction with the Office of Basic Energy Sciences, the Office of Energy Efficiency and Renewable Energy is interested in identifying and developing innovative concepts for advanced technologies for energy storage devices (batteries and electrochemical capacitors) that will improve the performance, extend the life, and significantly reduce the cost of the vehicles.

Battery-powered electric vehicles (EVs) require energy storage devices with high specific energy, and hybrid electric vehicles (HEVs) require devices that can deliver high power pulses. Advanced hybrids may require devices that both store significant energy and can deliver high power pulses. All of these devices must be able to accept high power recharging pulses from regenerative braking. For high specific energy systems, the near term goals are to develop cells that provide at least 150 Watt-hours/kg (Wh/kg), 230 Wh/l, 300 W/kg, and 460 W/l (with long term goals that exceed these targets); have a life of 1000 cycles at 80 percent depth of discharge; and have a calendar life of at least 10 years. For high power applications, the goal is to develop cells that provide peak power of 1000 W/kg or greater, have a cycle life of at least 300,000 shallow cycles, and have a calendar life of 15 years. For all systems, materials to be utilized should be plentiful, have low cost (< \$10/kg), be environmentally benign, and be easily recycled. Evaluation of the technology with regard to the above criteria should be performed in accordance with applicable U.S. Advanced Battery Consortium test procedures or Society of Automotive Engineers recommended practices (see references that follow).

Grant applications must show how proposed innovations would result in significant advances in performance and cost reduction over state-of-the-art technologies. Grant applications are sought only in the following subtopics:

a. Improved Electrolytes for Electrochemical Capacitors—The most common electrochemical capacitors, also known as "super" or "ultra" capacitors, use an aqueous or organic electrolyte solution. For vehicular applications, the higher cell voltages available with an organic electrolyte are attractive. Most organic electrolytes are based on acetonitrile. This solvent allows the preparation of electrolytes that have acceptable conductivity and function over a wide range of temperatures. Unfortunately, the solvent is quite flammable and under some circumstances can decompose to yield cyanide. Therefore, grant applications are sought to address the flammability and potential toxicity issues associated with acetonitrile. Replacement materials that result in reduced performance relative to the state-of-the-art (in areas such as power capability, energy stored, operating temperature, useful life, or cost) are not of interest. All proposals must provide a clear discussion based upon available data and theory to support an assertion that the materials to be developed will be improvements. Grant applications must include a demonstration of the materials' performance in laboratory cells by the end of Phase I and in capacitors suitable for use in a vehicle by the end of Phase II.

b. Technology to Improve the Performance of Lithium-Ion Cells at Low Temperatures—Lithium-ion cells and batteries discharged or charged at low temperatures (between -10 and - 20 degrees Celsius) exhibit poor

performance relative to performance at room temperature. Power capability is significantly reduced on discharge, and lithium plating on the negative electrode can occur upon charge. The loss of power below -10 Celsius is much more severe than would be predicted from the conductivity vs. temperature relationships for conventional Li-Ion electrolyte systems. Studies of cells being cycled at low temperatures indicate that the impedance increase is interfacial in nature and fairly evenly distributed between the positive and negative electrodes. Grant applications are sought for technology to address these concerns. Approaches that result in significantly reduced performance relative to the state-of-the-art (in areas such as room temperature performance, cycle life, calendar life, or cost) are not of interest. Grant applications must provide a clear discussion, based upon available data and theory, to support the assertion that the research will result in improved performance. The technologies being developed must be demonstrated in full electrochemical cells of at least 0.2 Ampere hour in size by the end of Phase I and in cells of at least 1.0 Ampere hour by the end of Phase II.

c. Technologies to Improve the Tolerance of Lithium-Ion Cells and Batteries to Thermal Runaway Provoked by Abusive Discharge or Overcharge—High energy and high power lithium-ion cells and batteries may be subject to inadvertent, abusive discharge or overcharge if the battery's control mechanism fails. For this subtopic, an abusive discharge is one that results in a cell going into thermal runaway sufficient to result in cell failures such as venting and/or fire. Depending upon the failure mode, cells may experience charging voltages that exceed the design specification by as little as 100 millivolts or by many volts. Even low levels of overcharge have been shown to make a cell more susceptible to thermal runaway. More extreme overcharge can produce rapid events such as venting with smoke and flames. Grant applications are sought to develop novel methods of improving the tolerance of lithium-ion cells to abusive discharge and/or overcharge. Grant applications may focus on changes in one or more of a cell's basic components (cell hardware, anode, electrolyte, separator, and cathode), or on materials added to a "standard" cell. Any standard, commercially available lithium-ion cell, suitable for vehicular use, may be used as the basis for the changes/improvements. (Note: some commercially available cells are not suitable for vehicular use because they contain costly components, operate only at low rates, have relatively limited cycle or calendar lives, etc.) Investigators that do not have access to specific information about the components of commercially available cells may use the specifications published by the Advanced Technology Development Program for its Generation 1 and Generation 2 cells as a starting point (see references 3 and 4).

Grant applications must be for novel research and development as defined in the introductory sections of this solicitation, provide a theoretical basis for the research, address the probable cost of using the technology in vehicular batteries, and address the impact of the technology on other performance parameters such as calendar life, power capability, and energy density – technologies that adversely affect these parameters are not likely to be adopted. Improvements must be demonstrated in cells of at least 0.2 Ampere-hour in size in Phase I and in cells of at least 1.0 Ampere hour in Phase II.

d. Methods for Rapidly Predicting the Calendar Life of Lithium-Ion Cells and Batteries—Lithium-ion cells and batteries proposed for vehicular use must meet goals related to both cycle life and calendar life. As described in the references, end-of-life is defined when an EV battery's capacity, as measured according to the procedures described in the EV Test Manual (reference 1), drops below 80% of its original capacity. For an HEV battery, the most common failure is the inability to provide the minimum power and energy for pulse cycles as described in the HEV battery test manuals. Cycle life can be experimentally evaluated within relatively short periods of time, typically less than one year. Quickly assessing calendar life, when the desired life is more than ten years, is much more difficult. Grant applications are sought to develop novel methods of rapidly assessing the calendar life of state-of-the-art lithium-ion cells. The ideal method would result in a reliable prediction within twelve to eighteen months. All grant applications must provide a clear discussion, based upon available data and theory, to support the assertion that the research is viable. Phase I efforts must include development of the basic approach and its preliminary evaluation on a commercially available cell. By the end of Phase II, the approach must be refined and demonstrated using at least two different types of

commercial cells. The deliverables under Phase II shall include a general, procedural manual that describes how one can assess the calendar life of lithium-ion cells other than those used to develop and demonstrate the approach.

References:

Please note: Paper copies of those references not available in the open literature or from NTIS may be obtained by addressing a request to Mr. Irwin Weinstock, Senior Engineer, Sentech, Inc., 7475 Wisconsin Avenue, Suite 9000, Bethesda, MD 20814. Where available, locations of the documents on the Internet are given.

- 1. Links to the following manuals are all available at: <u>http://ev.inel.gov/battery</u>. These documents provide a good general basis for understanding the performance requirements for electric and hybrid electric vehicle energy storage devices.
 - · FreedomCAR 42V Battery Test Manual
 - · FreedomCAR Battery Test Manual for Power Assist Hybrid Electric Vehicles
 - · PNGV Battery Test Manual, Revision 3
 - Electric Vehicle Capacitor Test Procedures
 - · USABC Electric Vehicle Battery Test Procedure Manual, Revision 2
- The internet site for the Batteries for Advanced Transportation Technologies (BATT) program at <u>http://berc.lbl.gov/BATT/BATT.html</u> includes quarterly and annual reports. This program addresses many long-term issues related to lithium batteries, including new materials and basic issues related to abuse tolerance.

References 3, 4, and 5 discuss issues related to more mature, high power, lithium-ion batteries. They include information about cell chemistries that have proven to be useful model systems for these applications along with discussions of issues related to abuse tolerance and cell life.

- Advanced Technology Development (High-Power Battery): 2001 Annual Progress Report, U.S. DOE, Office of Advanced Automotive Technologies, February 2002. (Full text available at: <u>http://www.eere.energy.gov/vehiclesandfuels/resources/fcvt_publications.shtml</u>. Scroll down to 2001, and select "Advanced Technology Development ...".)
- "Applied Research", in the 2002 Annual Progress Report, U.S. DOE, Office of Advanced Automotive Technologies, May 2003. (Full text available at: <u>http://www.eere.energy.gov/vehiclesandfuels/resources/fcvt_publications.shtml</u>. Scroll down to 2002, select "Energy Storage Research and Development," and go to Chapter III, "Applied Research".)
- 5. "Applied Research", in the 2003 Annual Progress Report, U.S. DOE, Office of Advanced Automotive Technologies, May 2004. (Full text available at: <u>http://www.eere.energy.gov/vehiclesandfuels/resources/fcvt_publications.shtml</u>. Scroll down to 2003, select "Energy Storage Research and Development," and go to Chapter III, "Applied Research".)
- 6. Information about requirements for vehicular batteries, separators for lithium-ion batteries, and abuse testing can all be found at the USABC section of the USCAR internet site. Go to <u>http://www.USCAR.org</u>; click on "Teams"; scroll down and click on "United States Advanced Battery Consortium (USABC)". This site provides a second source for many of the documents found at reference 1.
- The abuse test procedures, developed for FreedomCAR by Sandia National Laboratories may be accessed directly at: <u>http://www.uscar.org/consortia&teams/USABC/SAND99-</u> 0497%20USABC%20Safety%20Manual.pdf

18. TECHNOLOGIES FOR HYDROGEN TRANSPORT AND STORAGE

U.S. energy dependence is driven by transportation because at the present time nearly all of our vehicles run on either gasoline or diesel fuel. The transportation sector accounts for two-thirds of the 20 million barrels of oil our nation uses each day. Fifty five percent of this oil is now imported, and, without any change to the status quo, imports are expected to grow to 68% by the year 2025. This situation can be ameliorated only if alternative energy carriers are developed to promote future national energy security. Hydrogen is a leading candidate because it can be clean, efficient, and capable of production from diverse domestic resources, both renewable and non-renewable. Hydrogen can be employed in high-efficiency power generation systems, including internal combustion engines or fuel cells for both vehicular transportation and distributed electricity generation. The energy security and diversity benefits of hydrogen are the basis of the President Bush's Hydrogen Fuel Initiative in January 2003, which commits government funding for accelerated research, development, and demonstration programs, leading to an industry decision on the commercialization of hydrogen by 2015.

There are three primary technology barriers that must be overcome to realize the commercialization of hydrogen. First, the cost of safe and efficient hydrogen production and delivery must be lowered to be competitive with gasoline and diesel fuel. Second, fuel cell system costs must be significantly lowered while meeting performance and durability requirements. Third, on-board vehicular hydrogen storage systems must be developed that allow for driving ranges expected by consumers. Grant applications in response to this topic must show how proposed innovations would result in significant advances in performance and cost reduction over state-of-the-art technologies. Grant applications are sought only in the following subtopics:

a. Advanced Materials and Technologies for Hydrogen Pipelines—The transport and delivery of hydrogen in pipelines, as well as hydrogen storage in high pressure tanks in the near-term, will be an important part of the hydrogen infrastructure that will help enable a hydrogen economy. Although there are currently about 700 miles of hydrogen transmission pipelines in the U.S. and more in Europe, several technology issues need to be resolved and significant cost reductions are required for effective hydrogen pipeline transmission and distribution. These issues include: a better fundamental understanding of hydrogen embrittlement and diffusion to enable the development of lower cost metal alloys, plastics, or composites for hydrogen pipelines; improved metal welding or other joining techniques to reduce the material and labor costs associated with pipeline construction and repair; and improved seals to reduce hydrogen leakage in fittings and other components. It has also been suggested that interior or exterior coatings could be retrofitted on existing or new pipelines to achieve compatibility with hydrogen service. Grant applications are sought to develop advanced and novel approaches to significantly reduce the cost of new hydrogen pipelines (by as much as 50%) and/or technology to retrofit existing natural gas or petroleum pipelines for pure hydrogen transmission and distribution.

b. Hydrogen Compression Technology—Efficient and cost effective hydrogen compression technology has been recognized as a critical component of effective pipeline delivery. However, today's hydrogen compression technology is lacking in reliability and durability, which often requires the installation of spare compressors and adds significantly to cost. Current hydrogen compression can require energy use equivalent to as much as 15% of the hydrogen compressed. Grant applications are sought to develop advanced and novel hydrogen compression technology specifically for use in hydrogen transmission, analogous to the transmission in today's natural gas pipeline infrastructure. Areas of interest include lubricant free designs to avoid contamination and better sealing to reduce/eliminate hydrogen leakage. Grant applications must demonstrate that levels of compression from 0-500 psig to 800-1200 psig can be achieved, along with significant improvements in reliability/durability, energy efficiency, contamination, and sealing.

c. High-Pressure Hydrogen Tanks—Compressed hydrogen tanks (e.g. 5,000-10,000-psi) represent one of the best available, near-term commercial technologies for hydrogen storage systems for stationary and vehicular

applications. However, cost reduction is a critical issue that remains to be addressed, and there is a need for high strength materials such as carbon fiber composites that are amenable to high volume, low cost manufacturing methods. Grant applications are sought to develop novel materials or processes to significantly reduce the cost of high pressure hydrogen tanks. Areas of interest include methods to reduce the cost of carbon fiber materials, including carbonization/graphitization, surface treatments, spinning; alternate precursor routes and oxidation methods, such as microwave-assisted techniques; alternatives to carbon fiber; and/or alternative manufacturing approaches such as a fiber wrap approach; and materials amenable to high pressures (e.g. 1000 atm) and low temperatures (less than 100 K) that are viable for hydrogen tank technologies. All tank designs should have the potential of meeting the 2010 DOE/FreedomCAR system performance targets of 2kWh/kg [6 wt% hydrogen], 1.5 kWh/L, and \$4/kWh.

References:

- 1. *National Hydrogen Energy Roadmap*, U.S. Department of Energy, November 2002. (Full text available at: <u>http://www.eere.energy.gov/hydrogenandfuelcells/pdfs/national_h2_roadmap.pdf</u>)
- Hydrogen, Fuel Cells, & Infrastructure Technologies Program Multi-Year Research, Development, and Demonstration Plan, June 3, 2003 Draft, U.S. DOE Office of Energy Efficiency and Renewable Energy. (Full text available at: <u>http://www.eere.energy.gov/hydrogenandfuelcells/mypp/</u>)
- Annual Progress Reports, Hydrogen, Fuel Cells, & Infrastructure Technologies Program, U.S. DOE Office of Energy Efficiency and Renewable Energy. (Available at: <u>http://www.eere.energy.gov/hydrogenandfuelcells/pubs.html#progress</u>)
- 4. *FreedomCAR Technical Targets: On-Board Hydrogen Storage Systems*, U.S. Department of Energy Office of Energy Efficiency and Renewable Energy, 2004. (Available at: <u>http://www.eere.energy.gov/hydrogenandfuelcells/pdfs/freedomcar_targets_explanations.pdf</u>)

19. ENERGY EFFICIENT MEMBRANES

Separation technologies recover, isolate, and purify products in virtually every industrial process. Pervasive throughout industrial operations, conventional separation processes are energy intensive and costly. 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. Industrial efforts to increase cost-competitiveness, boost energy efficiency, increase productivity, and prevent pollution demand more efficient separation processes. In response to these needs, the Department of Energy supports the development of high-risk, innovative separation technologies. In particular, membrane technology offers a viable alternative to conventional energy intensive separations.

Successful membrane applications today include producing oxygen-enriched air for combustion, recovering and recycling hot wastewater, volatile organic carbon recovery, and hydrogen purification. Membranes also have been combined with conventional techniques such as distillation to deliver improved product purity at a reduced cost. Membrane separations promise to yield substantial economic, energy, and environmental benefits leading to enhanced competitiveness by reducing annual energy consumption, increasing capital productivity, and reducing waste streams and pollution abatement costs.

Despite the successes and advancements, many challenges must be overcome before membrane technology becomes more widely adapted. 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. The objective is better performance in existing industrial applications, as well as opportunities for new applications. To advance the use of membrane separations, research is needed to develop new, more effective membrane materials and innovative ways to incorporate membranes in industrial processes. Grant applications must address the potential public benefits that the proposed technology would provide, both from reduced energy consumption and from the reduction in one or more of the following: materials consumption, water consumption, and toxic and pollutants dispersion. Grant applications also should include a plan for introducing the new technology into the manufacturing sector, in order to access capabilities for widespread technology dissemination. **Grant applications are sought only in the following subtopics:**

a. Membrane Materials with Improved Properties—Grant applications are sought to develop lower cost inorganic, organic, composite, and ceramic membrane materials in order to improve one or more of the following properties: (1) increased surface area per unit volume, (2) higher temperature operation (e.g., by using ceramic or metal membrane materials), and (3) suitability for separating hydrophilic compounds in dilute aqueous streams. Particular membrane materials of interest include nano-composites, mixed organic/inorganic composites, and chemically inert materials. Particular processes/systems of interest include membranes for the separation of biobased products, membranes for hydrogen separation and purification, and membranes for industrial applications.

For industrial applications, high temperature separations of hydrocarbons and other mixtures are of particular interest. For example, low molecular weight hydrocarbons are separated from natural gas by condensing them as a liquid, and the liquid is distilled to fractionate it, or the liquid is hydrocracked to olefins. However, chilling the natural gas in order to recover the condensable portion and then reheating it is inefficient, because the energy used to chill it cannot be recovered. Membranes, either as stand alone systems or hybridized with other separation technologies, may provide an energy efficient means of separating mixtures at the high temperatures at which these industrial processes are carried out.

For all membrane processes/systems, grant applications must be targeted toward the development of specific membrane materials for carefully defined commercial applications; efforts focused on generalized membrane material research are not of interest and will be declined. In order to assure the rapid commercialization of the technology, especially for use by U.S. manufacturers, applicants are strongly encouraged to engage in partnerships, so that the costs of the technology development and commercialization can be shared among manufacturers, suppliers, and end users.

b. Membranes for Separations of Biobased Products—Grant applications are sought to develop membrane technology to enhance the production of large volume, value-added chemical products using biomass feedstocks. These processes may use either enzymatic or chemical catalysis, and may be conducted in either aqueous reaction media or organic solvents. Grant applications must demonstrate a clear connection to a cropbased feedstock and a large volume chemical product (one that would be manufactured at greater than 500 million pounds). Of particular interest are (1) novel membrane processes that use reactive separation technology, which combines the reactive transformation with the separation; and (2) novel membrane materials with higher flux or selectivity, and with improved chemical and thermal membrane stability. Again, applicants are strongly encouraged to form partnerships involving manufactures, suppliers, and end users, in order to promote and ensure the rapid development and commercialization of the technology in the U.S.

c. Hydrogen Production—Hydrogen can be produced from coal, natural gas, biomass, and biomass derivatives through the use of gasification, pyrolysis, reforming, and shift technologies. In all cases, a hydrogen-rich producer gas or syngas results, from which the hydrogen must be separated and purified. The most common approach today involves the use of pressure swing adsorption (PSA) technology. The use of membranes holds the promise of reducing costs by combining the separation and purification with the shift reaction in a reactive separation operation. Therefore, grant applications are sought to develop improved hydrogen membrane

separation and purification technology for use in the production of hydrogen; the focus of the research should be on low cost, high flux rate, durable membrane systems that can be integrated with the shift reaction. Membranes of interest include ceramic ionic transport membranes, micro-porous membranes, and palladium based membranes. Such membranes could be used for a wide range of production capacities, from large central production facilities (50,000-300,000 kgs/day of hydrogen) to small-distributed production units (50-1000 kgs/day of hydrogen). Grant applications must include a careful analysis of the overall hydrogen separation efficiency, to assure that the proposed membrane separation will maximize the hydrogen recovered by the proposed process. Technology partnerships with manufacturers, suppliers, and especially end users are encouraged, in order to assure rapid commercialization of the technology in the U.S.

d. Industrial Membrane Process Systems—Grant applications are sought to enhance the separation capabilities of membranes used in industrial process streams. Proposed research should be aimed at developing and commercializing innovative membrane systems, using new or currently existing membranes, that can be robust when integrated within real-world processes (e.g., inert gas removal, isomer separation, aromatic/nonaromatic separations, sulfur removal, and removal of trace metals). Grant applications should seek to address one or more of the following needs: (1) techniques for overcoming scale-up problems related to contaminants in industrial streams (fouling, oil misting, etc.), (2) manufacturing technologies that would reduce the cost of membrane modules, (3) anti-fouling and anti-flux schemes to improve the long-term operability of membrane systems, and (4) methods to regenerate membrane performance and lower membrane maintenance costs. Also of interest is the integration of membranes with other technologies (such as the integration of membranes with distillation systems, or with adsorption or extraction processes), in order to address specific process issues. For all grant applications, the overriding goal is to enhance U.S. industrial process efficiency to the maximum possible extent by increasing the separation process efficiency. Therefore, priority will be given to applications that carefully examine the efficiency of the proposed membrane technology within the targeted application. Grant applications also should include a process evaluation and an economic analysis along with the R&D effort. Lastly, technology partnerships involving U.S. manufacturers, suppliers, and end users are strongly encouraged.

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20. NANOTECHNOLOGY APPLICATIONS IN INDUSTRIAL CHEMISTRY

The U.S. chemical industry is poised to apply many of the recent discoveries in nanotechnology, undertaken at universities and national laboratories, which may have an important influence on the manufacture and uses of chemicals and materials. In this topic, small businesses are encouraged to take advantage of these discoveries by conducting further R&D, leading to marketable products of importance to the U.S. chemical industry. The subtopic areas focus on nanomaterials research in catalysis, on polymers and polymer manufacture, on composite materials, and on new materials with special properties that mimic properties of living organisms (i.e., "biomimetics" applications). Grant applications must demonstrate a significant energy benefit, either from saving energy in manufacture, conserving materials, or providing longer life in applications. Grant applications also must demonstrate how these nanotechnology innovations will be introduced into the marketplace in conjunction with major chemical companies that have capabilities for widespread technology implementation and manufacturing. **Grant applications are sought only in the following subtopics:**

a. Nanomaterials with Catalytic Activity—Recent discoveries suggest that some materials with nanosized features may exhibit novel heterogeneous catalytic activity. Grant applications are sought to develop new nanoscale materials with catalytic properties. Chemical transformations of interest include, but are not limited to isomerizations, halogenations, oxidations, reductions, stereospecific transformations, or combinations of these. Proposed approaches must demonstrate that (1) the materials exhibit catalytic behavior only when their functional properties are imparted at the nanoscale, and (2) the intended products of the chemical reactions have commercial value. Partnership with chemical companies that have the manufacturing capabilities needed to bring the technology to widespread commercial application is strongly encouraged.

b. New Nanoscale Polymer Materials, Polymer Composites, and Polymer Processes—Recent research has shown that polymer materials with controlled nanocrystalline features may exhibit special or new properties that are not exhibited otherwise when the polymer material's nanosize features are not controlled. Furthermore, a composite material comprising both polymers and nanosize organic or inorganic substances could exhibit useful properties that are not exhibited by the polymer alone. Grant applications are sought to develop novel polymer processes with the potential to control features of the polymer at the nanoscale, resulting in polymer materials that have properties unmatched by any other materials. (Examples of such naturally occurring processes include the spinning of a web by a spider or the clotting of blood.) Grant applications should (1) address commercial applications or markets for proposed approaches, (2) demonstrate a careful review of the relevant scientific literature, and (3) address possibilities for forming partnerships with industrial chemical companies willing to assist in the development and application of the technology.

c. Nanomaterials for Separations Technologies—Separations account for 60% or more of the energy and installed costs of industrial chemical manufacture. Recent developments in nanotechnology could contribute to more energy efficient separations technology in areas such as molecular sieves, membranes, and sorbents. Grant applications are sought to develop new nanotechnology-based separations technology for any industrial separation process, provided that significant increases in energy efficiency can be demonstrated, compared to the technology that is augmented or replaced. Grant applications that propose improvements or enhancements to existing technologies are not of interest and will be declined. Potential applicants are strongly urged to carefully review the scientific literature and patent databases related to the proposed technology, before submitting an application. In order to assure the rapid commercialization of the new technology, successful applicants will form partnerships with chemical manufacturers, suppliers to the industry, and end users.

d. Nanomaterials and Specialty Products Chemistry—In addition to the catalysts sought in subtopic a above, grant applications are sought to develop new products, based on nanoscience and nanotechnology, for use in specialty chemicals markets. These products include adhesives, antioxidants, biocides, corrosion inhibitors, dyes, flame retardants, flavorings and fragrances, specialty coatings, surfactants, and water-soluble polymers. Grant applicants must identify (1) specialty chemicals markets that will use the new materials, (2) energy benefits to be obtained from using the new materials, (3) the basis in nanoscience for the properties of the new materials, and (4) a specialty chemicals manufacturer that is prepared to assist in the commercialization of new materials technology.

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21. ALTERNATIVE REACTION MEDIA FOR INDUSTRIAL CHEMICAL PROCESSES

Many liquid phase chemical processes involve a solvent, which is usually recovered at the end of the process. Solvents are usually selected for their inertness to desired products and their ease of recovery. Because of environmental considerations, many solvent replacements are currently under investigation. Although environmental concerns are important, this topic seeks to develop solvent substitutes or alternative reaction media that would provide energy efficiency benefits as well. The challenge is to meet both goals with commercially viable costs.

This technical area has been explored extensively, and potential applicants are advised to thoroughly investigate the scientific and patent literature related to proposed ideas. Also, grant applications must demonstrate the possibility of saving energy by solvent elimination or substitution. In order to assure the rapid commercialization of the technology, successful small business applicants will form partnerships with U.S. suppliers to the chemical industry, as well as with U.S. chemical manufacturers and end users of the proposed technology. Although all sectors of the U.S. chemical industry are of interest (including pharmaceutical, agricultural, cosmetic, and specialty chemical), grant applications are sought only in the following subtopics:

a. Ionic Liquids—Ionic liquids, which entail a virtually endless number of chemical compositions, have attracted interest as reaction media due to their low vapor pressures. However, there exist many barriers to the commercial application of ionic liquids in the U.S. chemical industry: difficulty in separating final products, recycling concerns, system costs, and contamination issues. Grant applications are sought to overcome these barriers to the application of ionic liquids as reactive media in chemical processes. Areas of interest include processes in which ionic liquids have already been applied, as well as previously uninvestigated applications.

b. Solventless Polymerization—Although many polymerization reactions are carried out on an industrial scale in a condensed phase without solvents, many others still require the use of solvents. Grant applications are sought to develop technology to eliminate solvent usage in those polymerization processes that currently use solvents. Approaches of interest include, but are not limited to, (1) the development of new catalysts that would enable condensed phase industrial polymerization reactions, and (2) the conversion of a polymerization process, currently carried out in a liquid phase, to a vapor phase, which would eliminate solvent usage. Grant applications that propose solvent substitutions for polymerization reactions are not of interest, despite the possible benefits, and will be declined.

c. Supercritical Solvents—Supercritical solvents, such as carbon dioxide and water in their supercritical states, are used as solvents for a number of industrial chemical processes, providing important advantages over the traditional solvents they replace. Grant applications are sought to expand the use of these supercritical solvents in other chemical processes, and to develop other supercritical materials or mixtures for use as solvents. Grant applications must address the possible energy efficiency benefits of proposed supercritical processes,

accounting for the entire process, including materials of construction. For example, extreme demands are placed on materials for supercritical water processes, which limit the application of supercritical water on an industrial scale. Considerable R&D has already been carried out in the supercritical process area; therefore, a careful review of the scientific and patent literature related to the proposed technology development must be conducted.

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22. SOLID STATE INORGANIC AND ORGANIC LIGHT EMITTING DIODES FOR GENERAL LIGHTING

The current generation of solid state lighting (SSL) products (monochromatic) are commercially viable and, in some limited instances, may contribute to energy conservation. However, they are most often used in applications that do not produce the large energy conservation results sought by the DOE for general illumination. The DOE has engaged the rapidly expanding SSL industry and research community in several workshops^(1,2,3,5) that have identified high priority research needs. The objective of this topic is to encourage small business participation in addressing these needs, in order to overcome the significant technical challenges that restrict the application of SSL to only relatively low luminous output products. **Grant applications are sought only in the following subtopics:**

a. High Efficiency Visible and Near UV (>380 nm) Semiconductor Materials for LED-Based General Illumination Technology—Current nitride compound semiconductors are incapable of achieving the price and performance targets to be competitive in general illumination applications, primarily due to limitations in materials and packaging. In particular, significant advances in the basic materials technology associated with visible and near UV light emitting diodes (LEDs) will be needed for current devices to achieve performance characteristics beyond their present limitations of 50 to 80 lumens per watt (LPW). These advances not only must produce the substantial gains in light production efficiency, but also must reduce the significant costs normally associated with the complex and labor intensive epitaxial growth required to produce these devices.

Grant applications are sought to develop significant improvements in conventional nitride systems performance (e.g., >80 LPW) or explore novel material systems to achieve this goal. Approaches of interest include (1) advancements in P-doping efficiency and novel charge introduction structures, which may produce significant fundamental improvements to existing materials systems; and (2) advancements in high purity process materials and growth structures, which also may improve device performance by limiting the photon inhibiting processes thought to be associated with defects, dislocations, and other crystalline artifacts. In order to achieve practical solutions, grant applications must demonstrate that improvements by several orders of magnitude, in the price and performance of these devices, are likely. Anticipated device performance should be compared to benchmark devices available today (i.e., Luxeon $III^{(4)}$).

b. Advanced Architectures and Designs for High Power Conversion Efficiency Emitters—Grant applications are sought to develop advanced device architectures and designs that optimize both the electrical transport and optical properties of SSL devices, in order to achieve long-term efficiencies in excess of 160 lumens per watt, leading to meaningful energy savings. Areas of interest include (1) more advanced light emitting designs such as micro-cavities, photonic lattices, quantum dots, and edge emitting and vertical-cavity laser structures; and (2) fundamental advancements and novel innovations associated with chip-level architectures and high power conversion efficiencies, believed by many to be the key for producing significant increases in power handling capability. Grant applications may be directed at any advanced architecture approach for achieving the desired increase in power capability including, but not limited to, novel chip scaling, production of practical and cost efficient multi-color chips, or building resonant cavity devices such as lasers or directional emitters. Grant applications also must include a complete discussion of anticipated price and performance impacts compared to baseline devices available today⁽⁴⁾.

c. High Efficiency, Low-Voltage, Stable Materials for OLED-Based General Illumination Technology— Today, the designs for organic light emitting diodes (OLEDs) used for general illumination purposes are usually derived from designs associated with display applications. This is not ideal. General illumination OLEDs will require different price and performance levels to perform as viable alternatives to conventional luminous sources. Current OLED materials simply do not have the efficiency or lifetime performance necessary to qualify them as viable candidates for the demanding general illumination market. Estimates of lifetime and efficiencies necessary for OLED-based general illumination are roughly 50,000 hours and 100 lumens per watt (LPW), respectively. However, state-of-the-art white OLEDs (at 850 cd/m²) have a lifetime and efficiency of approximately only 500 hours and 5 LPW, respectively. In addition, innovative device structures and materials are needed to reduce high-luminance (~1000 cd/m²) drive voltages from 10-20V to 4-5V. To realize the full potential of OLED technology, new materials and systems are needed that offer the promise of vastly improved efficiency and stability.

Experimental OLED systems in the laboratory have already achieved luminous efficiencies of in excess of 200 LPW with external quantum efficiencies greater than 10%. However, many challenging technical issues still remain to achieve the targeted OLED lifetime and performance at the relatively high intensities needed for general illumination applications. A recent workshop ⁽⁵⁾ was held in Salt Lake City, UT (sponsored by DOE, Basic Energy Sciences) and a list of high priority research issues was identified. Therefore, grant applications are sought to achieve the above OLED requirements for general illumination, by addressing one or more of these high priority issues: (1) carrier injection, related to ohmic and non-ohmic contacts; (2) spin effects, such as organic/metal, organic/dielectric and organic/organic; (4) quenching of electroluminescence processes, such as quenching by metallic electrodes, by injected polarons and triplets, and by electric field; (5) theory and modeling; (6) morphology effects on OLED performance; (7) light extraction theory and techniques for improvement, including novel approaches that provide a substantial increase over the 10% extraction that is characteristic of today's devices; (8) the relationship between constituent material purity and OLED

performance; and (9) new ways of producing the requisite white light, i.e., a more thorough understanding of how OLED materials systems produce broad visible emissions.

Grant applications must include a complete discussion of the anticipated improvement in efficiency, the potential impacts on cost and lifetime, and the compatibility with practical methods of current distribution and controls. Although packaging considerations should be considered, they should not be the primary subject of grant applications submitted under this topic.

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23. NEUTRON AND ELECTRON BEAM INSTRUMENTATION

The Department of Energy supports a number of large-scale, national user facilities that provide intense beams of neutrons and electrons for the characterization of materials. Grant applications are sought only in the following subtopics:

a. Neutron Facilities—As a unique and increasingly utilized research tool, neutrons have made invaluable contributions to the physical, chemical, and biological sciences. The Department is committed to enhancing the operation and instrumentation of its present and future neutron science facilities so that their full potential is realized.

Grant applications are sought to develop improved neutron detectors and associated electronics needed for DOE's existing and proposed steady-state and pulsed neutron scattering facilities (References 1-2, 5). New detectors must represent substantial improvements in one or more of the following parameters: efficiency at short wavelengths, high counting rate capability, high spatial resolution in one or two dimensions, cost per unit area, or adaptability to unique geometries. Detectors for pulsed neutron applications must be able to identify the time of arrival of each neutron. All detectors must have low intrinsic dark count rates and low sensitivity to gamma radiation.

Grant applications are also sought to develop novel or improved neutron optical components for use in neutron scattering instruments (References 2-3, 5). Such components include, but are not limited to, neutron choppers, neutron guides, neutron lenses and focusing mirrors, neutron monochromators, or neutron polarization devices including ³He polarizing filters. Applications are also sought for novel use of such components in neutron scattering instruments.

b. Electron Beam Microcharacterization Facilities—The Department of Energy supports four collaborative research centers for electron beam microcharacterization of materials. These tools are important in the materials and biological sciences and are used in numerous research projects funded by the Department. Innovative instrumentation developments offer the promise of radically improving the capabilities of electron beam microcharacterization and thereby stimulate new innovations in materials science. Grant applications submitted to this subtopic must address improvements in electron beam instrumentation capabilities beyond the present state-of-the-art.

Grant applications are sought to develop stages, holders, and/or detectors with new capabilities for quantifying data and collection efficiency in electron beam instruments. Areas of interest include: (1) extremely stable holders and stages that allow long exposure/analysis times, with accurate tilting and alignment capability (to an angle accuracy ± 0.005 degrees on two axes while maintaining eucentricity to within 20 nm); (2) fast CCD camera systems that allow electron imaging exposure times in the millisecond range and kHz frame rates; (3) high sensitivity electron imaging systems based on CCD technology that provide 16 bit dynamic range or better over large areas; and (4) improved electron and x-ray detectors that are robust and not susceptible to electron beam damage. Proposed approaches for electron detectors must show suitability for either low- or high-energy electrons, and address one or more of the following three aspects: high quantum efficiency, high spatial resolution, and high temporal resolution. Proposed approaches for x-ray detectors should show significant improvement in sensitivity or spectral resolution for elemental analysis in electron microscopes.

Grant applications are also sought to develop stages and holders with new capabilities for *in situ* experiments or sample manipulation in the transmission electron microscope. Stages and/or holders must provide for one or more of the following: (1) application of magnetic field up to 5000 Oe in the plane of the specimen, with capability to rotate field orientation in the specimen plane with respect to the sample; (2) manipulation or measurement of the sample using a 4-probe nanomanipulator, including capability to measure deflection or strain, or capability to apply electric fields or current; and (3) precision control of specimen temperature (to an accuracy of 10° C in the range 5-2000K), ambient gas pressure and flow rate (to within several percent for each), and alignment (to an angle accuracy ± 0.005 degrees on two axes).

Grant applications are also sought to develop electron sources for scanning transmission electron microscopy with brightness on the order 10⁹ Amp/cm²/steradian or higher. Current sources are based on tungsten emitters, and it is hoped that higher brightness can be achieved with new materials and designs. Proposed electron sources must be suitably robust for practical applications, have long lifetimes (greater than 6 months), and offer a significant increase in brightness over existing sources.

Grant applications are also sought for systems for automated data collection, processing, and quantification. Systems should include hardware and platform-independent software for data collection and visualization, including automated measurement and mapping of crystallography, internal magnetic or electric field, or strain, and for multi-spectral analysis. Software and quantification routines for image reconstruction and for interpretation of interference patterns/holography are encouraged.

Finally, grant applications are sought for extremely stable power supplies to improve lens stability in electron beam instruments. Power supplies should be capable of producing 15 amperes with current stability exceeding

0.1 ppm, or 5 amperes with current stability exceeding 0.05 ppm, and should exhibit voltage stability of 0.1 ppm in the range of 1 kV to 200kV.

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- Report: Second TEAM [Transmission Electron Aberration-corrected Microscopy] Workshop: Materials Research in an Aberration-Free Environment, Lawrence Berkeley National Laboratory, July 18-19, 2002. (Full text available at: http://ncem.lbl.gov/team/TEAM%20Report%202002.pdf)

24. MATERIALS FOR ADVANCED NUCLEAR ENERGY SYSTEMS

The Generation IV nuclear energy initiative is an international collaboration to identify, assess, and develop sustainable nuclear energy technologies that are competitive in most markets, while further enhancing nuclear safety, minimizing the nuclear waste burden, and further reducing the risk of proliferation (reference 1). Many nuclear energy systems have been proposed to advance the goals of the Generation IV program (see references 2-8), including designs that use liquid-metal coolants such as sodium and lead, gas coolants such as helium, water coolants such as supercritical water, and molten salt coolants. For these systems, operation at higher temperature has been identified as a means to improve economic performance and to support the thermochemical production of hydrogen. However, the move to higher operating temperatures will require the development and qualification of advanced materials to perform in the more challenging environment. As part of the process of developing advanced materials for these reactor concepts, a fundamental understanding of materials behavior must be established and a database that defines the critical performance limitations of these materials under irradiation must be developed. A recent workshop details many of the research challenges for higher temperature materials associated with proposed Generation IV systems (reference 9). **Grant applications are sought only in the following subtopics:**

a. Advanced Radiation Resistance Ferritic-Martensitic Alloys—Because of their resistance to void swelling, 9 Cr and 12 Cr ferritic-martensitic steels are considered prime candidates for intermediate temperature reactors such as the proposed liquid metal and supercritical water concepts operating in the temperature range of 400-750°C. However, many ferritic-martensitic steels are limited by poor higher temperature creep strength, typically degrading at temperatures greater than 550-600°C (reference 10). Grant applications are sought to improve the creep strength of 9 Cr and 12 Cr ferritic-martensitic steels through alloying, dispersion strengthening, or precipitation hardening. Innovative alloys with protective coatings are also of interest. Proposed approaches must provide for (1) isotropic creep properties with strength greater than that of Sandvik HT9 steel, (2) a ductile to brittle transition temperature less than room temperature, and (3) a minimum planestrain fracture toughness of $0.25\sigma_y$. Alloying elements that act as neutron poisons (e.g., boron) or that become highly activated in a neutron spectrum (e.g, cobalt) must be minimized or eliminated. Because the ferriticmartensitic steels likely would be used in conjunction with sodium-cooled, lead- or lead-bismuth-cooled, or supercritical water-cooled reactor concepts, approaches that optimize corrosion performance while achieving improved high temperature strength would be considered high priority. Lastly, approaches that also address irradiation performance are strongly encouraged.

b. Advanced Refractory, Ceramic, Ceramic Composite, or Coated Materials—Some Generation IV concepts aim for very high temperature (>900°C) operation. However, with the exception of limited data on SiC-based systems, the radiation resistance of construction materials subjected to very high temperatures has not been identified or proven. Grant applications are sought to develop advanced refractory, ceramic, ceramic composite, or coated materials that can meet the very demanding conditions required to operate at temperatures greater than 900°C in a fast spectrum nuclear energy system. For these conditions, the materials should have low thermal expansion coefficients, excellent high temperature strength, excellent high temperature creep resistance, and good thermal conductivity. For post-irradiation handling at lower temperatures, sufficient room temperature fracture toughness must be maintained. Additionally, the materials need to be easily fabricated and capable of being joined. Because the reactors operating in this temperature regime are expected to be helium cooled, the materials must have low erosion properties in flowing helium and be able to survive an air ingress condition. Because sustainable nuclear energy systems are likely to be based on fast spectrum systems, the materials must avoid low atomic mass components such as hydrogen and carbon. Because the high temperature strength and corrosion resistance may be difficult to achieve with a single material, composite or coated systems may be required. Finally, because sustainable nuclear energy systems may be based on fast spectrum (i.e., fast flux) designs, materials intended for fast reactor concepts should minimize the use of low atomic mass components such as hydrogen and carbon.

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- * Abstracts of papers and ordering information available through ASME at: <u>http://store.asme.org/category.asp?catalog%5Fname=Conference+Papers&category%5Fname=Tenth+Intern</u> <u>ational+Conference+on+Nuclear+Engineering&Page=1</u>. In SEARCH boxes in upper right corner, search "Conference Papers" for Paper No. given in citation above.

PROGRAM AREA OVERVIEW -OFFICE OF NUCLEAR ENERGY, SCIENCE AND TECHNOLOGY

http://www.nuclear.gov http://www.ne.doe.gov http://gen-iv.ne.doe.gov/

Continued use of nuclear power is an important part of the Department's strategy to provide for the Nation's energy security, as well as to be responsible stewards of the environment. Nuclear energy currently provides over 20 percent of the U.S. electricity generation and will continue to provide a significant portion of U.S. electrical energy production for many years to come. Also, nuclear power in the U.S. makes a significant contribution to lowering the emission of gases associated with global climate change and air pollution.

The Office of Nuclear Energy, Science and Technology (NE) enables the Department of Energy to provide the technical leadership necessary to address critical domestic and international nuclear issues by administering research and development and technical assistance in the following general areas: (1) the Generation IV Nuclear Energy Systems Initiative seeks to develop and demonstrate of one or more Generation IV nuclear energy systems that offer advantages in the areas of economics, safety and reliability, sustainability, and could be deployed commercially by 2030, (2) the Nuclear Energy Research Initiative (NERI) Program addresses key issues affecting the future of nuclear energy in order to preserve U.S. nuclear science and technology leadership, (3) the Radioisotope Power Systems Program develops new state-of-the-art radioisotope power systems to support the NASA space missions and terrestrial applications for other agencies, (4) the Nuclear Energy Plant Optimization (NEPO) Program conducts research to assure the continued safe and reliable operations of over 100 of the Nation's nuclear power plants, (5) the University Reactor Fuel and Educational Assistance Program is designed to help retain the U.S. nuclear engineering capability for conducting nuclear research, addressing pressing nuclear environmental challenges, and preserving the nuclear energy option, (6) the Isotope Production Program produces and sells hundreds of stable and radioactive isotopes that are widely used by domestic and international customers for medicine, industry and research applications, and (7) the Advanced Fuel Cycle Initiative supports the growth of nuclear energy by developing and demonstrating technologies that enable transition to a stable, long-term, environmentally, economically and politically acceptable advanced fuel cycle.

25. ADVANCED TECHNOLOGIES FOR NUCLEAR ENERGY

Nuclear power provides over 20 percent of the U.S. electricity supply without emitting harmful air pollutants, including those that may cause adverse global climate changes. New methods and technologies are needed to address key issues that affect the future deployment of nuclear energy and to preserve the U.S. leadership in nuclear technology and engineering. This topic addresses several of these key technology areas: improvements in nuclear reactor technology for existing reactors and evolutionary designs, advanced instrumentation and control (I&C) for very high temperature reactor applications, advanced I&C for use in high radiation environments, and advanced core/reactor physics computer simulations and modeling for Generation IV reactor designs. **Grant applications are sought only in the following subtopic:**

a. New Technology for Improved Nuclear Energy Systems—Improvements and advances are needed for reactor systems and component technologies that ultimately would be used in the design, construction, or operation of existing and future nuclear power plants and Generation IV nuclear power systems [See References 1-5]. Grant applications are sought: (1) to improve, optimize, and control nuclear power plant systems and component instrumentation, and to more accurately measure key reactor and plant parameters, by developing and improving the reliability of advanced instrumentation, sensors, and controls; (2) to improve the monitoring of plant equipment performance and aging, using improved diagnostic techniques for in-service and non-

destructive examinations; (3) for advanced instrumentation, sensors, and controls for very high temperature Generation IV reactor designs that can withstand temperatures in excess of 1000°C; (4) for advanced instrumentation, sensors, and controls for very high irradiation environments that will be encountered in evolutionary and Generation IV reactor designs, and (5) for advanced reactor/core computer simulation methods for new Generation IV reactors, major reactor components, and reactor core and fuel assemblies – areas of interest include advanced reactor design model code development, coupled/parallel thermal-hydraulic-reactor physics tools, safety and performance evaluation methods, and engineering calculations. Please note that the following areas of investigation are NOT of interest and will be declined: concepts for complete or partial reactor plant designs; generalized thermal-hydraulics analysis (e.g. CFD or two-fluid codes) and probabilistic risk assessment tools or methods; reactor/core computer simulation methods for existing light water reactor designs, nuclear power plant security, or building/containment enhancements; and NRC licensing and site permit issues. In addition, grant applications that deal with nuclear materials, chemistry, and/or corrosion research are also not of interest for this topic and should be submitted instead under Topic 24.

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PROGRAM AREA OVERVIEW OFFICE OF ENERGY EFFICIENCY AND RENEWABLE ENERGY

http://www.eere.energy.gov

The mission of the Office of Energy Efficiency and Renewable Energy (EERE) is to strengthen America's energy security, environmental quality, and economic vitality through public-private partnerships that enhance energy efficiency and productivity; strengthen the U.S. manufacturing sector with advances in innovation; bring clean, reliable, and affordable energy technologies to the marketplace; and make a difference in the everyday lives of Americans by enhancing their energy choices and their quality of life.

In order to accomplish this mission EERE has streamlined and integrated its program and business management by creating 11 programs to most effectively address the needs of the industry, transportation, buildings and power sectors: Biomass; Buildings; Distributed Energy and Electricity Reliability; Federal Energy Management; FreedomCar and Vehicle Technologies; Geothermal; Hydrogen, Fuel Cells, and Infrastructure Technologies; Industrial Technologies; Solar Energy Technology; Wind and Hydropower Technologies; and Weatherization and Intergovernmental. One of EERE's core mission priorities is to engage and partner with the small business technology sector, in so doing, "leapfrog the status quo" by facilitating the development of new technologies that will dramatically reduce or end dependence on foreign oil; increase the viability and deployment of renewable energy technologies; increase the reliability and efficiency of electricity generation, delivery, and use; increase the efficiency of buildings and appliances; and increase the efficiency/reduce the energy intensity of industry.

It is estimated that the energy technologies and practices supported by the EERE programs have saved Americans billions of dollars in energy costs over the past decade. These savings are projected to dramatically increase as emerging and new energy technologies are developed and commercialized. These energy savings are accompanied by parallel reductions in emissions and pollutants that affect human health and in the production of greenhouse gases. The EE program in renewable energy has advanced the state of technologies in such areas as solar, wind, and biomass to the point where renewables have been projected to supply as much as 28 percent of the Nation's energy by 2030.

26. INNOVATIVE WASTE HEAT RECOVERY TECHNOLOGY AND NOVEL COOLING SYSTEMS

Many processes, especially in industrial applications, produce large amounts of excess heat – i.e., heat beyond what can be efficiently used in the process. Waste heat recovery methods attempt to extract some of the energy as work that otherwise would be wasted. Typical methods of recovering heat in industrial applications include direct heat recovery to the process itself, recuperators, regenerators, and waste heat boilers. In many applications – especially those with low-temperature waste heat streams, such as automotive applications – the economic benefits of waste heat recovery do not justify the cost of the recovery systems. Innovative, affordable methods that are highly efficient, applicable to low-temperature streams, and/or suitable for use with corrosive or "dirty" wastes could expand the number of viable applications of waste heat recovery, as well as improve the performance of existing applications. The focus of this topic is on the development of innovative waste heat recovery processes and techniques that are (1) more efficient than conventional methods, yet still cost-effective; and (2) applicable to waste streams from which heat cannot be recovered easily with conventional methods.

Turning to cooling, air conditioning systems consume approximately 10% of the energy used in U.S. buildings and are key contributors to peak demand. Consequently, improving the energy efficiency of air conditioning systems would substantially reduce overall energy consumption and enhance grid reliability. For example, compressors require cooling to dissipate the heat produced during compression and could benefit from improved surface heat transfer – innovative designs could increase the available heat-transfer area or materials enhancement could increase the heat flux between the hot and cool sides of a heat exchanger. Similarly, a reduction in the requirement for condenser cooling could provide significant energy savings if more-efficient, cost-effective technologies were developed. **Grant applications are sought only in the following subtopics:**

a. Novel Equipment and Materials for Industrial Waste Heat Recovery—The recovery of waste heat from exit gases can significantly increase the energy efficiency of industrial processes. Energy can be recovered from flue and stack gases, vent gases, and combustion gases at a variety of temperatures at large-scale industrial plants (chemical plants, petroleum refineries, biorefineries, pulp and paper mills, etc.). Grant applications are sought to develop novel equipment and materials for the recovery of this waste-heat energy. Areas of interest include: (1) waste heat boilers capable of recovering heat from corrosive streams, including the development of corrosion-resistant coatings for both low and high temperature applications; (2) improved heat transfer from new heat exchanger geometries and innovative fluids (used in closed-loop systems), for use in waste heat rather than direct gas firing; (4) development of advanced cycles and working fluids, which would increase temperature lift in absorption cycles and improve overall heating and cooling performance; and (5) cost-effective thermoelectric or thermoionic materials capable of producing electricity from heat, with at least 15% thermal efficiency.

b. Automotive Waste Heat Recovery—The growing demand for electric power in vehicles is currently being met with inefficient, pulley-driven mechanical generators that are driven off of the vehicle engine. Although improvements in generator efficiency have been on-going, it is the nature of such systems to rob the engine of shaft power, thereby decreasing overall system efficiency. In contrast, extracting electricity from the energy lost to engine exhaust or from the coolant loop would be, essentially, "free energy" and would improve overall system efficiency. As an example, in a spark-ignited automobile, 30% to 40% of the fuel energy is lost out the exhaust pipe, and an additional 30% is lost through the radiator. Recovering a portion of these heat losses as electricity could enable radical hybridization and allow spark-ignition technology to compete with diesel on an efficiency basis. Therefore, grant applications are sought to develop:

(1) Thermoelectric or thermionic energy conversion devices for the direct conversion of exhaust or coolantrejected heat to electricity with conversion efficiencies greater than 15%. The devices should be able to provide power generation or heating/cooling for automotive applications within the cost criteria for commercial production.

(2) New approaches to recuperative or regenerative engine operating cycles, including modified compression/expansion ratio control. Such approaches would decrease the amount of energy expended, and consequently increase the proportion and amount of useful work produced, during the combustion process.

(3) Electric turbo-compounding systems that produce more electric power and provide higher overall engine efficiencies than current turbocharger systems. These electric turbo-compounding technologies should deliver over 1.5 kW of electric power for 2500 hours and increase overall engine efficiency by 10 percent or more.

Applications for technologies that merely reiterate currently-commercial technologies will not be considered.

c. Novel Cooling Systems for Buildings—Nearly all air conditioners sold in the U.S. are based on vapor compression technology, and the service, installation, and technical infrastructure to support this technology is well-established. Achieving air conditioner efficiency breakthroughs will require entirely new (non-vapor compression) approaches, revolutionary changes to traditional vapor compression systems, or new ways of operating conventional vapor compression systems. Therefore, grant applications are sought to design, develop, and demonstrate: (1) high efficiency non-vapor compression technologies, including but not limited to those listed above, that have the long term potential to achieve efficiencies much higher than conventional vapor compression systems in system efficiency at modest cost—systems with reduced global warming potential are also desirable; or (3) technologies that facilitate new operational strategies for conventional vapor compression cooling, in order to substantially reduce energy consumption and possibly provide other non-energy benefits such as enhanced comfort, at modest cost. All grant applications must provide detailed estimates of the cost-effectiveness of the proposed technologies.

With respect to (1) above, numerous non-vapor compression cooling system approaches have been explored in the past, including thermally-activated absorption and adsorption, Stirling cycle, magnetic refrigeration, thermoacoustic refrigeration, Malone refrigeration, and others. Aside from specialty applications where particular characteristics (e.g. very long life, ultra-high reliability) are necessary, few of these alternatives have gained significant commercial acceptance due to the high costs and low projected efficiencies. However, advances in materials, electronics, sensors and controls may provide new opportunities for improved efficiency at acceptable costs. In particular DOE's Zero Energy Home (ZEH) project has called for the development of high efficiency systems with low cooling capacities (e.g. 1 ton) – improvements to some of the alternative approaches listed in this paragraph may be effective at these lower capacities. With respect to (2) above, Direct Expansion (DX) systems like unitary central residential and commercial rooftop air conditioners, which are available in a variety of efficiency levels, account for the bulk of air conditioner energy consumption. Residential systems are available with Seasonal Energy Efficiency Ratio (SEER) levels from 10 (the minimum efficiency allowed by standards) to approximately 18, while rooftop units are available with Energy Efficiency Ratios (EERs) from approximately 9-12. However, the units with the highest efficiencies are too expensive to achieve any significant market acceptance, particularly in residential capacities. These high efficiencies are often achieved by adding large amounts of heat exchanger coil area and/or multiple compressors, leading to system sizes and costs that are unacceptable to consumers. Achieving dramatic increases in the efficiency of these vapor compression systems will require completely new designs for key components such as compressors, heat exchangers, fans, blowers, and motors. Examples might include variable capacity compressors that maintain high efficiency throughout their operating range, without the need for expensive inverters; new approaches for enhancing the heat transfer of heat exchanger coils using new materials or fabrication processes; or the application of advanced electronics and sensors.

With respect to (3) above, the energy consumption of conventional air conditioning systems could be reduced by adding features that allow the systems to operate more intelligently. Examples include: using adaptive/fuzzy logic controls to enhance comfort and indoor environmental quality while reducing energy consumption, providing real-time energy-use feedback to consumers in order to change their usage patterns, optimizing operations based on current or predicted outdoor and occupancy conditions, and improving zone control using approaches such as microenvironments or automated ductwork-damper systems with occupancy sensing.

d. Air-Cooled Condenser Enhancements—Air-cooled condensers, using banks of finned tubes with forced or inductive cooling airflow, are used in binary (organic Rankine cycle) geothermal power plants, in bottoming cycles for combined cycle power plants, and for waste heat recovery. A major challenge is to maximize the airside heat transfer at fixed or reduced airside pressure drop. Grant applications are sought to: (1) enhance the airside heat transfer coefficient via boundary layer renewal or flow control, using innovative devices such as small transverse fins (tabs) on the major fins, unique fin types such as pleated fins with flow through small holes in the fins, or vortex generators to direct flow into the wake region; (2) increase the effective temperature difference by using a water stream in contact with the incoming air to reduce the air temperature by evaporative cooling, or by dripping or flowing a limited amount of water over the fins and tubes (deluge cooling); or (3) decrease the parasitic power requirement by minimizing the pressure drop while maintaining constant heat transfer through an improved the airside flow path, or by innovative changes in the fan so that it moves more air with less energy.

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27. ADVANCED MATERIALS

Advanced materials play a fundamental role in technology advance, underpinning the development of new technological capabilities as well as whole new industries for the transformation and production of new energy

carriers, services, and products. The following have been identified as critical areas for the development of advanced materials. Grant applications are sought only in the following subtopics:

a. Advanced Materials for Hydrogen and Fuel Cell Technologies—In his 2003, State of the Union address, President Bush expressed a goal to reverse America's growing dependence on foreign oil by developing commercially-viable, hydrogen-powered fuel cells. This subtopic addresses two major materials challenges for fuel cells: (1) the need for materials/coatings for low-cost bipolar plates; and (2) materials/concepts to address freeze/thaw and cold startup issues for improved durability.

The bipolar plate is a major component of the Proton Exchange Membrane (PEM) fuel cell stack and plays a critical role in performance, durability, and cost. New developments in materials, along with low-cost fabrication processes, would ultimately lead to commercially viable fuel cell systems. Therefore, grant applications are sought to develop new materials that can be used for the bipolar plate or new corrosionresistant coatings for use with inexpensive base materials for the bipolar plate. These materials must be lowcost, durable in the fuel cell environment (i.e., under acidic, oxidizing, and reducing conditions), and suitable for high-volume manufacturing processes. Materials proposed as coatings must be rugged, corrosion-resistant, and defect-free, and capable of being formed on complex shapes (including sharp corners and perforations) using commercial fabrication techniques. Such coatings must be resistant to temperature changes because fuel cell stacks undergo frequent start, stop, and dynamically varying load cycles. All of these materials, including the coatings, must be excellent electronic conductors so that they can be formed into tough, flexible, thin, and low-mass bipolar plates, capable of surviving low ambient temperatures (down to -40° C) with normal operating temperatures up to 120°C or higher. Performance targets for the bipolar plates are: conductivity greater than 100 S/cm; corrosion rate less than 16 : A/cm²; hydrogen permeability less than 2×10^{-6} cm³/(cm²·s) at 80°C and 3 atm or equivalently 0.1 mA/cm²; flexibility greater than 5 %; crush strength greater than 4200 kPa; and weight less than 1 kg/kW. The high-volume production cost target for bipolar plates is \$10/kW.

In transportation applications, fuel cell systems will undergo frequent startups and shutdowns, will operate under variable load conditions, and may be used under sub-freezing conditions. In such cases, these fuel cells would need to survive sub-freezing temperatures, perhaps as low as -40°C in northern North America, and be able to startup from such low temperatures. Therefore, grant applications are sought to develop new materials for use in fuel cells, fuel cell stacks, or in the system's balance-of-plant. The materials must resist degradation by exposure to sub-freezing conditions, and help to improve the fuel cell's performance during the start up and warm up periods. One particular area of interest is the development of new membrane materials that are intrinsically tolerant of repeated freeze/thaw conditions, while maintaining high performance and durability. In addition to the material development effort itself, grant applications must consider how these new materials would be used to address the freeze/thaw and cold startup issues.

b. Advanced Materials for Bioproducts—Materials derived from lignocellulosics, and/or from resins that result from the chemical or biological conversion of biomass components, can serve as value-added co-products from an advanced lignocellulose-based biorefinery. Grant applications are sought to: (1) develop and demonstrate new co-product materials, based on improved methods to functionalize fibers or to prepare compatible fiber-resin combinations; (2) develop corrosion and abrasion resistant materials for components used in the processing of aggressive streams associated with the pretreatment of lignocellulosic feedstocks and the thermochemical conversion of black liquor; and (3) facilitate the efficient physical, chemical, and structural characterization of fibrous or resinous intermediates, residues, or materials derived from biomass processes. Of particular interest are fibrous lignocellulose/cellulose (for fiber) high molecular weight polymers or reactive systems that can be converted to high performance materials, especially methods for improving the strength of interactions between the hydrophilic lignocellulosic materials and the more hydrophobic resins.

c. Advanced Phosphor Technology for General Illumination—Phosphors are widely used in many lighting and display applications, ranging from conventional fluorescent lighting to more contemporary solid state devices. All of these applications have important implications for energy conservation. For example, modern fluorescent lighting consumes more than 40% of the total energy attributed to lighting -60% of the lighting in commercial and industrial spaces. Modern lamps, especially T-8 linear fluorescent lamps (LFLs) are good at producing very high light quality with acceptable energy efficiency over an extensive lifetime, and compact fluorescent lamps (CFLs) are not far behind. However, even the best of today's T-8 LFLs convert less than 30% of the power consumed into visible radiation. Solid state lighting (SSL) devices, such as light emitting diodes (LEDs), also may depend upon phosphors to convert some of their blue or near ultraviolet radiation into useful visible light. As bright and efficient as these devices have become in recent years, the conversion of monochromatic light into broad spectrum, white light is not particularly efficient – less than 40% of the light produced is actually released from the device. Other potential applications of phosphor technology may exist, both in general illumination and within the building envelope. One possibility is the conversion of infrared radiation into visible light, using nanocrystalline phosphor structures that alter emissive wavelengths; another is the development of infrared capture mechanisms for potential use in semiconductor devices such as LEDs and photovoltaics.

Grant applications are sought to increase phosphor efficiency or range of application. Areas of research interest include: (1) multi-photon phosphors (MPP) that employ novel conversion schemes to increase long wavelength photonic emissions, using quantum splitting phosphors (QSPs) or other molecular effects such as nanoscale properties; and (2) novel macro-scale effects such as unusual phosphor material structures or different manufacturing methods.

d. Advanced Materials for Lightweight Vehicles—Lightweight materials in automobile structures can provide significant fuel savings, but they also must be able to withstand or absorb the energy of impact in order to protect occupants in collisions.

Grant applications are sought to develop rapid processing technologies for reinforced polymers that can be used in primary and secondary structures of passenger vehicles. Areas of interest include: (1) rapid cure technologies, for use with thermoset-based composites, using UV, IR, E-beam, acoustic, or any other nonthermal methods; (2) rapid forming of thermoplastic composites, including production technologies where composites are molded to a rough shape and then thermally-assisted methods are used to complete the forming; and (3) non-liquid molding process technologies for continuous and discontinuous fiber reinforced composites. Grant applications must show that the concept(s) can be cost-effectively incorporated into the high-rate, highvolume manufacturing of commercial passenger vehicles.

Grant applications also are sought to develop energy absorbing metal foams to be used in conjunction with aluminum beams for enhancing energy absorption in automotive crash scenarios. Areas of interest include: (1) new foamed metallic systems that demonstrate consistent, well-characterized structure and properties; (2) cost-effective processing technologies for existing foamed metals, which demonstrate sufficient control to reliably deliver materials of consistent, well-characterized structure and properties, covering a range of required performance scenarios; and (3) manufacturing processes for incorporating metal foams into useful automotive structures. Grant applications must demonstrate that the foams can be cost-effectively produced with properties sufficiently uniform to reach full-scale commercialization. In addition, the foams must be cost-effectively incorporated into automotive component designs, consistent with the high-rate, high-volume manufacturing of commercial passenger vehicles.

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28. NEW ENERGY SOURCES

To meet national energy needs, diversify energy supplies, reduce security and reliability risks, and reduce environmental impacts, there is a need to develop new, clean, and domestic sources of energy. Renewable energy technologies have achieved significant advances in recent years, but further improvements are needed if they are to realize their full potential. Advances are needed in solar photovoltaic systems, hydrogen energy carriers, ocean hydrodynamic systems, and wind turbines. **Grant applications are sought only in the following subtopics:**

a. Solar Photovoltaics Technology—Further development of solar photovoltaic (PV) systems is needed through creative and innovative approaches in engineering and design, new materials and processes, and cross-cuts from other fields. The following areas would complement and enhance the existing research activities:

(1) Thin film photovoltaic modules of copper indium selenide (CIS) or cadmium telluride (CdTe) have the potential to reach energy-significance and produce over 100 GW/yr of PV modules at some future date. To accomplish this, the CdTe and CuInSe₂-alloy layers must be thinned from today's 2-5 microns to less than 1 micron, and preferably below 0.5 microns, to avoid severe price and availability pressure on the rare elements, indium and tellurium. The use of thinner layers would also reduce materials costs, processing times and costs, maintenance costs, and waste and waste treatment costs in the manufacturing process. Grant applications are sought to fabricate ultra-thin layers of CIS and CdTe for PV modules, leading to the manufacture of these modules at the end of three years. The thin layer technology is expected to sustain high efficiencies (over 15% cells) and good manufacturability, despite the potential for increased pin-hole and uniformity problems.

(2) Current solar concentrators that utilize troughs, heliostats, and dishes utilize relatively conventional materials and designs of glass and steel. Grant applications are sought to develop new concentrator designs that could lower first costs, potentially lower operating costs, be easy to manufacture and install, and be replicable for large fields of troughs, heliostats, and/or dishes. Designs must accommodate trough concentrators of at least 4 meters aperture, heliostats of at least 100 m², and dishes of at least 100 m².

(3) Grant applications are sought to develop easily manufactured PV systems that can capture waste solar thermal energy (that heats the PV cell, especially the concentrating cell) at high efficiency for use in other processes or co-generation applications. The grant application must show that the design will provide significant value-added benefits.

(4) Grant applications are sought to develop and manufacture solar cells based on polymers, small molecules, dyes, chromophores, or other materials (e.g. quantum structures of inorganic materials). The goal is to develop solar cells with efficiencies above 10%, using designs capable of achieving good reliability, low cost, and easy manufacturability.

(5) The ability of crystalline silicon PV systems to continue rapid market growth will be partly determined by the ability to supply sufficient silicon feedstock at a low cost and at sufficient quality for producing high efficiency cells. Therefore, grant applications are sought to develop low-cost rapid processes for the production of crystalline silicon. Grant applications must demonstrate significant improvements over current technologies.

b. Novel Carrier Technologies for Hydrogen—For the nation to move toward a hydrogen economy, cost issues must be addressed. For example, the target cost for the delivery of hydrogen from the central production facility to the point of use at a refueling station or stationary power facility is less than \$1.00/kg hydrogen. This

includes handling and compression at the refueling station or stationary power facility. To enable this delivery cost, the following material performance targets have been established: hydrogen content by weight 10%; hydrogen content of 150 kg H_2/m^3 ; and energy efficiency of 85%.

Grant applications are sought to develop novel materials for use as high energy density, low-cost energy "carriers" for vehicles, fuel delivery, stationary power, and off-board energy storage applications. Approaches of interest will store hydrogen absorbed in the form of a chemical compound or adsorbed on a high-surface area sorbent. All approaches must be able to release the hydrogen as needed. In addition, grant applications must address issues of material durability and cycle life, hydrogen uptake and discharge kinetics, process conditions during operation, and requirements for heat removal and addition. Technologies excluded from this topic include on-board or off-board reformation of fuel to make a hydrogen rich stream; ammonia, hydrazine, and borate based chemistries; and materials for use as primary energy sources.

For on-board vehicular storage, the material approaches must be consistent with the range (greater than 300 miles), weight, volume, and cost constraints posed by customer expectations. In particular, approaches that have the potential to meet or exceed the 2015 DOE/FreedomCAR storage system performance targets of 3kWh/kg (9wt.% hydrogen); 2.7 kWh/L; and \$2/kWh are desired. Additional information on hydrogen storage performance targets can be found in the references.

For storage concepts that require off-board regeneration, the disposition of the "spent" fuel (e.g., reclamation and regeneration) must be addressed. Approaches must meet optimum life-cycle cost, efficiency, and environmental requirements for the regeneration of the spent fuel, while meeting the cost and volumetric/gravimetric energy capacity targets for the hydrogen-storing system.

c. Hydrodynamic Ocean Energy—Ocean hydrodynamic energy – which depends upon the kinetic and potential energy in waves, tides, and currents, either in deep ocean or near coast lines – is a potentially significant energy resource. For example, the California Energy Commission has estimated that wave energy resources on the order of 17 MW per mile exist along the northern coast of California. Grant applications are sought for energy technology systems that can tap ocean wave, tidal, or current energy resources. Desired designs will be non-obtrusive and robust, have lifetimes on the order of 10 years or greater, be low maintenance, and have relatively high energy density. Grant applications must address the life cycle cost of energy, which will be a primary evaluation criterion, and clearly demonstrate how the research effort will proceed to hardware development, fabrication, testing, and manufacture of ocean energy devices.

d. Sensors for Monitoring and Controlling Wind Turbine Components—Improving the operation and maintenance of wind turbines can greatly increase system reliability and have a significant impact on the cost of wind energy. To achieve this improvement, remote systems are needed that can accurately monitor and control component performance, and predict pending failure based on actual physical measurements. Grant applications are sought to develop the following monitoring and control instrumentation: (1) a wind turbine gearbox monitor to determine the state-of-health and predict impending failures of gearboxes – this would greatly increase gearbox reliability and reduce Operation and Management costs; (2) a blade deflection sensor to detect the deflection of the turbine rotor blade – based on actual physical measurements or imputed values based on stresses or strains – and feed this information to the control systems for blade pitch, in order to protect against possible tower strikes in extreme conditions; and (3) a rotor control sensor and actuator capable of high speed aerodynamic control of rotor blades in rapidly changing wind conditions. Sensors and controls must be low cost and capable of extended operation in remote and sometimes harsh environmental safety; and clearly demonstrate how the research effort will proceed to hardware development, fabrication, and testing of a prototype system.

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29. ADVANCED POWER ELECTRONICS TECHNOLOGIES

Unique applications for conversion of power, either from electrical to mechanical form or vice versa, often require unique approaches. With recent advances in power electronics and generator/motor technology, several new areas of emphasis have evolved that require innovation to achieve their expected effect on energy conversion technology. This topic solicits new materials technology for power electronics components, as well as technology for using power electronics in new applications. Grant applications must clearly show how the research effort will proceed to hardware development, fabrication, testing, and manufacture of power electronics components and devices. **Grant applications are sought only in the following subtopics:**

a. Advanced Power Electronics Component Materials—Over the past 10 years, advanced silicon power chips have revolutionized power conversion with the use of new power semi-conductor devices such as Integrated Gate Bi-Polar Transistors (IGBTs). Although these devices continue to improve in performance and power handling capability, there exist alternative materials that could revolutionize the performance of power electronic components. Materials such as gallium-arsenide, diamond, and, in particular, silicon-carbide (SiC) offer potentially outstanding properties for power conversion: large band-gap, high breakdown field, good thermal conductivity, and a high saturation velocity. In addition, SiC has high elastic modulus and toughness, and SiC devices can operate at temperatures up to 600°C. Grant applications are sought to develop technology to further the use of these materials in improved power electronics devices. Areas of interest include: overcoming micro-pipe defects in SiC wafers (i.e., small tubular voids that run through the wafers in a direction normal to the polished wafer surface), innovative thermal management, advanced bonding and soldering techniques that can withstand higher temperatures, incorporating long-life capacitors in advanced SiC components, insulated metal substrates, elimination of wire bonds, automated manufacturing, and innovative packaging.

Another target of opportunity relates to the thermal properties of materials used in existing power modules. These modules are constructed by bonding the die, copper layers, substrate, and the base plate together. The whole module is then mounted on a heat sink using thermal interface materials. Unfortunately, existing thermal interface materials that can withstand high temperatures have very low thermal conductivities; in fact, the thermal interface material represents 30 to 40 percent of the total thermal resistance between the junction and the heat sink. Grant applications are sought to reduce this resistance by developing thermal interface materials with increased thermal conductivity. This requirement becomes even more important for power electronics components using SiC, which operate at higher temperatures.

For both of the above areas, special consideration will be given to grant applications that address the special operating conditions and requirements (reduced size, weight, and adverse environmental operating conditions) of electric vehicles, fuel cells, and wind turbines.

b. Permanent Magnet (PM) Drives, Motors, and Associated Power Electronics—The rapidly declining cost of rare earth permanent magnets (e.g., neodymium-iron-boron), along with their improved magnetic properties, is rapidly revolutionizing the use of permanent magnet motors and generators. Rare earth PM generators and motors offer improved power-to-weight characteristics for use in electric and hybrid vehicles, wind generators, gas turbines, gas compressors, and a wide range of other applications. Increases in the magnetic properties of the magnets would allow such devices to be applied to generators in the size range of 1 to 10 MW. Improved PM generators could be more easily designed and built as direct drive units, thereby eliminating gear boxes and oil lubrication systems while improving efficiency. These improved devices also could find use as prime movers in compressors and variable speed drives. Grant applications are sought to further improve the performance of rare earth PM generators/motors by integrating them with improved power converters. This combination would provide for variable speed operation, allowing devices such as gas turbine generators and wind turbines to run at optimum operating speeds. Areas of interest include advanced design, design tools, assembly processes, alternate fabrication materials, optimized cooling, improved reliability, electrically-insulating thermally conducting materials for cooling and thermal modeling techniques – all necessary to develop units with high power density, high efficiency, and low cost of manufacture and operation.

c. Power Electronics for Renewable Energy Applications—Improved power electronic components and circuit topologies present ever changing opportunities for improving modules for a wide range of applications in renewable energy. Power converters/conditioners and controllers could provide improved performance and integration of renewable energy technologies such as photovoltaics, wind, and hydrogen.

With respect to photovoltaics (PV), a new concept known as "AC Photovoltaic Module" could revolutionize the PV industry through improved building integration. As a first step toward commercialization, grant applications are sought to develop innovative DC-to-AC micro-inverters (in the watts range) that can be integrated into a PV panel for roof-top mounting or into other small PV-powered systems on buildings (window frames, roofs, etc.). These inverters must be rugged, able to withstand the brutal environments associated with rooftops, and must have long lifetime. Goals for the concept are to significantly reduce balance-of-system (BOS) costs, improve reliability and ease of installation, reduce the cost of the micro-inverter to the range of \$0.15 to \$0.30 per watt, and increase the efficiency to 94% or higher, while maintaining all Underwriters Laboratory and interconnection requirements.

Most modern wind turbines operate at variable speeds and use power electronics to condition the power, changing it from variable frequency AC to DC, and back to fixed frequency AC. A key aspect of the controller is that it is an active part of the wind turbine load-control, used to control the torque on the wind generator and rotor. The existence of the DC link within the control system offers an opportunity to use the power output of the wind turbine to directly drive an electrolyzer for H₂ production. An electrolyzer requires DC input and normally has a separate power converter that draws power from the electrical grid. By eliminating one set of power electronics, the cost of H₂ production could be significantly reduced. Therefore, grant applications are sought to design, fabricate, and test a wind-hydrogen electrolyzer system, focusing on the development of an integrated power electronics package that simultaneously converts a wind turbine's output into grid quality power and controls hydrogen generation at the 100 kW to 1 MW scale. The challenge of this approach is to develop a device that can provide load control for the wind turbine while simultaneously producing DC for an

electrolyzer and AC for the grid. No existing device can currently provide all three functions, and its design will require a thorough understanding of wind turbine and electrolyzer operations, as well as the requirements for grid connection including adherence to IEEE 519 grid interconnection standards. To be successful, such a device must be able to perform the described functions without adding more than 10% to the cost of a normal wind turbine power converter, for which current costs are approximately \$70/kW. Grant applications should include projections for capital and operating costs and should clearly show how the research effort will proceed to hardware development, fabrication, and testing of a prototype wnd-H₂ power converter in Phase II, with demonstration in Phase III.

d. Improved Illumination—Numerous applications for efficient, power electronics exist today in lighting applications. The most pervasive opportunity is the application of power electronics to ordinary linear fluorescent lamp (LFL) ballasts, especially ballasts with dimming capability. Grant applications are sought to reduce the complexity and component count of ordinary LFL ballasts, while simultaneously conserving electricity and providing new functionality (such as integrated controls for networking, dimming, or diagnostics) at little or no additional costs. Advanced ballast features of interest include programmed controlled start, lumen-driven current controls to minimize output variations near the end of lamp life, continuous power factor correction, and automatic adaptation to differing lamp types and currents. These features may all be possible with new, novel ballast designs that also could increase lamp life, installation value, and most importantly, system efficacy.

In addition to fluorescent lamps, improved power electronics offer opportunities for other types of high power discharge lamps. For example, advanced power electronics may enable the use of low-power, high-intensity-discharge (HID) lamps that may be more energy efficient, have longer life cycles, and be more cost-competitive than the conventional lamps they may replace. Most significantly, the magnetic ballasts of conventional lamps possess limited functionality: while these ballasts may be adequate for many of today's industrial applications, they fail to provide the flexible service demanded by other markets, such as retail and residential. Therefore, grant applications are sought to integrate advanced power electronics into these high intensity lighting systems to provide new service features such as programmed controlled start, dimming (even within a limited range), networking, lumen maintenance, and diagnostic interfaces. Of particular interest are approaches that also reduce the cost differential between fixed-output ballasts and dimming ballasts.

Finally, innovations in power electronics and controls could have application for solid state lighting (SSL). Existing power supplies for SSL are derived from commercial, off-the-shelf (COTS) supplies that are not optimized for the SSL devices, applications, or controls. Grant applications are sought to apply power electronics technology to efficiently power and control SSL, such that the range of performance is extended beyond, and yet costs remain competitive to, the COTS options.

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30. REACTIONS AND SEPARATIONS

Advances in oxidation catalysis and separation process technologies can increase energy efficiencies in a variety of industries. In the petroleum and petrochemicals industries, oxidation catalysis is a leading technology for chemical synthesis, with great potential for improved feed stock efficiencies, environmental impact, and energy savings. New developments in oxidation catalysis also would be likely to influence catalytic developments for many other commercial catalytic transformations. The Department of Energy supports R&D in oxidation catalytic technology to overcome current limitations of selectivity and efficiency, leading to substantial energy savings, improved economic performance, enhanced utilization of feedstocks, and reduced requirements for materials of construction.

Separation technologies recover, isolate, and purify products in virtually every industrial process. Pervasive throughout industrial operations, conventional separation processes are energy intensive and costly. 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. Industrial efforts to increase cost-competitiveness, boost energy efficiency, increase productivity, and prevent pollution, demand more efficient separation processes. In response to these needs, the Department of Energy is seeking the development of high-risk, innovative separation technologies applicable to the exploration and use of geothermal energy as a heat and power resource, the conversion of biomass to fuels and chemicals, the petroleum refining and petrochemicals industries, and the mining industry.

Grant applications must address the potential public benefits that the proposed technology would provide from reduced energy consumption and from the reduction in one or more of the following: materials consumption, water consumption, and toxic and pollutants dispersion. Grant applications also should include a plan for introducing the new technology into the manufacturing sector, in order to access capabilities for widespread technology dissemination. Grant applications are sought only in the following subtopics:

a. Catalytic Oxidation—All industrial syntheses of oxygenated compounds from hydrocarbons involve the cracking of paraffins to olefins and the subsequent direct or indirect addition of oxygen. The direct addition of oxygen to olefins is exothermic, and, therefore, energy savings can result from saving hydrocarbon feedstock through increased selectivity. Indeed, the enhancement of oxidation selectivity represents the largest potential improvement of energy efficiency in the chemical industry (Parshall, 1994). Grant applications are sought for the research and development of technologies for improving the efficiency of industrial catalytic oxidations. Areas of particular interest are: (1) selective oxidation of petroleum feedstocks for commodity chemicals, thereby enhancing efficiency by reducing over-oxidation; (2) alkane activation for direct oxidation with molecular oxygen, e.g., methane to methanol; (3) heat integration of catalytic oxidations with other processes; and (4) improvements in the syntheses or use of reactive intermediates. Item (4) above could involve the use of peroxides; the *in situ* generation and consumption of reactive intermediates to achieve steady state benign operations, e.g., phosgene; or the full replacement of these intermediates, e.g. phosgene, HCN, chorine, etc.

b. Distillation—Significant quantities of inorganic acids, and all commodity organic chemicals, are purified by distillation at some stage in their manufacture. Distillation accounts for more than 60% of the total process energy used for the manufacture of commodity chemicals and is therefore a meaningful target for improvements in energy efficiency. Grant applications are sought to develop new technologies for significantly enhancing the energy efficiency of existing distillation systems used in the U.S. for the manufacture of any major commodity chemical, both inorganic and organic. Areas of interest include: (1) systems integration in commodity

chemical manufacture that could be implemented at an attractive cost and reduces currently needed distillation capacity; (2) hybridization of distillation with other more efficient means of separation such as membranes – but before developing this approach, the history of commercial attempts to introduce efficient hybrid distillation systems should be carefully reviewed; (3) design and development of new column externals, such as the reboiler and the condenser, provided that the technology can be demonstrated at an acceptable cost and pay back period; and (4) processes that take advantage of the excess reactive distillation capacity that may result from regulations on oxygenated fuel additives in the chemical industry, provided that the new processes enhance energy efficiency over the processes replaced.

Grant applications should include a review of the state of the art of the targeted distillation application in the U.S., including a review of its current inefficiencies, in order to provide a sound technical basis for the efficiency gains to be expected from the technology development effort. Strategies to overcome the inefficiencies should be identified and practical means to address them developed. The number of distillation units in the U.S. that could apply the new technology should be identified, along with the energy savings that could be derived by reasonable market penetration. The cost of applying the new technology and the ease of implementation also are important: approaches must demonstrate an attractive cost, maintain (or enhancing) system reliability and safety, be capable of retrofit at attractive cost, and meet or exceed the performance characteristics demanded of distillation systems. Incremental improvements to existing distillation technologies are not of interest, nor is technology that is not broadly applicable to distillation as applied today in commodity chemical manufacture.

c. Biomass Separation Process Technologies—Process streams resulting from the primary

fractionation/saccharification of lignocellulosic biomass are typically highly complex slurries that are difficult to process and separate. Such slurries often contain substantial levels (10-20% w/w) of insoluble lignocellulosic solids as well as high concentrations of soluble biomass sugars (>10-20%) along with a variety of other soluble components (organic and inorganic acids, aldehydes, phenolics, etc.) that are typically present at lower levels. Advanced separation process technologies, which would enable more cost effective solid/liquid (S/L) separations of such slurries, are needed for bulk or primary S/L separations, as well as for secondary/polishing S/L separations. Therefore, grant applications are sought to develop: (1) improved upstream fractionation, to recover products and/or facilitate bio/catalysis and to reduce the cost of downstream recovery and purification; (2) advanced concepts such as reactive separations schemes that will enable in situ combination with bio/catalysis steps, or approaches that are substantially more energy efficient and/or require much less capital equipment; (3) techniques to remove smaller suspended particles or high molecular weight compounds from partially clarified liquors, in advance of further purification by chromatography or concentration and/or purification by evaporation and/or crystallization; and (4) efficient membrane separation systems that enable more economic and efficient separation and recovery of specific components (e.g., specific sugars or organic acids) or classes of components (e.g., mixed sugars or mixed phenolics) from clarified biomass hydrolyzate liquors. Progress in these areas will reduce the need for bio/catalysts to tolerate impurities and interfering components, and will help reduce the cost of producing fuels and chemicals from biomass processing streams.

d. Innovative Mineral Processing—Americans currently use 3.5 million pounds of minerals, metals, and fuels per capita in the course of a lifetime (Mining Journal Ltd., Mining Annual Review 1999). To reduce the energy consumption and environmental impacts associated with producing those materials, existing processes must be improved, and new ones must be developed. As used here, the term 'process' refers to methods used to clean, separate, prepare, and recover minerals from mined ores and from geothermal brines. Mineral preparation, physical separation, and chemical separations are key technology areas in need of research to achieve energy and productivity savings in the next twenty years. The greatest potential improvements are associated with the optimization of combined processes and the resulting synergies. For example, combining beneficiation, dewatering, and agglomeration into a single process would reduce flow sheet complexity and materials handling. Recovering minerals from geothermal brines, produced primarily for electric power generation, could enhance the economics of both power generation and mineral production.

Grant applications are sought to develop chemical separation process technologies that would reduce or eliminate processing steps in the mining industry, leading to improvements in overall efficiency. Specific areas of research interest include improved reaction kinetics and heat efficiency, and increased direct conversion and *in situ* recovery. Typical processes of interest include pelletizing or briquetting, smelting, refining, leaching, solvent extraction, bioleaching and electro winning.

Grant applications also are sought to develop mineral recovery technology from geothermal electricity generation facilities. In particular, small prototype systems for the commercial production of silica, manganese, hydrogen or other materials (other than zinc and carbon dioxide) associated with geothermal fluids are desired. The cost and quality of the produced materials and a market for them must be clearly defined.

Grant applications are not sought for improving process efficiencies primarily through emissions controls or through waste disposal, remediation, or treatment. However, this limitation does not apply to approaches that target materials recycling or by-product utilization as their primary focus.

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31. SENSORS AND CONTROLS FOR EFFICIENCY AND RENEWABLE ENERGY APPLICATIONS

Innovative sensor and control technologies could significantly improve the performance, reliability, and economics of energy use in a variety of applications, including the generation of electricity from renewable energy. The integration of sensors and controls would allow feedback systems to continuously respond to system changes, reducing operations and maintenance costs and mitigating technical risk. For example, fault detection and diagnostics systems that provide early warning of system problems could prevent costly repairs or replacement of equipment in wind turbines and HVAC systems. Likewise, the effective monitoring of process conditions, combined with methods for controlling the process, could enable process optimization or problem mitigation in geothermal power generation, biomass conversion, and automotive combustion. Because these process stream, sensors and controls that can work in these harsh environments would significantly contribute to minimizing wasted energy and damage to key equipment. **Grant applications are sought only for the following subtopics:**

a. Geothermal Two-Phase Flow Instrumentation and Control—The fluid produced from geothermal wells is often a two-phase flow consisting of solids along with non-condensable and corrosive gasses. Development of improved two-phase flow monitoring and logging instruments would help reduce the cost of geothermal power, increase the effectiveness of reservoir management, reduce operator risks, and improve the economics of geothermal power production. Such instrumentation must be capable of providing reliable measurements in the high-temperature, physically and chemically aggressive environment of geothermal process streams. Grant applications are sought for the following innovative two-phase monitoring and control equipment: (1) a meter to acquire accurate, real-time measurements of two-phase mass flow at individual producing geothermal well

installations – approaches of interest must not involve such established methods as orifice plate, choke flow, and grab sample technologies; (2) instrumentation for accurately sampling and monitoring geothermal steam quality and purity, in order to protect power plants against process upsets – the instrumentation must signal such occurrences and initiate corrective action to mitigate impending damage; (3) a control valve for throttling two-phase geothermal fluids at the well site – the valve must be resistant to erosion, corrosion, and scaling; have throttling ability from 0 to100% of opening; and have a large, full-opening control valve coefficient, Cv, where Cv is the capacity of a valve in terms of the number of gallons of water per minute that will flow through the valve with a pressure of 1 psi; and (4) a steam quality and flow logging tool for installation in geothermal production wells.

With regard to item (4) above, tool specifications include: outer diameter less than 2 inches; temperature rating of 250°C without the need for heat-shielding; temperature rating of 350°C for 16 hrs with or without heat-shielding (Dewar); pressure rating of 10,000 psi; ability to operate in either memory or real-time mode. The ideal ranges for the measured parameters include: steam quality, 10 to 90%; flow, 0 to 400 tons/hour; pressure, 0 to 10,000 psia; and temperature, 0 to 500°C. Particular consideration will be given to approaches that provide a permanently installed system for monitoring and controlling multi-lateral production values, so as to isolate zones for enhanced well performance.

b. Automotive Sensors, Controls, and Automation—In order to optimize the efficiency, performance, and emissions profile of current and near-term advanced vehicle engines, advances in sensors, controls, and automation are necessary. For example, robust, low-cost sensors for engine-exhaust constituents such as NOx, ammonia, and particulate matter are desired. Also, low-cost sensors for measuring in-cylinder conditions can play an important role in combustion management and control for these engines; these sensors may be either direct or virtual, and may be used to determine when the engine is at the boundary of a particular combustion regime. Although progress has been made in these technologies, commercial devices that meet all of the required performance and cost criteria are not available. Grant applications are sought to develop:

(1) Low-cost, robust sulfur sensors. The purpose of these sensors are to protect two types of systems: first, near-term (2007 - 2010) engine and emission-control systems that use exhaust sulfur traps or other sulfur removal techniques; and, second, the fuel system (which uses, e.g., interlocks), to prevent fuel containing more than 15 PPM sulfur from contacting sulfur-sensitive components.

(2) Broadband fuel sensors that can provide representative chemistry information. The information provided must account for the increasing broad range of chemistries found in heavier fuel sources and for their impact on combustion kinetics, so as to meet high efficiency and low emissions requirements.

(3) A low-cost pressure transducer to enable the detection of cycle-to-cycle variance in peak cylinder pressure, along with the associated crank location of the pressure peak. This transducer would allow on-line, real-time calculation of heat-release rate and other combustion parameters.

(4) Practical, small, cost-effective, and real-time broadband sensors for monitoring engine combustion, exhaust gas, and related parameters needed to control combustion process in an automotive engine. Durable sensors for pressure, temperature or other variables would provide closed-loop control for homogenous charge compression ignition engines. Sensors that provide measurement of exhaust species or intermediates, which may serve as markers of advanced combustion regimes, are of particular interest. Sensors of interest could be installed either within the cylinder or external to it; if installed in the cylinder of an engine, there should be no disruption of the hydrodynamics or thermodynamics of the combustion event.

(5) Practical, durable, and cost effective sensors to monitor exhaust gas species, such as hydrocarbons, oxides of nitrogen, aldehydes, and other compounds created by low temperature combustion regime engines. These would be suitable for on-board diagnostics as well as for feedback loop control systems.

c. HVAC Sensors, Controls, and Automation—New cooling equipment must meet certain efficiency standards when manufactured. However, faulty installation and operating conditions can degrade efficiency. For example, grass clippings from lawn mowing can get sucked into the outside condensing unit coil of a brand new unit and cause the efficiency to degrade for the life of the unit. Although the early warning of problems could prevent unneeded equipment repairs or replacement, there is no easy way to check the efficiency of the system once the equipment is installed. The development of HVAC sensors and controls could allow equipment performance to be measured, and efficiency could be maintained by proper corrective action. Information regarding the equipment being monitored could be communicated over the Internet via modem for remote monitoring in real time by a service company or the owner. Therefore, grant applications are sought to develop: (1) low-cost, remote fault detection and diagnostics systems for HVAC systems, including commercial rooftop and residential systems, that can continuously monitor performance and detect such faults as charge leakage, economizer malfunction, heat exchanger fouling, burner condition, and controls malfunctions; (2) new sensor, electronics, and software technologies that leverage wireless networks, mobile computers, and the Internet to provide user-friendly, low cost systems - for example, intelligent wireless controls, possibly combined with low cost thermal storage, to reduce peak electricity demand from HVAC systems; (3) variable speed motor and drive technologies with low applied costs, using adaptive/fuzzy logic controls to enhance comfort and indoor environmental quality, while reducing energy consumption; (4) modules, for integration with HVAC systems, that can respond to price and peak demand signals; and (5) automated ductwork damper systems with occupancy sensing to improve zone control – with mass production, these FDD (fault detection and diagnosis) systems should add no more than \$50-100 to the final consumer cost of a unitary residential HVAC system.

d. Sensors for Industrial Manufacturing Applications—Real-time measurement and control is needed to optimize the performance of a number of industrial processes: petroleum refining and petrochemical manufacturing; the production of bioproducts and biofuels, forest products, aluminum, steel, and glass; metalcasting and mining. The development of new sensing technologies would enable industry to measure critical process and/or product properties such as temperature and pressure profiles and/or chemical compositions and stoichiometry in real time during the production process itself. The sensors and controls must be capable of withstanding the harsh (corrosive, very high or very low temperatures) conditions found in industrial processing and manufacturing. In addition, the measurements must be made *in situ*, as opposed to the current indirect methods.

Grant applications are sought for the on-line monitoring and control of: (1) reaction conditions and constituent byproduct concentrations in reactors under harsh operating conditions (e.g. extreme pH, high temperature, two or three phase flow, high solids); and (2) biologically compatible conditions on complex slurry streams (e.g. mixtures of biomass sugars in presence of soluble acids, phenolics, and fermentation products/byproducts). Grant applications are also sought for sensor development approaches that use engineered materials solutions, such as molecular scale tailoring, for selectivity and sensitivity; or nanostructured materials/coatings for sensor viability and robustness in harsh environments. Possible applications include but are not limited to the measurement of: (1) temperature and/or composition in cryolite or black liquor; (2) temperatures greater than 600°C, or less than -40°C, (3) sulfur compositions less than 50 ppm, (4) pressures greater than 200 atmospheres.

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PROGRAM AREA OVERVIEW OFFICE OF FUSION ENERGY SCIENCES

www.ofes.fusion.doe.gov

The Department of Energy sponsors fusion science and technology research as a valuable investment in the clean energy future of this country and the world, as well as to sustain a field of scientific research - plasma physics - that is important in its own right and has produced insights and techniques applicable in other fields of science and industry. The mission of the Fusion Energy Sciences (FES) program is to acquire the knowledge base needed for an economically and environmentally attractive fusion energy source. FES research efforts seek to: (1) understand the physics of plasmas, the fourth state of matter – plasmas constitute most of the visible universe, both stellar and interstellar, and progress in plasma physics has been the prime engine driving progress in fusion research; (2) identify and explore innovative and cost-effective development paths to fusion energy – the current fusion program encourages research on a wide range of approaches including the Tokamak (the leading power plant candidate), other magnetic configurations, and inertial fusion energy using particle beams or lasers; and (3) explore the science and technology of energy producing plasmas, the next frontier in fusion research, as a partner in a international effort – reducing costs, avoiding duplication of efforts, and bringing the best available scientific and engineering talent together to seek solutions to complex problems can best be done through the cooperative efforts of the world fusion community.

This is a time of important progress and discovery in fusion research. The FES program is making great progress in understanding turbulent losses of particles and energy across magnetic field lines used to confine fusion fuels, identifying and exploring innovative approaches to fusion power that may lead to more economical power plants, and encouraging private sector interests to apply concepts developed in the fusion research program. It is felt that small businesses, by performing research within the following technical topics, can make significant contributions to these efforts. This solicitation is restricted to science and technology relevant to magnetically confined plasmas and inertial fusion energy. Grant applications pertaining to fusion energy concepts not based specifically on the use of plasmas for producing energy/electricity for non-defense purposes will be declined.

32. FUSION SCIENCE AND TECHNOLOGY

The Fusion Energy Sciences program currently supports several fusion experiments with many common objectives. These include expanding the scientific understanding of plasma behaviour and improving the performance of high temperature plasma for eventual energy production. The goals of this topic are to develop and demonstrate innovative techniques, instrumentation, and concepts for measuring magnetic plasma parameters; for plasma processing; for magnetic plasma simulation, control, and data analysis; and for innovative approaches to fusion. It is also intended that concepts developed as part of the fusion research program will have application to industries in the private sector. A list of items under the heading "Goods and Services that are needed by the Fusion laboratories" can be found in the Office of Fusion Energy Sciences (OFES) Website (**URL:** <u>www.ofes.fusion.doe.gov</u>). **Grant applications are sought only in the following subtopics:**

a. Diagnostics for Magnetic and Inertial Fusion Plasma Research—Grant applications are sought to develop: (1) measurement techniques for parameters such as plasma density, electron and ion temperature, plasma current and current density, plasma position and shape, impurity density, magnetic field strength. ambipolar potentials, and radiation from the plasma; (2) new diagnostics for measurements in the threedimensional plasmas characteristic of stellarators, as well as diagnostics especially adapted to other innovative concept experiments; (3) diagnostic methods for examining the edge and divertor regions in tokamak plasmas, and for understanding electron thermal transport (high-k fluctuation diagnostics, core magnetic fluctuation diagnostics, and profile diagnostics on smaller devices); and (4) diagnostics applicable to the management of particle and energy inventory, to profile control and thermal barrier formation, and to burning plasmas including ITER (International Thermonuclear Experimental Reactor). Approaches of interest include new techniques and methods to improve the accuracy and resolution of existing diagnostics (e.g., improving the signal-to-noise ratio or extending the range of measured parameters), visualization of turbulence in two and three dimensions, and imaging of non-thermal electrons in two dimensions. Measurements must be both spatially and temporarily resolved for both the absolute values of parameters and for small relative differences. Real-time measurements of the pertinent parameters will be required for providing feedback and plasma control. Further information on experiments on innovative fusion concepts is available at the OFES website.

Grant applications also are sought to develop sets of miniature (non-perturbing) magnetic probes and associated circuitry as an integrated package, suitable for detecting the magnetic oscillations often associated with changes in plasma transport properties. The ranges of interest for the frequency and amplitude of these magnetic fluctuations are 10 kHz to 100 MHz and 0.01 to 100 G, respectively, as shown by research on fusion plasma experiments. Approaches of interest must account for the complex mode structure of these fluctuations – i.e., fluctuation amplitudes and phases differ markedly with spatial position. In addition, the probes should be moveable, ultra high vacuum compatible, and able to withstand exposure to conditions expected in the edge of fusion research devices.

Grant applications also are sought to apply diagnostics technology, developed for fusion energy, to the use of plasmas in manufacturing. These grant applications should show how the application of these diagnostics would contribute to the understanding of plasmas used in manufacturing, as well as provide an improved basis for modelling these plasmas.

Lastly, grant applications are also sought to develop instrumentation and time-resolved measurement techniques of high-charge-density heavy-ion beams of energy greater than 0.5 MeV and radius ~1 to 5 cm. Beam parameters of interest include current, density distribution, beam position, energy, energy distribution, emittance, and space potential in the Injector, Transport, and Final Focus sections. Of particular interest are innovative non-intercepting position detectors and optical (including scintillator-based) beam diagnostics suitable for rapid characterization of beams in both the present (0.5 to 2 MeV) and higher energy ranges, and diagnostics for characterizing trapped secondary electron distributions. Further information may be obtained in the HIF Symposia series (see reference for 12th International Symposium).

b. Components for Heating and Fueling of Fusion Plasmas and Tokamak Facility Operations—Grant applications are sought to develop components related to the generation, transmission, and launching of high power electromagnetic waves in the frequency ranges of ion cyclotron resonance heating (50 to 300 MHz), lower hybrid resonance heating (2 to 20 GHz), and electron cyclotron resonance heating (100 to 300 GHz). Components of interests include power supplies, fault protection devices, antenna and launching systems, tuning and matching systems, unidirectional couplers, circulators, mode convertors, windows, output couplers, loads, energy extraction systems from spent electron beams and particle accelerators, and diagnostics to evaluate the performance of these components. In addition, grant applications are sought to explore concepts that would generate energetic neutral beams.

Grant applications also are sought to (1) develop computer codes for the simulation of maintainability/reliability assurance technologies and for plant operations, applicable to fusion experiments; and (2) apply artificial intelligence to the monitoring of tokamak plant operation and real-time or impending fault condition.

c. Plasma Simulation and Data Analysis—The simulation of fusion plasmas is important to the development of plasma discharge feedback and control techniques. The simulations can be used to make reliable predictions of the performance of proposed feedback and control schemes and to identify those that should be tested experimentally. Unfortunately, accurate simulations of fusion plasmas are very difficult because of the enormous range of temporal and spatial scales involved in plasma behaviour. Considerable progress has been made in recent years in understanding and simulating plasma turbulence, along with associated transport, macroscopic equilibrium and stability, and the behaviour of the edge plasma. However, there remains a need to integrate the various plasma models. Grant applications are sought to develop computer algorithms applicable to plasma simulations that account for an expanded number of plasma features and an integration of plasma models. Examples of possible approaches include algorithms that incorporate mathematical techniques such as neural networks, sparse linear solvers, and adaptive meshes; algorithms for coupling disparate time and space scales; efficient methods for facilitating comparison of simulation results with experimental data; and visualization tools for local and remote analysis, and presentation of multi-dimensional time dependent data.

Grant applications are also sought to develop software tools useful for the analysis and distribution of fusion data. Areas of interest include methods for coupling codes across architectures and through the Internet; techniques for making highly configurable scientific codes; data management and analysis techniques for large data sets; and remote collaboration tools that enhance the ability of a geographically distributed group of scientists to interact in real-time.

The computer algorithms and programming tools should be developed using modern software techniques and should be based on the best available models of plasma behaviour.

d. Components and Modeling Support for Innovative Approaches to Fusion—Innovative Confinement Concepts is a broad-based, long-range, research activity that specifically addresses parameters that could lead to the attractive and practical use of fusion power. This research includes investigations in stellarators, spherical torus, reversed field pinches, field reversed configurations (FRC), spheromaks, magnetized target fusion, levitated dipole, flow-stabilized (long-pulse) z-pinch, rotationally stabilized magnetic mirror, inertial electrostatic confinement, and magneto-Bernoulli confinement. Grant applications are sought for scientific and engineering developments, including computational modeling, in support of any aspect of these research activities. Of particular interest are grant applications that explore the feasibility of plasma injection into magnetic fields and/or magnetized plasmas, generation of plasma rotation, and disruption mitigation. Plasma initiators and accelerators also are of interest. Further information on experiments on innovative fusion concepts is available at the OFES Web site.

Grant applications also are sought to develop innovative, high economic value, non-electric applications of fusion reactions. Of particular interest are grant applications that explore space applications of fusion reactions (e.g., space propulsion).

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33. ADVANCED TECHNOLOGIES AND MATERIALS FOR FUSION ENERGY SYSTEMS

An attractive fusion energy source will require the development of superconducting magnets and materials as well as technologies that can withstand the high levels of surface heat flux and neutron wall loads expected for the in-vessel components of future fusion energy systems. These technologies and materials will need to be substantially advanced relative to today's capabilities in order to achieve safe, reliable, economic, and environmentally-benign operation of fusion energy systems. A list of items under the heading "Goods and Services that are needed by the Fusion laboratories" can be found in the Office of Fusion Energy Sciences Website (URL: www.ofes.fusion.doe.gov). Grant applications are sought only in the following subtopics:

a. Plasma Facing Components—The plasma facing components (PFCs) in energy producing fusion devices will experience 5-15 MW/m² under normal operation (steady-state) and off-normal energy deposition up to 1 MJ/m^2 within 0.1 to 1.0 ms. Refractory solid surfaces represent one PFC option. These PFCs are envisioned to have a refractory metal heat sink cooled by helium gas and a plasma facing surface, consisting of an engineered refractory metal surface or a thin coating of refractory material, that minimizes thermal stresses. The materials being considered include tungsten and molybdenum. Grant applications are sought to develop: (1) innovative refractory alloys having good thermal conductivity (similar to Mo, at a minimum), resistance to recrystallization and grain growth, good mechanical properties (e.g., strength and ductility), and resistance to thermal fatigue; (2) innovative refractory metal heat sink designs for helium gas cooling; (3) efficient fabrication methods for engineered surfaces that mitigate the stresses due to high heat flux; and (4) joining or coating methods, for attaching the plasma facing material to the heat sink, that are reliable, efficient to manufacture, and capable of high heat transfer.

Another option for plasma facing components is a flowing liquid surface; therefore, in the near term, plasma interactions with thin flowing films are of critical interest. This will require the production and control of thin, fast flowing, renewable films of liquid lithium (less than 1 mm in thickness) for particle control at divertors. Grant applications are sought to develop: (1) techniques for the production, control, and removal of flowing (velocity 0.01 to 10 m/s) liquid lithium films (0.5-5 mm thick) over a temperature controlled substrate or free surface liquid jets (velocity 1.0 to 10 m/s); (2) advances in materials that are wet by lithium at temperatures near the lithium melting point and that produce uniform, well-adhered films; (3) techniques for active control of lithium flow and stabilization in the presence of plasma instabilities (time and space varying magnetic field); (4) computational tools that model flow and magnetohydrodynamic response of flowing liquid metals; and (5) cost-effective experimental techniques that integrate items (1) to (4) above to allow advanced plasma-material interaction testing and simulation.

b. **Blanket Materials**—The pebble-bed solid breeder configuration introduces several operational limits: thermo-mechanical uncertainties caused by pebble bed wall interaction, potential sintering and subsequent macro-cracking, and a low pebble bed thermal conductivity – all of which result in small characteristic bed dimensions and limit windows of operation. A new form of solid breeder morphology is required that holds the promise for increased breeding ratios, dictated by increased breeder material density; long term structural reliability; and enhanced operational control, compared to packed beds. Grant applications are sought for new solid breeder material concepts that include: (1) increased breeder material densities (>80%); (2) higher thermal conductivities (provided by a fully interconnected structure as opposed to point contacts between pebbles); (3) bonded contacts to cooling structures (instead of point contacts between pebbles and wall); (4) the absence of major geometry changes between beginning-of-life and end-of life (such as sintering in pebble beds)

in the presence of high neutron fluence; and (5) structural integrity in freestanding and self-supporting structures with significant thermo-mechanical flexibility.

Flow channel inserts (FCIs) act as magnetohydrodynamic and thermal insulators in ferritic steel channels containing, for example, a slowly flowing tritium breeder such as molten Pb-17Li alloy. The insert geometry is approximately C-shaped in straight channels, with more complex shapes possible for insertion in manifolds and other complex-geometry elements in the flow path. Although SiC/SiC composite is a candidate FCI, its use would differ from its application as a structural material, in that high thermal and electrical conductivity is not desirable; in particular, electrical conductivity should be as low as possible, with a target range from 1 to $10 \Omega^{-1}$ 1 m⁻¹. In addition, strength requirements are reduced compared to its application as a structural material because the primary stresses and pressure loads will be very low; however, the insert must be able to withstand thermal stresses from temperature gradients in the range of 10-20 C/mm. Grant applications are sought to develop manufacturing techniques for radiation resistant, low thermal/electrical conductivity SiC/SiC composites that would not allow the Pb-17Li alloy to penetrate any porosity in the matrix. For instance, a final "sealing" layer of SiC matrix material is envisioned that would be near theoretical density and cover any porosity or exposed fibers in the main body of the insert. Two-dimensional weaves are generally thought to be satisfactory, and an effective way to reduce electrical conductivity normal to the insert interface with the Pb-17Li (the more important of the directions). In addition, grant applications are sought to experimentally determine the compatibility between the SiC/SiC composite and such breeder materials as Pb-17Li alloy, as well as the insert integrity under cyclic thermal loading.

One of the missions of the International Thermonuclear Experimental Reactor (ITER) project is the integrated testing of fusion blanket materials and components in a true integrated fusion environment. This ITER fusion environment includes radiation and magnetic fields, along with surface and volumetric heating, under pulsed and/or steady-state plasma operation. The "test blanket modules" (TBMs) will be complicated systems of different functional materials (breeder, multiplier, coolant, structure, insulator, etc.) in various configurations with many responses and interacting phenomena (e.g., thermomechanical, thermofluid, nuclear). As part of the design and validation process for these various experiments [5], the overall simulation of a "virtual" TBM is required to integrate all of the individual simulations at the system level. Such a project would be inherently multi-scale and multi-physics and will require careful code and algorithm design. Therefore, grant applications are sought to develop a TBM simulation code that can provide visual animations of: (1) fluid flow and thermal hydraulic characteristics; (2) the thermal response of all materials (structure, breeder, multiplier, coolant, insulator, etc); (3) structural responses such as stress and deformation magnitudes with respect to different loadings, including both steady-state surface heat flux and dynamic loadings; and (4) other important performance characteristics of the TBM. The overall code framework/structure must effectively link all of the simulation components of the virtual TBM and serve as an efficient, useful, and user-friendly tool.

c. Superconducting Magnets and Materials—New or advanced superconducting magnet concepts are needed for plasma fusion confinement systems; i.e., high field magnets (12 to 20 T) and low loss pulsed magnets. Grant applications are sought for: (1) innovative and advanced materials and manufacturing processes that have a high potential for improved conductor performance and low fabrication costs; (2) cryogenic superconductor materials with high critical current density, low sensitivity to strain degradation effects, and radiation resistance; (3) novel, low-cost cable designs and fabrication techniques, which minimize conductor strain; (4) superconducting joints for high field and pulsed applications; (5) novel, advanced sensors and instrumentation for non-invasively monitoring magnet and helium parameters (e.g., pressure, temperature, voltage, mass flow, quench, etc.); (6) thick (15-30 cm), weldable, structural case materials with high strength and toughness at 4 K; (7) welding techniques for such thick cryogenic structural materials; and (8) radiation-resistant electrical insulators (e.g., wrapable inorganic insulators and low viscosity organic insulators, which exhibit low out gassing under irradiation).

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34. HIGH ENERGY DENSITY PHYSICS FOR INERTIAL FUSION ENERGY

Inertial fusion seeks to produce fusion reactions by creating plasmas of extremely high density and using inertia to contain momentarily the extreme pressure generated by the fusion burning plasma. In order for inertial fusion to achieve significant energy production, it will be necessary to develop attractive physics pathways for providing the necessary conditions for ignition and burn. In turn, these conditions will require states of matter with extremely high energy density (HED). For this purpose, HED states are defined as states of matter with energy densities exceeding about 10¹¹ J/m³ and temperature exceeding 1 eV. However, the physics of matter at such high energy densities is not well established – it is an emerging field that cuts across many areas of science. Therefore, the Office of Fusion Energy Sciences (OFES) sponsors research in heavy ion beams to produce these HED states, along with studies of the physics of fast ignition and high-temperature dense magnetized plasmas. This topic seeks to supplement the on-going research activities as well as to develop new techniques for creating or studying HED states relevant to the pursuit of inertial fusion energy. A list of items under the heading "Goods and Services that are needed by the Fusion laboratories" can be found in the Office of Fusion Energy Sciences Website (**URL:** <u>www.ofes.fusion.doe.gov</u>). **Grant applications are sought only in the following subtopics:**

a. Beam Generation, Compression, and Focusing—In current OFES programs, ion beams are produced by induction linear accelerators with components to produce, accelerate, transport, and focus beams of required energy and intensity. Over the next few years, the research will concentrate on developing intense ion sources and on studying the physics of spatial compression, neutralized transport, and focusing of the beam. The research is led by the Virtual National Laboratory for Heavy Ion Fusion, a collaboration among Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, and the Princeton Plasma Physics Laboratory. Grant applications are sought to support the development of high current, high brightness ion sources for heavy ion induction linacs. Grant applications also are sought for research in the spatial compression and focusing of high-current, high brightness ion beams. Research of interest includes theoretical, computational, and/or experimental investigations.

b. Fast Ignition—The Fast Ignition concept employs two drivers to create inertial fusion: one for compression, and one for the ignition of a small portion of the compressed fuel. The main requirement and challenge for Fast Ignition is to deliver the ignition energy to the compressed fuel. In the most common approach, petawatt laser energy is nominally deposited in the coronal plasma surrounding the compressed fuel, resulting in a relativistic electron beam. Ignition depends on the successful propagation of that electron beam to the fuel and the effective heating of a small portion of that fuel. In this approach, the energy transport by relativistic electrons to the high-density fuel to achieve ignition is a key physics issue. An alternative approach, in which energetic proton beams are used as igniter beams, also is under consideration. These Fast Ignition concepts are being

funded by the OFES at the University of Rochester, Lawrence Livermore National Laboratory, General Atomics, Ohio State University, University of Texas at Austin, and the University of Nevada at Reno. Grant applications are sought for computational, experimental, and component development in support of these on-going Fast Ignition research efforts at these institutions. Grant applications that address the development of petawatt lasers are outside the scope of this solicitation and will be declined.

c. Innovative Approaches for Creating and/or Studying States of High Energy Density—Grant applications are sought to develop innovative approaches for creating and/or understanding HED states. Areas of interest include, but are not limited to: (1) transport of thermal energy, kinetic energy, momentum and particles in these states, especially the effects of externally applied or self-generated magnetic fields on the transport processes; (2) and theoretical, computational, and/or experimental investigations for creating and/or using dense, high Mach-number, high velocity plasma jets/beams to create HED states. However, grant applications that address the development of petawatt lasers are outside the scope of this solicitation and will be declined.

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PROGRAM AREA OVERVIEW OFFICE OF HIGH ENERGY PHYSICS

http://www.science.doe.gov/hep/index.shtm

Through fundamental research, scientists have found that all physical matter is composed of apparently pointlike particles, called leptons and quarks. These constituents of matter were created following the "big-bang" which originated our universe, and they are components of every object that exists today. We also understand a great deal about the four basic forces of nature: electromagnetism, the strong nuclear force, the weak nuclear force, and gravity. For example, in the past we have learned that the electromagnetic and weak forces are two components of a single force, called the electro-weak force. This unification of forces is analogous to the unification in the mid-nineteenth century of electric and magnetic forces into electromagnetism. History shows that, over a period of many years, the understanding of electromagnetism has led to many practical applications that form the technical basis of modern society.

The goal of the Department of Energy's (DOE) High Energy Physics (HEP) program is to provide mankind with new insights into the fundamental nature of energy and matter and the forces that control them. This program is a major component of the Department's fundamental research mission. Such fundamental research provides the necessary foundation that enables the nation to advance its scientific knowledge and technological capabilities, to advance its industrial competitiveness, and possibly to discover new and innovative approaches to its energy future.

Experimental research in HEP is largely performed by university scientists using particle accelerators located at major laboratories in the U.S. and abroad. Under the HEP program, the Department operates the Fermi National Accelerator Laboratory (Fermilab) near Chicago, IL and the Stanford Linear Accelerator Center (SLAC) near San Francisco, CA. Furthermore, the Department has a significant role in the Large Hadron Collider project under construction at the CERN laboratory in Switzerland. The Tevatron at Fermilab is currently the world's highest energy accelerator. SLAC also provides unique experimental capabilities.

While much progress has been made during the past five decades in our understanding of particle physics, future progress depends to a great degree on the availability of new state-of-the-art technology for accelerators, colliders, and detectors operating at the high energy and/or high intensity frontiers.

Within HEP, the High Energy Technology subprogram supports the research and development required to extend relevant areas of technology in order to support the operations of highly specialized accelerators, colliding beam facilities, and detector facilities which are essential to the goals of the overall HEP program. The DOE SBIR program provides a focused opportunity and mechanism for small businesses to contribute new ideas and new technologies to the pool of knowledge and technical capabilities required for continued progress in HEP research, and to turn these novel ideas and technologies into new business ventures.

35. HIGH-FIELD SUPERCONDUCTOR AND SUPERCONDUCTING MAGNET TECHNOLOGIES FOR HIGH ENERGY PARTICLE COLLIDERS

The Department of Energy High Energy Physics (HEP) program supports a broad research and development (R&D) effort in the science, engineering, and technology of charged particle accelerators, storage rings, and associated apparatus. Advanced R&D is needed in support of this research in high-field superconductor and superconducting magnet technologies. This topic addresses only those superconductor and superconducting magnet development technologies that support dipoles, quadrupoles, and higher order multipole corrector magnets for use in accelerators, storage rings, and charged particle beam transport systems. Grant applications that propose the use of third party resources (such as a DOE laboratory) must include in the application a letter of certification from an authorized official of that organization. **Grant applications are sought only in the following subtopics:**

a. High-Field Superconductor Technology—Grant applications are sought for new or improved materials and related processing techniques for high critical-current, high critical-field superconductors for the production of low alternating current (AC) (ramped) loss conductors used in very high-field magnets. Grant applications for the improvement of starting raw materials and the basic superconductor are of particular interest. While improvements are sought for magnets above 12 Tesla (T), the engineering goal for the near future (five to eight years) is at least 16 Tesla. Vacuum requirements in accelerators and storage rings favor operating temperatures below 20K and more likely 5K.

Advanced conductors must demonstrate such property improvements as higher critical-current densities and higher critical fields, as well as the manageable degradation of these properties as a function of applied strain. Stability requirements for magnets dictate that effective filament diameters (d_{eff}) should be minimized while maintaining a highly conductive normal metal matrix – the goal is for d_{eff} to be less than 30 micrometers. Advanced conductor fabrication techniques of interest include methods to utilize high aspect ratio stranded conductors, such as Rutherford cables, or low AC loss tape geometries in particle accelerator applications under the above conditions. Any proposed process improvements must result in equivalent performance at reduced cost. Advanced materials of interest include: the so-called "A-15" compounds (e.g., niobium-tin (Nb₃Sn) and niobium-aluminum (Nb₃Al)), and high temperature superconductors (HTS). Regarding HTS materials, a minimum current density of 1200 A/mm² (not cm²) in the superconductor itself and a minimum current density of 250 A/mm² over the total conductor cross section, at 12 Tesla minimum and 4.2K, must be achieved.

 MgB_2 is emerging as a conductor material with inexpensive raw materials and the ability to be fabricated into conductors using relatively conventional metal-working processes. However, present prototype wires are characterized by a filling factor that is too low, too few filaments, and an H_{C2} value that is too low, especially in the perpendicular field direction at lower H_{C2} values. Therefore, grant applications are sought to extend the use of MgB_2 to round-wire, multifilament conductors, suitable for the 12-16 T range of applications with current densities of >1200 A/mm².

Because high performance niobium-titanium (NbTi) alloys operating above 8 T continue to be required for focusing quadrupole magnets or for "low field" graded windings in higher field dipoles, grant applications are sought to develop NbTi composite superconductors with properties optimized at the higher field portion of the short sample curve.

Lastly, grant applications are sought for innovative insulating materials which would enable employment of new superconductors, such as the A-15 or HTS types, in practical devices. Insulating materials must be compatible with high temperature reactions in the 750-900°C range and must be capable of supporting high mechanical loads at cryogenic temperatures.

All grant applications must focus on conductors that will be acceptable for accelerator magnets, especially with regard to the operating conditions mentioned above, and must address plans to physically deliver a sufficient amount of material for winding and testing in small dipole or quadrupole magnets.

b. Superconducting Magnet Technology—Grant applications are sought to develop: (1) improved instrumentation to measure properties (such as local strain, temperature, and magnetic field) which are directly applicable to the testing of superconducting magnets; (2) improved current leads based on high-temperature superconductors for application to high-field accelerator magnets, which have requirements that include an operating current level of 5 kA or greater, stability, low heat leak, and good quench performance; (3) alternative designs, to traditional "cosine theta" dipole and "cosine two-theta" quadrupole magnets, that may be more compatible with the more fragile A-15, and the HTS, high-field superconductors; (4) designs for bent (e.g., bending radius in the range 0.75 to 1.25m) solenoids (e.g., 2 T, 30 cm inside diameter) with superimposed dipole fields (e.g., 1 T) for dispersion generation in large emittance beams; (5) improved industrial fabrication methods for magnets such as welding and forming; or (6) improved cryostat and cryogenic techniques.

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36. ADVANCED CONCEPTS AND TECHNOLOGY FOR HIGH ENERGY ACCELERATORS

The DOE High Energy Physics (HEP) program supports a broad research and development (R&D) effort in the science, engineering, and technology of charged particle accelerators, storage rings, and associated apparatus. Advanced R&D is needed in support of this program in the following areas: (1) new concepts for acceleration, (2) novel device and instrumentation development, (3) inexpensive electron sources, and (4) computer software that will contribute to overall advances in accelerator technology applicable to HEP research. Relevance to applications in HEP must be explicitly described in the submitted grant applications. Advanced accelerator R&D more appropriate to applications in nuclear physics is specifically excluded from this topic and should be submitted under Topic 45. Grant applications that propose using resources of a third party (such as a DOE laboratory) must include, in the application, a letter of certification from an authorized official of that organization. **Grant applications are sought only in the following subtopics:**

a. New Concepts for Acceleration—Grant applications are sought to develop new or improved acceleration concepts. Designs should provide very high gradient (>100 MV/m for electrons or >10 MV/m for protons) acceleration of intense bunches of particles, or efficient acceleration of intense (>50 mA) low energy (of order <20 MeV) proton beams. One possible concept might include the fabrication of accelerator structures from materials such as Si or SiO₂, using integrated circuit technology; in this case, power sources might include lasers. For all proposed concepts, stageability, beam stability, manufacturability, and high wall plug-to-beam power efficiency should be considered. Grant applications must address the marketability of any systems, technologies, and devices to be developed.

b. Novel Device and Instrumentation Development—Grant applications are sought for the development of electromagnetic, permanent magnet, or silicon microcircuit-based charged particle optical elements for particle beam focusing. Examples include, but are not limited to, dipoles, quadrupoles, higher order multipole correctors for use in electron linear accelerators, and solenoids for use in electron-beam or ion-beam sources or for klystron or other radio frequency amplifier tubes operating at wavelengths from 0.7 to 10 cm. In these optical elements, permanent magnets or hybrid magnets incorporating magnetic materials that have very high residual magnetization, radiation resistance, and thermal stability (low variation of field strength with temperature) are of particular interest.

Grant applications are also sought for: (1) novel charged particle beam monitors to measure the transverse or longitudinal charge distribution or emittance, or phase-space distributions of small radius (0.1 μ m to 5 mm diameter), short length (10 μ m to 10 mm) relativistic electron or ion beams; (2) devices capable of measuring and recording the Schottky or transition radiation spectrum of these beams (proposed techniques should be nondestructive or minimally perturbative to the beams monitored and have computer-compatible readouts); and (3) lasers for laser-accelerator applications that provide substantial improvements over currently available lasers in one or more of the following parameters: longer wavelengths (up to 2 to 2.5 μ m for use with Si transmissive optics), very short wavelengths (< 200 nm) with low mode numbers (M-squared < 100) and high pulse energy (> 0.1 J) for photo-ionized plasma sources, higher power, higher repetition rates, or shorter pulse widths.

Grant applications are sought to develop high density (range of 10^{18} - 10^{20} cm⁻³), high repetition rate (10 Hz) pulsed gas jets, capable of producing fan-shaped gas plumes with long lengths on the centimeter scale and narrow widths of a few hundred microns. These gas jets are to be used in laser wakefield accelerators. The gas

plumes should have sharp edge gradients, on the order of 100 μ m. The gas jet system should have the flexibility to offer longitudinal density profile control using, for example, multi-nozzle systems produced, potentially, with Micro-Electro-Mechanical Systems technology. Ideally, the pulse duration of the jets should be less than 1 ms to minimize the amount of gas loading in vacuum chambers.

Grant applications also are sought for the development of novel devices and instrumentation for use in the cooling (transverse and longitudinal emittance reduction) of muon beams. Approaches of interest include the development of: concepts or devices for ionization cooling, including emittance exchange processes; instrumentation for muon cooling channels with muon intensities of 10^{12} muons/pulse; or fast (of order 10 picosecond) timing detectors for muon cooling experiments with low muon intensity (of order 10^5 muons/second).

c. Inexpensive High Quality Electron Sources—Grant applications are sought for the design and prototype fabrication of small, inexpensive (<\$1 million) electron sources for use in advanced accelerator R&D laboratory experiments. The following parameters are target values for accelerator research experiments: (1) energy range of 5 to 35 MeV providing, at a minimum, on the order of 10⁹ electrons in a bunch less than 5 picoseconds long; (2) normalized transverse beam emittance less than or equal to 5 pi mm-mrad; and (3) pulse repetition rate greater than 10 Hz. Grant applications are also sought for significantly lower bunch charges, energies, and emittances – yet with comparable or greater peak currents and significantly higher repetition rates – for bunches from a matrix cathode. In addition, grant applications are sought to develop a bright DC/RF photocathode electron source that combines a pulsed high electric field DC gun and a high field rf accelerator, operates at a repetition rate of several kHz, and has electron bunch specifications that are similar to those listed above.

Grant applications are also sought for the development of radio frequency photocathodes (robust, with quantum efficiencies >0.1 percent) or other novel rf gun technologies operating at output electron beam energies >3 MeV. Laser or electron driven systems for such guns are also sought.

Finally, grant applications are sought for research and development of electron sources to be used as polarized beam injectors for linear accelerators, including linear colliders. These sources should be gated with pulses or pulse trains larger than 0.1 μ s at about 100-200 pulses per second, and on semiconductor photocathode sources of electrons with polarization greater than or on the order of 80 percent and energy in the range of a few volts to several hundred kilovolts. In addition, intensity stability <1 percent is required for polarized beams in pulsed linacs.

d. Computer Software and Control Systems—Grant applications are solicited for developing new or improved computational tools specifically for the design, study, or operation of charged particle beam optical systems, accelerator systems, or accelerator components. Such applications should incorporate the innovative development of user-friendly interfaces with emphasis on graphical user interfaces and windows. Grant applications also are solicited for the conversion of existing codes to incorporate such interfaces, provided that existing copyrights are protected and that applications include the authors' statements of permission where appropriate.

Grant applications are sought for improved simulation packages for injectors or photoinjectors. Specific examples include: (1) improved space-charge algorithms; (2) improved algorithms for computing self-consistently the effects of wakefields and coherent synchrotron radiation on the detailed beam dynamics; (3) improved fully 3-D algorithms for the modeling of transversely asymmetric beams; and (4) explicit end-to-end simulations that provide for more accurate beam-quality calculations in full injector systems.

Grant applications are also sought to improve (1) software systems for command and control functions, real time database management, real-time or off-line modeling of the accelerator system and beam, and status display systems encountered in state-of-the-art approaches to accelerator control and optimization; and (2)

decision and database management tools, specifically for use in planning and controlling the integrated cost, schedule, and resources in large HEP R&D and construction projects.

In addition, grant applications are sought to develop optical real-time networks for pulsed-accelerator control. These networks require combining timing information with data-communication functions on a single optical fiber connected to pulsed device-controllers. The single fiber should provide each controller with an RF-synchronized clock that has the following features: an arrival time phase-locked to the temperature-stabilized RF reference phase, a similarly-locked machine pulse fiducial point, digital data for machine pulse-type selection and specific pulse identification, and real-time-streaming pulsed waveform data-acquisition capabilities. These controllers provide interfaces to systems for such functions as low-level RF signal generation, modulator control, beam position monitors, and machine protection system sensing. The network should provide real-time, fast feedback loop closure and TCP/IP connectivity for slow control functions, such as database access, device configuration, and code downloading and debugging.

Finally, proposals are sought to develop real-time processors and software for pulsed accelerator control and monitoring, based on a multiprocessor architecture that can be deeply embedded within pulsed device-controllers employing system-on-a-chip, field-programmable gate-array, or application-specific integrated circuit technologies. These architectures should feature distinct processors for pulse-to-pulse, real-time functions and conventional slow control functions. Architectural provisions for supporting machine protection functions via an additional processor or dedicated hardware should also be included.

For the preceding two paragraphs, proposed solutions should be engineered for both: (1) resistance to electromagnetic interference generated by nearby, large, pulsed-power systems; and (2) maximum availability in remote deployment locations. Further information on the preceding two paragraphs can be obtained from Ray Larsen at Stanford Linear Accelerator Center (email: <u>larsen@SLAC.Stanford.edu</u>; phone: 650-926-4907; fax: 650-926-5124).

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37. RADIO FREQUENCY ACCELERATOR TECHNOLOGY FOR HIGH ENERGY ACCELERATORS AND COLLIDERS

The DOE High Energy Physics (HEP) program supports a broad research and development (R&D) effort in the science, engineering, and technology of charged particle accelerators, storage rings, and associated apparatus. Advanced R&D is needed in support of this research in: (1) high gradient accelerator structures, (2) high peak power radio frequency (rf) technologies, and (3) new concepts for low-cost, very efficient, pulse power modulators. Relevance to applications in HEP must be explicitly described. Advanced accelerator R&D more appropriate to applications in nuclear physics is specifically excluded from this topic and should be submitted under Topic 45. Grant applications that propose using resources of a third party (such as a DOE laboratory) must include, in the application, a letter of certification from an authorized official of that organization. **Grant applications are sought only in the following subtopics:**

a. Radio Frequency Acceleration Structures—Grant applications are sought for research on very high gradient rf accelerating structures, normal or superconducting, for use in accelerators and storage rings. Gradients >100 MV/m for electrons and >10 MV/m for protons in normal cavities are of particular interest, as are means for suppressing unwanted higher-order modes and reducing costs. For use in muon accelerator R&D, achieving gradients of 5-10 MV/m for cavities with frequencies between 20 and 200 MHz is also of interest. Means for achieving unloaded voltage gradients >40 MV/m and reducing costs in superconducting cavities are also of interest, as are methods for reducing surface breakdown and multipactoring (such as surface coatings or special geometries) and for suppressing unwanted higher order modes. Grant applications should be applicable to devices operating at frequencies from 1 to 40 GHz or between 20 and 300 MHz for muon accelerators.

b. Radio Frequency Power for Linear Accelerators—Grant applications are sought to develop new concepts, high-power rf components and instrumentation to be used in producing high peak power in narrow band, low duty-cycle, and low pulse repetition frequency (approximately 0.1 to 1 kHz) pulsed rf amplifiers. The principal application is to future large electron/positron linear colliders. Potential electrical efficiencies greater than 45 percent are considered essential. Of particular interest are innovations related to cost saving, manufacturability, and electrical efficiency. Examples include, but not limited to:

- (1) One way of providing rf power is the cluster klystron, a device consisting of a "cluster" of separate gun driven klystrons that share a common focusing field and accelerating gap. Such a device could give high total pulsed power with relatively small individual beam currents, and thus be capable of high efficiency. The electron gun used must allow the many beams to be enclosed in a compact space, and have modulation anodes that allow the current to be switched, thus eliminating the need for a pulsed high-voltage modulator.
- (2) Another approach is through the use of sheet beam klystrons. Therefore, grant applications are sought for the development of cluster klystrons, highly stable electron guns for cluster klystrons, as well as rf components such as single or dual sheet beam gridded or diode guns, sheet beam klystron rf structures, or whole single channel or dual channel sheet beam klystrons.

Upgrades to the next generation linear collider will require many rf power handling components which are not presently available, e.g., rf windows, couplers, mode transformers, rf loads, and high power rings capable of operating at high pulse powers (10 - 100 MW), high frequencies (1 - 40 GHz), and pulse lengths of several microseconds. Therefore, grant applications also are sought for passive and active rf components such as over-moded mode converters from rectangular to circular waveguide and vice versa, high-power rf windows, circulators, isolators, switches, and quasi-optical components.

Lastly, grant applications are sought for the initial design, modeling, and development of a compact multi beam klystron (MBK) at 201.25 MHz to support proton drift tube linacs. The source must produce 5 MW pulsed rf at 201.25 MHz for 500 µs at 15 Hz repetition rate. For application at Fermilab, this power source, together with its low and high level systems, must fit into a footprint of 12 feet by 24 feet with a ceiling height of 12 feet. Output power must be supplied via a 9-inch coaxial hard line that can be pressurized to 12 psig. Also, because the MBK would be part of phase and amplitude feedback loops, it must operate linearly 15 percent below saturation. An efficiency of about 50 percent and gain of at least 50 dB are required. Tube lifetimes of about 30,000 hrs are very desirable.

c. New Concepts or Components for Pulsed Power Modulators and Energy Storage—Most rf power sources for future linear colliders require high peak-power pulse modulators of considerably higher efficiency than presently available. Grant applications are sought for new types of modulators in the 400 kV – 1 MV range for driving currents of 200 - 800 A, with pulse lengths of $0.2 - 4.0 \mu$ s, and rise- and fall-times of less than 0.5 μ s. Innovation related to cost saving, manufacturability, and electrical efficiency in modulators is especially important. Modulators with improved voltage control for rf phase stability in some alternate rf power systems

are also sought. Of particular interest is the development of cathode modulators for driving single or double sheet beam diode gun klystrons, based on the Marx multiplier principle. This design should produce 400-500 kV, $3-5 \mu s$ pulses; have rise- and fall-times less than 600 ns; and be compact and cost competitive compared to present cathode pulse modulator schemes.

Grant applications also are sought to develop improved high power solid-state switches for pulse power switching. For some applications, requirements will include the ability to switch high current pulses (2-5 kA) at voltage levels of 2 to 6 kV with switching times of less than 300 nsec. These switches must handle very high di/dt (20 kA/ μ s) at low duty cycle (<0.1%).

Existing Insulated Gate Bipolar Transistor (IGBT) packages for high voltage (> 3.3kV) and high pulsed current (> 3 kA peak, 59 A average) are not optimized for very high speed pulsed power applications (6.6 MW peak for $3.2 \mu s$ at 120 Hz) due to failure modes induced by very rapid fall time (di/dt >10 kA/ μ s) and/or rise time (dV/dt >15 kV/ μ s) upon device turn-off. Therefore, grant applications are sought to reduce these failure modes through improved packaging of commercial IGBT chips, by incorporating appropriate protective circuitry in a high voltage power package designed specifically for high-speed transients. Additional information can be provided by Richard Cassel or Saul Gold at Stanford Linear Accelerator Center (Cassel: email rlc@slac.Stanford.edu; phone 650-926-2299; fax 650-926-3588; Gold: email slg@slac.Stanford.edu; phone 650-926-4450; fax 650-926-3654).

Lastly, grant applications are sought to develop and optimize high reliability, high energy density energy storage capacitors for future solid state pulse power systems. The capacitors must: (1) deliver high peak pulse current (5 - 8 kA) in the partial discharge region (less than 10 percent voltage droop during pulse); (2) be designed with very low inductance connections to allow fast rise and fall time discharge without ringing (di/dt $\sim 20 \text{ kA/}\mu\text{s}$); and (3) be packaged to meet the requirements of high power solid state board layouts and have minimum production cost.

Further information regarding the last two paragraphs can be obtained from either Ron Koontz or Saul Gold at Stanford Linear Accelerator Center (Koontz: email <u>rfkap@SLAC.Stanford.edu</u>; phone 650-926-2528; fax 650-926-3654; Gold: email <u>slg@slac.stanford.edu</u>; phone 650-926-4450; fax 650-926-3654).

d. Radio Frequency Power for Muon Colliders—Grant applications are sought for new concepts, approaches, or designs for radio frequency amplifiers or pulse compression schemes for use in the acceleration and ionization cooling channels of a future muon collider. The amplifiers or compressors must have high peak power (>30 MW) and pulsed, low frequency (from 2 ms pulses at 20 MHz to 0.1 ms pulses at 200 MHz). Higher power (>100 MW) pulsed sources at higher frequencies (from 30 µs at 400 MHz to 10 µs at 800 MHz) are also of interest. All muon collider amplifiers must have moderate repetition rate capability (e.g., 15 Hz). Another important factor is the cost per unit of peak power, including the cost of required power supplies.

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38. HIGH ENERGY PHYSICS DETECTORS

The DOE supports research and development in a wide range of technologies essential to experiments in HEP and to the accelerators at DOE high energy accelerator laboratories. The development of advanced technologies for particle detection and identification for use in HEP experiments or particle accelerators is desired. Principal areas of interest include particle detectors based on new techniques and technological developments (e.g., superconductivity or solid-state devices) or detectors which can be used in novel ways as a consequence of associated technological developments in electronics (e.g., sensitivity or bandwidth), with particular interest in

devices exhibiting insensitivity to very high radiation levels. Also of interest are novel experimental systems that use new detectors, or use old ones in new ways, that either extend basic HEP experimental research capabilities or result in less costly and less complex apparatus. Grant applications must clearly and specifically indicate their particular relevance to HEP programmatic activities.

Although particle physics detector development is often concentrated at major national particle accelerator centers, there are many developmental endeavors, especially in collaborative efforts, where small businesses can make creative and innovative contributions that further develop the required advanced technologies. Nonetheless, applicants are encouraged to collaborate with active high energy elementary particle physicists at universities or national laboratories to establish mutually beneficial goals. On-line directories of appropriate researchers are available at http://www.hep.net/sites/directories.html. **Grant applications are sought only in the following subtopics:**

a. Particle Detection and Identification Devices—Grant applications are sought for novel devices in the areas of charged and neutral particle detection and identification. Examples include, but are not limited to, semiconductor particle detectors (silicon, CVD diamond, or other semiconductors), light-emitting particle detectors (scintillating materials including fibers and crystals or Cherenkov radiators), photosensitive detectors that could be used with light-emitting detectors (photomultipliers, micro-channel plates, photosensitive semiconductors), gas or liquid-filled chambers (used for particle tracking or in electromagnetic or hadronic calorimeters, Cherenkov or transition radiation detectors).

The proposed devices must be explicitly related to future high-energy physics experiments, either accelerator or non-accelerator based, or to future uses in particle accelerators. **Relevant potential improvements over existing devices and techniques must be discussed explicitly** (e.g., radiation hardness, energy, position, and timing resolution, sensitivity, rate capability, stability, dynamic range, durability, cost). Electromagnetic calorimeters, also called shower counters or gamma ray detectors, must be optimized for photons with energies above 1 GeV. X-ray detectors are not relevant to this topic.

b. Detector Support and Integration Components—HEP experiments frequently require high performance detector support that will not compromise the precision of the detectors. Therefore, grant applications are sought for components used to support or integrate detectors into HEP experiments. The support components must be well matched to the detectors and possess some or all of the following features: low mass, high strength or stiffness, low intrinsic radioactivity, exceptionally high or exceptionally low thermal conductivity, and low cost. Grant applications also are sought for alignment and cooling systems.

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39. HIGH ENERGY PHYSICS DATA ACQUISITION AND PROCESSING

The DOE supports the development of advanced electronics and computational technologies for the recording, processing, storage, distribution, and analysis of experimental data that is essential to experiments and particle accelerators used for HEP research. Areas of present interest include event triggering, data acquisition, scalable clustered computer systems, distributed collaborative infrastructure, distributed data management and analysis frameworks, and distributed software development useful to HEP experiments and particle accelerators. Grant applications must clearly and specifically indicate their relevance to present or future HEP programmatic activities.

Although particle physics detector instrumentation, data processing and analysis, and software development typically occur in large collaborative efforts at national particle accelerator centers, there are efforts where small businesses can make innovative and creative contributions to further development of the required advanced technologies. Applicants are encouraged to collaborate with active high energy elementary particle physicists at universities or national laboratories to establish mutually beneficial goals. On-line directories of appropriate researchers are available by institution at http://www.hep.net/sites/directories.htlml. Grant applications that propose using the resources of a third party (such as a DOE laboratory) must include, in the application, a letter of certification from an authorized official of that organization. Grant applications are sought only in the following subtopics:

a. High-Speed Electronic Instrumentation—Grant applications are sought to develop components, electronics, systems, and instrumentation modules as follows:

(1) Special purpose chips and devices are sought for use in the internal circuitry employed in large particle detectors. Desirable features include low noise, low power consumption, high packing density, radiation resistance, very high response speed, and/or high adaptability to situations requiring multiple parallel channels. Desirable functions include amplifiers, counters, analog pulse storage devices, decoders, encoders, analog-to-digital converters, controllers, and communications interface devices.

(2) Circuits and systems are sought for rapidly processing data from particle detectors such as proportional wire chambers, scintillation counters, silicon microstrip detectors, particle calorimeters, and Cerenkov counters. Representative processing functions and circuits include low noise pulse amplifiers and preamplifiers, high

speed counters (>300 MHz), and time-to-amplitude converters. Compatibility with one of the widely used module interconnection standards (e.g., VMEbus, PCIExpress, or high speed serial interfaces) is highly desirable, as would be low power consumption, high component density, and/or adaptability to large numbers of multiple channels.

(3) Advanced, high speed logic arrays and microprocessor systems are sought for fast event identification, event trigger generation, and data processing with very high throughput capability. Such systems should be compatible with or implemented in one of the widely used module interconnection standards (e.g., VMEbus, PCIExpress, or high speed serial interfaces).

(4) Much of the electronics instrumentation in use in HEP is packaged in one of the international module interconnection standards (e.g., VMEbus, PCIExpress, or high speed serial interfaces). Therefore, grant applications are sought for modules that will provide capabilities not previously available; for substantial performance enhancement to existing types of modules; and for components, devices, or systems that will enhance or significantly extend the capability or functionality of one of the standard systems. Examples include large and/or fast buffer memories, single module computer systems (either general purpose or special purpose), display modules, interconnection systems, communication modules and systems, and disk-drive interface modules.

b. Large Scale Analysis Computer Systems—Grant applications are sought to develop: (1) computer system components and supporting software enabling large scale and open use of storage networks, especially for magnetic disks, optical disks, and magnetic tapes; (2) computer system components and supporting software enabling the use of TCP/IP protocols in a more efficient manner over a local area network; (3) computer software or systems for monitoring and operating heterogeneous computer systems and networks for functionality, performance, and manageability criteria (also, ease of software installation on hundreds of computers would be desired); (4) methods for integrating distributed authority and access control into distributed data systems; and/or (5) improvements to the quality, reliability and cost effectiveness of petabyte storage systems. Proposed efforts must address identified computing problems related to diverse, large scale computing systems that support particle physics analysis or accelerator control.

c. Distributed Collaborative Infrastructure and Distributed Data Management and Analysis

Frameworks—Advanced computational tools and software are needed to strengthen the ability of dispersed particle physics researchers to collaborate and to address problems related to the acquisition, handling, storage, analysis, and visualization of large datasets by these distributed collaborations. Grant applications are sought to develop: (1) client-server frameworks and Web tools for creating collaborative environments, facilitating remote participation of detector experts at the data collection stage, and allowing collaborators to remotely monitor experiments; (2) software project management tools; (3) computer system components and supporting software incorporating the use of Quality of Service features generally available in wide area networks; (4) portable systems to hold very large collections of data of the type created in connection with the operation of very large detectors, along with data management tools; (5) visualization and software environments appropriate for physics analysis; (6) software to support data systems distributed over a wide area network; (7) framework, interconnects, and other peripherals which allow the use and orderly aggregation of commodity computers and computer peripherals at larger than normal scales, or at higher performance levels than usual; (8) software development tools for the production of computer software to meet identified problems related to distributed, large scale software development, configuration management, and data analysis – approaches of interest include distributed portable testing and Computer Aided Software Engineering, including configuration management tools for a portable, distributed environment; (9) Web tools for remote data selection ("skimming"); and (10) neural nets for optimization of data cuts and pattern recognition.

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- 13. PCI Express: Performance Scalability for the Next Decade, http://www.pcisig.com/specifications/pciexpress
- 14. Regler, M., et al., *Data Analysis Techniques in High Energy Physics Experiments*, Cambridge, MA: Cambridge University Press, 1990. (ISBN: 0521341957)

PROGRAM AREA OVERVIEW OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

http://www.sc.doe.gov/ascr/home.html

The primary mission of the Advanced Scientific Computing Research (ASCR) program, which is carried out by the Mathematical, Information, and Computational Sciences subprogram, is to discover, develop, and deploy the computational and networking tools that enable researchers in the scientific disciplines to analyze, model, simulate, and predict complex phenomena important to the Department of Energy. To accomplish this mission the program fosters and supports fundamental research in advanced scientific computing – applied mathematics, computer science, and networking – and operates supercomputer, networking, and related facilities. The applied mathematics research efforts provide the fundamental mathematical methods to model complex physical and biological systems. The computer science research efforts enable scientists to efficiently run these models on the highest performance computers available and to store, manage, analyze, and visualize the massive amounts of data that result. The networking research provides the techniques to link the data producers; e.g., supercomputers and large experimental facilities with scientists who need access to the data.

In fulfilling this primary mission, the ASCR program supports the Office of Science Strategic Plan's goal of providing extraordinary tools for extraordinary science as well as building the foundation for the research in support of the other goals of the strategic plan. In the course of accomplishing this mission, the research programs of ASCR have played a critical role in the evolution of high performance computing and networks.

40. HIGH PERFORMANCE NETWORKS

The Office of Science (SC) in the U.S. Department of Energy (DOE) relies on a wide range of advanced network technologies to support its scientific activities. This topic addresses the development and deployment of advanced high-speed network technologies needed to support distributed tera-scale supercomputing, the remote controls of scientific instruments, distributed data storage, and large-scale secure scientific collaboration in SC programs. In particular, emerging large-scale science experiments in many SC programs (such as highenergy physics, nuclear energy, computational genomics, climate modeling, etc.) are expected to generate several petabytes of data, which will be transferred to geographically distributed tera-scale computing facilities for analysis and visualization by thousands of scientists. These distributed large-scale science activities require networks with unprecedented bandwidth and capabilities. This topic focuses primarily on system-level, ultra high-speed (10 Gbps and beyond) network technologies. Current areas of interest include, but are not limited to: (1) ultra high-speed transport protocols, (2) dynamic provisioning of Dense Wave Division Multiplexing (DWDM)-switched networks, and (3) ultra high-speed cyber security systems. Additional information on the DOE networking requirements can be found in the reports of the following workshops: DOE Science Networking Challenge: Roadmap to 2008 (http://www.es.net/hypertext/welcome/pr/Roadmap/), DOE workshop on High-Speed Transport Protocols and Dynamic Provisioning for Large-Scale Science Applications (http://www.csm.ornl.gov/ghpn/wk2003), and the High-Performance Network Planning Workshop (http://www.doecollaboratory.org/meetings/hpnpw/). Grant applications are sought only in the following subtopics:

a. Ultra High-Speed Network Technologies—Emerging large-scale distributed science applications increasingly depend on networks with unprecedented bandwidth capabilities to support distributed tera-scale computing and scientific collaboration. These networks are expected to securely deliver guaranteed ultra high-speed end-to-end throughputs (10-100 Gbps) to distributed high-end science applications. Achieving such levels of end-to-end performance will require advanced network technologies that are radically different from today's commercial Internet protocol (IP) networks, which are designed to deliver best-effort services. Grant applications are sought to develop system-level network technologies (hardware and software) that can securely

deliver multi-Gigabits/sec throughput to high-end scientific applications. Technical areas of interest include, but are not limited to, cost effective 10 Gbps network Interfaces, Transmission Control Protocol (TCP) and User Define Protocol (UDP) extensions for ultra high-speed data transfers, non-TCP transport protocol technologies, high-speed I/O and storage systems, and Operating System (OS)-bypass over wide-area networks, and ultra high-speed cyber security systems. Device-level network technologies (such as laser, optical signal processors, low-level hardware components, etc.) are beyond the scope of the current announcement.

b. Dynamic Provisioning Network Technologies—DOE recently funded a nation-wide high-capacity optical network testbed called *Ultra-Science Net* for developing, testing, and deploying user-controlled, dynamic provisioned, DWDM-based, optical network technologies. The goal of Ultra Science Net is to develop, test, and deploy advanced DWDM networks that are transparent to transport protocols and can be dynamically provisioned to provide on-demand end-to-end circuits and related services. The testbed, which is based on the Generalized Multiple Protocol Label Switching (GMPLS) standard for optical internetworking, has a switching capacity of 20 Gbps and expected to reach 40 Gbps capacity by 2006. Grant applications are sought to develop network technologies to support dynamic provisioning of secure end-to-end optical channels, bandwidth reservation and scheduling, and security mechanism for GMPLS services. Technical areas of interest include, but are not limited to: resource discoveries; bandwidth scheduling; GMPLS security; integration of end-to-end signaling technologies [Transaction Language 1 (TL1), GMPLS, and Multiple Protocol Label Switching (MPLS)], and conceptual frameworks such as inter-domain signaling architectures; circuit/wavelength routing; circuits exchange; and GMPLS traffic engineering. Further information on the Ultra-Science net testbed can be found at http://www.csm.ornl.gov/ultranet/.

c. High-Speed Network Security Systems—Grant applications are also sought to develop scalable cyber security systems that can operate at speeds up to 10 Gbps and beyond. Technologies of interest include ultra high-speed Intrusion Detection Systems (IDS), firewall systems, authentication systems for GMPLS control plane, and optical layer security services. Grant applications must address the scalability issues associated with their proposed approaches by demonstrating how the resulting security system be will operated at 10 GigE and OC-192 (Optical Carrier Level 192).

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- 2. ESnet: The Energy Sciences Network, U.S. DOE Office of Science, http://www.es.net
- 3. IEEE P802.3ae 10Gb/s Ethernet Task Force, http://grouper.ieee.org/groups/802/3/ae/public/index.html
- 4. *IETF RFC2823: PPP Over Simple Data Link (SDL) Using SONET/SDH with ATM-Like Framing,* <u>http://www.faqs.org/rfcs/rfc2823.html</u>
- 5. National Coordination Office for Information Technology Research and Development, <u>http://www.itrd.gov</u>
- Networked Computing for the 21st Century, Washington, DC: National Science and Technology Council, August 1998. (Available at: <u>http://www.itrd.gov</u>. Click on "Publications." Scroll down and click on "Supplement to the President's Budget," and then on "FY 1999 Blue Book".)
- 7. Next Generation Internet (NGI), <u>http://ngi.gov</u>
- 8. *QBONE* (Cooperative Advanced Quality of Service Testbed), <u>http://qbone.internet2.edu/</u>

- 9. Rajagopalan, B., et al., *IP Over Optical Networks: A Framework*. (URL: <u>http://www.faqs.org/rfcs/rfc3717.html</u>)
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41. SCALABLE MIDDLEWARE AND GRID TECHNOLOGIES

Advances in high performance network capabilities and collaboration technologies are making it easier for large geographically dispersed teams to collaborate effectively. This is especially important for research teams that use major computational resources, data resources, and experimental facilities supported by DOE. The importance of collaboratories is expected to increase in the future. However, significant research questions must be addressed if collaboratories are to achieve their potential, namely, by providing: (1) remote access to facilities that produce petabytes per year; (2) remote users with an experience that approaches "being there;" (3) remote visualization of terabyte to petabyte data sets from computational simulation; and (4) effective remote access to advanced scientific computers. Research and software tool development are needed to support coordinated and dynamic resource sharing in areas such as resource discovery, resource access, authentication, authorization, accounting, etc., in the areas listed below. Any tools or services developed should be interoperable according to emerging standards from the Global Grid Forum. Also, it should be noted that the high performance network environment does not include wireless elements. **Grant applications are sought only in the following subtopics:**

a. Scalable Middleware Technologies—Grant applications are sought to develop scalable middleware technologies that will: (1) enable universal, ubiquitous, easy access to remote computing resources and scientific instruments; (2) facilitate collaboration among distributed science teams; and (3) enable a new generation of distributed high-end applications. Areas of interest include, but are not limited to, secure directory services, scalable authentication services, authorization services, deployable LAN and WAN QoS services, wide-area distributed data management, efficient multicast capabilities, automatic resource discovery protocols, remote data access services, and network-attached memory and storage systems.

b. Scalable Grid Technologies—Grant applications are sought to develop scalable grid technologies to support the emerging distributed computing network that provides reliable, secure, consistent, pervasive, scaleable, and efficient access to various resources integrated into a distributed infrastructure, which can be accessed wherever and whenever by DOE scientists. These resources include visualization systems, computer systems, data storage and archive systems, and scientific instruments. Areas of interest include, but are not limited to, collaborative visualization systems, collaborative problem solving services, application level fast data transfer toolkits or services, group collaboration, co-scheduling of distributed resources, grid accounting and billing mechanisms, data management tools, science portals, and real-time instrumentation services.

- 1. U.S. DOE Collaboratories, U.S. DOE Office of Science, http://www.doecollaboratory.org
- Foster, I. and Kesselman, C., eds., *The Grid: Blueprint for a New Computing Infrastructure*, San Francisco, CA: Morgan Kaufmann Publishers, 1999. (ISBN: 1-55860-475-8)
- 3. Foster, I. and Kesselman, C., eds., *The Grid 2: Blueprint for a New Computing Infrastructure*, 2nd ed., San Francisco, CA: Morgan Kaufmann Publishers, 2003. (ISBN: 1-55860-933-4)
- 4. Berman, F., et al., eds., *Grid Computing: Making the Global Infrastructure a Reality*, John Wiley & Sons, 2003. (ISBN: 0-470-85319-0) (Resource site at: <u>http://www.grid2002.org</u>)

- 5. *Global Grid Forum (GFF)*, <u>http://www.globalgridforum.com/</u>
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- 7. Particle Physics Data Grid, U.S. DOE Office of Science, http://www.ppdg.net
- 8. Earth System Grid Project, U.S. DOE Office of Science, http://www.earthsystemgrid.org/
- 9. FusionGRID, National Fusion Grid Project, U.S. DOE Office of Science, http://www.fusiongrid.org
- 10. *SciDAC (Scientific Discovery through Advanced Computing)*, U.S. DOE Office of Science <u>http://www.osti.gov/scidac</u>
- 11. U.S. Department of Energy, Office of Science, http://www.science.doe.gov/

42. TECHNOLOGY FOR SOFTWARE LIBRARIES

The Advanced Scientific Computing Research (ASCR) program has been fully or partially responsible for funding the research and development of a wide range of robust high-quality numerical algorithms for scientific computation. These include the development of libraries such as EISPACK, LINPACK, LAPACK, ScaLAPACK, ARPACK, CLAWPACK, PETSc, TAO, CHOMBO, ebCHOMBO, SALSA, MPSALSA, LOCA, HYPRE, SuperLU, FronTier, and many others. However, critical issues still require resolution to ensure that the value of such scientific software is maintained and that the large investment in the research and development of these algorithms is maximized. These issues include enhancing user interfaces, providing distribution support, providing maintenance activities such as collecting and tracking bug reports, fixing bugs, and providing portability across platforms (including porting to new computational architectures). Grant applications are sought only in the following subtopic:

a. Deployment and Maintenance of Robust Numerical Software Libraries—Grant applications are sought to: (1) develop new maintenance and distribution mechanisms to ensure that updated scientific libraries are subjected to validation and verification testing; (2) implement formal tracking mechanisms for bug reports, bug fixes, and update notification for a wide range of scientific algorithm libraries; (3) develop and maintain mechanisms for providing cost effective portability of scientific libraries across a wide range of computer architectures, from desktop systems to massively parallel leadership-class supercomputers; (4) develop and maintain high-quality user documentation for each component of scientific software, including advice on domains of applicability for each module; and (5) develop comprehensive email- or Web-based user support services for scientific libraries. The ASCR program will assure that successful grant applicants will obtain access to relevant computational facilities, as needed for their research.

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- 2. Dongarra J. and Walker, D., "Software Libraries for Linear Algebra Computations on High Performance Computers," *SIAM Review*, 37: 151-180, 1995. (ISSN: 0036-1445)

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- 5. Geist, A., et al., eds., *PVM: Parallel Virtual Machine. A Users' Guide and Tutorial for Networked Parallel Computing*, Cambridge, MA: MIT Press, 1994. (ISBN: 0262571080)
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- Balay, et al., *PETSc Users Manual*, Argonne National Laboratory, 2002. (Report No. ANL-95/11 Rev. 2.1.6) (Full text available at: <u>http://www-unix.mcs.anl.gov/petsc/petsc-2/snapshots/petsc-current/docs/manual.pdf</u>)
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- Benson, S., et al., *TAO Users Manual*, Technical Report, Argonne National Laboratory, August 2004. (Report No. ANL/MCS-TM-242-Revision 1.7) (Full text available at: <u>http://www-unix.mcs.anl.gov/tao/docs/manual/manual.html</u>)
- 16. Shadid, J., et al., MPSalsa Version 1.5: A Finite Element Computer Program for Reacting Flow Problems: Part 1 – Theoretical Development, Technical Report, Sandia National Laboratories, 1998. (Report No. SAND98-2864) (NTIS Order No. DE00002641. See Solicitation Program Information, Instructions, and Requirements, Section 7.1.)
- Salinger, A. G., et al., LOCA 1.1: Library Of Continuation Algorithms: Theory and Implementation Manual, Technical Report, Sandia National Laboratories, October 2002. (Report No. SAND2002-0396) (Full text available at: <u>http://www.cs.sandia.gov/loca/loca1.1_book.pdf</u>)

18. *Hypre*, <u>Advanced CompuTational Software Collection</u>, U.S. Department of Energy National Energy Research Scientific Computing Center, undated. (Available at: <u>http://acts.nersc.gov/hypre/main.html</u>)

PROGRAM AREA OVERVIEW OFFICE OF NUCLEAR PHYSICS

http://www.sc.doe.gov/production/henp/np/index.html

Nuclear physics 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 determine the essential physical characteristics of the universe. The primary mission of the Nuclear Physics program is to develop and support the scientists, techniques, and facilities that are needed for basic nuclear physics research. Attendant upon this core mission are responsibilities to enlarge and diversify the Nation's pool of technically trained talent and to facilitate transfer of technology and knowledge to support the Nation's economic base.

Nuclear physics research is carried out at National accelerator facilities and through university programs. The Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility (TJNAF) and the Bates Linear Accelerator at MIT allow detailed studies of how quarks and gluons bind together to make protons and neutrons. CEBAF is planning a future upgrade in which the electron beam energy is doubled from 6 to 12 GeV. The Relativistic Heavy Ion Collider (RHIC), now in operation at Brookhaven National Laboratory (BNL), will instantaneously form submicroscopic specimens of quark-gluon plasma by colliding gold nuclei, thus allowing a study of the primordial soup of quarks and gluons thought to make up the early universe. RHIC is planning a beam luminosity upgrade in the future; a new electron-ion collider is also being discussed. The nuclear physics program supports research and facility operations that are directed towards 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), the Holifield Radioactive Ion Beam Facility (HRIBF) at Oak Ridge National Laboratory (ORNL) and the 88-Inch Cyclotron at Lawrence Berkeley National Laboratory (LBNL), which provide complementary facilities for stable and radioactive beams as well as a variety of species and energies. In addition, the operations of accelerators for in-house research programs at four universities (Yale University, Washington University, Texas A&M University, and Triangle Universities Nuclear Laboratory (TUNL) at Duke University) provide unique instrumentation with a special emphasis on training of students. The nuclear physics program also supports non-accelerator experiments such as the Sudbury Neutrino Observatory (SNO) facility, constructed by a collaboration of Canadian, English, and U.S. supported scientists, now taking data on solar neutrino fluxes and providing the first results on the "appearance" of oscillations of electron neutrinos into another neutrino type. A proposed Rare Isotope Accelerator (RIA) facility is being designed that would provide a way to explore the limits of nuclear existence. By producing and studying highly unstable nuclei that are now formed only in the stars, scientists could better understand stellar evolution and the origin of the elements.

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

43. NUCLEAR PHYSICS SOFTWARE AND DATA MANAGEMENT

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 and the Thomas Jefferson National Accelerator Facility. The experiments at such facilities are extremely complex and expensive, involving thousands of detectors that produce raw experimental data at rates of up to several hundred MB/sec, resulting in the annual production of data sets on the order of several hundred Terabytes (TB), with Petabytes (PB) of data in the near future. Many 10s of Terabytes of data per year are distributed to many institutions around the U.S. and other countries for analysis by the scientific collaborators. Research on large scale data management systems is required to support these large nuclear physics experiments. All grant applications must explicitly show relevance to the nuclear physics program. **Grant applications are sought only in the following subtopics:**

a. Large Scale Data Storage—Projections of the cost of data storage media show that magnetic disk media will soon be competitive with magnetic tape for storing large volumes of data. Because current technology keeps all disk drives powered and spinning, the infrastructure costs of operating a petabyte disk storage system could be prohibitive. However, one characteristic of nuclear physics datasets is that most of the data is accessed infrequently. Therefore, grant applications are sought for new techniques for petabyte-scale magnetic disk systems optimized for infrequent data access, emphasizing lower cost and lower power usage. To the extent feasible, it is desirable that the cost should scale with the amount of data accessed rather than the total storage capacity.

Grant applications are also invited for development of innovative new storage technologies with high reliability, low cost, and geared toward infrequently accessed petabyte-scale data.

b. Large Scale Data Processing and Distribution—Some nuclear physics facilities produce 100s of TB of data per year, soon to be PB per year. Many 10s of TB of data per year are distributed world-wide for analysis by the scientific collaborators. A recent trend in nuclear physics is to construct these data handling and distribution systems using data grid infrastructure software such as Globus and Condor. In the near future. these systems will use the Open Grid Services Architecture (OGSA), which is based upon Web Services. At that time, it will be necessary for any proposed infrastructure software solutions to integrate well with this new data grid technology. 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 data volumes, including, but not limited to, automated data replication coupled with application data catalogs, and distributed storage systems of commercial off-the-shelf (COTS) hardware; (2) hardware and/or software techniques to improve the effectiveness of computational and data grids for nuclear physics (see reference 3 for these uses) – examples include integrating the management of distributed open source Relational Data-Base Management System (RDBMS) with OGSA and developing application level monitoring services for status and error diagnosis; (3) effective new approaches to data mining, automatic structuring of data and information, and facilitated information retrieval; and (4) distributed authorization and security systems enabling single sign-on access to data distributed across many sites. Applicants that propose data distribution projects are encouraged to contact the U.S. National Nuclear Data Center to determine relevance and possible future migration strategies into existing infrastructures.

c. Large Scale Data Archiving and Maintenance—One of the legacies of experimental nuclear physics experiments is the data produced. Large projects like RHIC, Gammasphere, or Jefferson Laboratory produce unique data, reflecting measurements that may never be repeated. Although results are usually obtained and published from this data, it may take several years before the data is analyzed and the results are published; then, in subsequent years, there may be a need to present the data in different forms, in order to facilitate comparison with new theoretical descriptions or newer experimental measurements. Therefore, it is important to preserve the data and its documentation over many years, through changes in storage technology and the

evolution of experimental groups. Grant applications are sought to develop permanent archiving and userfriendly Internet dissemination procedures for the data from nuclear physics experiments along with associated detector description and calibration information. A complete data package would include raw data and the programs to read and process it; ROOT trees or n-tuples with derived physics quantities; and documentation, analysis notes, email archives, and web pages that detail the information and procedures used with the data for existing results. Examples of relevant technologies include (but are not limited to) systems for collecting, recording and preserving data-provenance metadata, tools to verify data integrity over long lifetimes, annotation tools, and data access portals to enable searching and retrieving relevant and related data and metadata.

d. Cluster Interconnects—Large scale (thousands of CPU's) computing platforms are needed to perform theoretical calculations of Lattice Quantum ChromoDynamics (LQCD), a method of extracting the predictions of the fundamental theory of the interactions of quarks. While these science applications can use virtually any supercomputer architecture efficiently, the computational demands are such that the cost effectiveness of the platform (measured in floating point operations per second per dollar, as sustained by a large scale parallel application) is a significant consideration. Clusters would be an appropriate platform for these calculations because of their low cost per compute node, but only if the cluster interconnects were of high bandwidth, low latency, and low cost. Although current offerings fall short on at least one of these metrics, the science applications are such that nearest-neighbor communications predominate in a three or four dimensional torus; therefore, a fully interconnected switch fabric is not essential – a torus mesh with routing also would be a feasible design. Grant applications are sought to develop mesh-communication-optimized cluster interconnects scalable to thousands of nodes at modest cost. The interconnects must be well coupled to next generation commodity compute nodes (to achieve high bandwidth and low latency on future systems) and must have a cost well below the cost of the compute node.

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44. NUCLEAR PHYSICS ELECTRONICS DESIGN AND FABRICATION

The DOE seeks developments in detector instrumentation electronics with improved energy, position and timing resolution, sensitivity, rate capability, stability, dynamic range, durability, pulse shape discrimination capability, and background suppression. Of particular interest are innovative readout electronics for use with the nuclear physics detectors described in Topic 46. All grant applications must explicitly show relevance to the nuclear physics program. **Grant applications are sought only in the following subtopics:**

a. Advances in Digital Electronics—Digital signal processing electronics are needed to replace analog signal processing in nuclear physics applications. Grant applications are sought to develop: (1) digital pulse processors that simplify or replace analog designs and have sufficient flexibility to incorporate such features as pile-up rejection and ballistic deficit correction; (2) digital pulse processing electronics, including pulse-shape discrimination, for commonly used nuclear physics detectors in general, and for position sensitive solid-state detectors or highly segmented CdZnTe detectors in particular; and (3) fast digital processing electronics that improve the accuracy of the analog electronics, such as in determining the position of interaction points (of particles or photons) to an accuracy smaller than the size of the detector segments.

b. Circuits—Grant applications are sought to develop custom designed integrated circuits, as well as for circuits (including firmware) and systems, for rapidly processing data from highly segmented, position-sensitive germanium detectors (pixel sizes of approximately 1 cm²) and from particle detectors (e.g., gas detectors, scintillation counters, silicon drift chambers, silicon strip detectors, particle calorimeters, and Cherenkov counters) used in nuclear physics experiments. Areas of specific interest include: (1) representative circuits such as low noise preamplifiers, amplifiers, peak sensors, analog storage devices, analog-to-digital and time-to-digital converters, transient digitizers, and time-to-amplitude converters; (2) multiple sampling ASICs, to allow for pulse shape analysis; (3) readout electronics for solid-state pixilated detectors, including interconnection technologies and amplifier/sample-and-hold integrated circuits; and (4) constant fraction discriminators with uniform response for low and high energy gamma-rays. These circuits should be fast; low-cost; high-density; configurable in software for thresholds, gains, etc.; easy to use with commercial auxiliary electronics; low power; compact; and efficiently packaged for multichannel devices.

In addition, planned luminosity upgrades at RHIC and experiments at the Large Hadron Collider will require fine-grained vertex and tracking detectors (both silicon and gas) for high particle multiplicity environments. Therefore, grant applications are sought for advances in microelectronics that are specifically designed for low noise amplification and processing of detector signals, and that are suitable for these next generation detectors. The microelectronics and associated interconnections must be lightweight and have low power dissipation. Of particular interest are designs that minimize higher gate leakage currents due to tunneling and maintain dynamic range.

c. Advanced Devices and Systems—So called Active Pixel Sensors in CMOS (complementary metal-oxide semiconductor) technology are replacing Charge Coupled Devices as imaging devices and cameras for visible light. Several laboratories are exploring the possibility of using such devices as direct conversion particle detectors. The charge produced by an ionizing particle in the epitaxial layer is collected by diffusion on a sensing electrode in each pixel. The charge is amplified by a relatively simple low noise circuit in each pixel and read out in a matrix arrangement. If successful, this approach would make possible high-resolution, position-sensitive particle detectors with very low mass (only about 100 microns of silicon in a single layer). This approach would be clearly superior to the present technology that use hybrid vertex detectors, which

consist of a separate silicon detector layer bump-bonded to a CMOS readout circuit. Grant applications are sought to attempt this very significant advance in integrated detector-electronics technology, using CMOS monolithic circuits as particle detectors. The new active pixel detector with its integrated electronic readout should be based on a standard CMOS process. The challenge is to design the sensor and low noise readout circuits to have sufficiently high sensitivity and low power dissipation in order to detect the charge signal developed in a thin epitaxial layer (~10 microns), as available in some of the standard CMOS processes.

Grant applications also are sought for the next generation of active pixel, or even strip, sensors which use the bulk silicon substrate as the active volume. This more advanced approach would have the advantage of developing relatively larger signals and allowing sensitivity to non-minimum ionizing particles such as MeV-range gamma rays.

Lastly, 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 devices include radiation-hardened, wide-bandgap semiconductors (i.e., semiconductor materials with bandgaps greater than 2.0 electron volts, including Silicon Carbide (SiC), Gallium Nitride (GaN), and any III-Nitride alloys), inhomogeneous semiconductors such as SiGe; and device processes such as silicon-on-insulator (SOI) or silicon-on-sapphire (SOS). Areas of interest regarding systems include 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., >500Gb/s), advanced high-bandwidth data links are of interest. Also of interest are generalized software and hardware packages, with improved graphic and visualization capabilities, for the acquisition and analysis of nuclear physics research data.

d. Manufacturing and Advanced Interconnection Techniques—Grant applications are sought to develop: (1) manufacturing techniques for large, thin, multiple-layer printed circuit boards (PCBs) with plated-through holes, dimensions from 2m x 2m to 5m x 5m, with thickness from 100 to 200 microns (these PCBs would have use 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 (this 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 interdensity 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 parasites [13]; (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 [14]; 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 the goal of reusing the developed circuits in future experiments.

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45. NUCLEAR PHYSICS ACCELERATOR TECHNOLOGY

The Nuclear Physics program of the Department of Energy (DOE) 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 superconducting Relativistic Heavy Ion Collider (RHIC) with heavy ion beam energies up to 100 GeV/amu and polarized proton beam energies up to 250 GeV, technologies associated with RHIC luminosity upgrades and the development of an electron-ion collider, superconducting radio frequency (srf) linear accelerators such as the electron machine at the Thomas Jefferson National Accelerator Facility (TJNAF), and development of devices and/or methods that would be useful in the generation of intense accelerated beams of radioactive isotopes related to the construction of a Rare Isotope Accelerator (RIA) facility. Relevance of applications to nuclear physics must be explicitly described. Grant applications that propose using the resources of a third party (such as a DOE laboratory) must include, in the application, a letter of certification from an authorized official of that organization. **Grant applications are sought only in the following subtopics**:

a. Materials and Components for Radio Frequency Devices—Grant applications are sought to improve or advance superconducting and room temperature materials or components for radio frequency (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, cryogenic radio frequency windows, rf power couplers, and magnetostrictive or piezoelectric cavity tuning mechanisms; (2) materials that efficiently absorb microwaves from 2 to 90 GHz and are compatible with ultra-high vacuum, particulate-free environments at 2 to 4 K; (3) methods for manufacturing superconducting materials that have lower RF losses, operate at higher temperatures, and/or have higher RF critical fields than sheet niobium; (5) innovative designs for hermetically sealed helium refrigerators and other cryogenic equipment that simplify procedures and reduce costs associated with repair and modification; (6) development of simple, low-cost mechanical techniques for damping length oscillations in accelerating structures, effective in the 10-300 Hz range at 2 Kelvin; and (7) development of techniques to create a layer of niobium on the interior of a copper elliptical cavity, such as by energetic ion deposition, so that the resulting 700-1500 MHz structures have $Q_0 > 8 \times 10^9$ at 2 K and so that overall fabrication costs are reduced relative to using sheet niobium.

Grant applications also are sought for the design, computer-modeling, and hardware development of 5 kW and 13 kW cw power sources at 1497 MHz and 1 MW cw rf power sources at 704 MHz. Examples of candidate technologies include (but are not limited to): solid-state devices, multi-cavity klystrons, Inductive-Output Tubes (IOT's), or hybrids of those technologies. The devices for 1497 MHz should: (1) be capable of operating efficiently over a range of output power levels; (2) include a method for power adjustment other than using the rf drive signal and the voltage of any primary dc source – for example, a klystron should include a gun-current modulating electrode; and (3) have an ac-to-rf conversion efficiency greater than 50%. Interested

parties should contact Dr. Leigh Harwood at Jefferson Laboratory [harwood@jlab.org] or Dr. Ilan Ben-Zvi at Brookhaven National Laboratory (<u>ILAN@BNL.GOV</u>) for further specifications.

Lastly, grant applications are sought for a new generation of high-voltage (up to 200 k VDC) electronic switching devices with peak current capability on the order of 100 A. Such devices should also be capable of operating as very high power (tens of Megawatts), low-frequency (below 100 MHz) rf power amplifiers with suitable external rf circuits. A possible technology is the Hobetron. Interested parties should contact Abbi Zolfaghari (*abbi@bates.mit.edu*) at MIT-Bates Laboratory.

b. Design and Operation of Radio Frequency Beam Acceleration Systems—Grant applications are sought for the design, fabrication, and operation of radio frequency accelerating structures and systems for heavy-ion accelerators. Areas of interest include: (1) continuous wave (cw) structures, both superconducting and non-superconducting, for the acceleration of beams in the velocity regime between 0.001 and 0.01 times the velocity of light and with charge-to-mass ratios between 1/30 and 1/240; (2) superconducting rf accelerating structures appropriate for RIA drivers, for particles with speeds in the range of 0.02-0.8 times the speed of light; (3) innovative techniques for field control of ion acceleration structures (1° of phase and 0.1% amplitude) and electron acceleration structures (0.1° of phase and 0.01% amplitude) in the presence of 10-100 Hz variations of the structures' resonant frequencies (0.1-1.5 GHz); (4) multi-cell, superconducting, 0.5-1.5 GHz accelerating structures that have sufficient higher-order mode damping for use in energy-recovering linac-based devices with ~1 A of electron beam; (5) 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 (6) methods and/or devices for reducing the emittance of relativistic ion beams – such as electron or optical-stochastic cooling.

c. Particle Beam Sources and Techniques—Grant applications are sought to develop: (1) particle beam ion sources with improved intensity, emittance, and range of species (areas of interest include high-charge-state sources for heavy ions, sources for negative and light ions, and polarized sources for hydrogen ions and electrons); (2) ion sources for radioactive beams (emphasizing aspects such as high efficiency, high-charge-state ions, small emittance and energy spread, high temperature operation for coupling to high temperature production targets, and element selectivity -e.g., through the use of laser ionization); (3) techniques for secondary radioactive beam collection, charge equilibration, and cooling; (4) methods and devices to increase the charge state of ion beams (e.g., by the use of special electron-cyclotron-resonance ionizers or special stripping techniques); (5) high brightness electron beam sources utilizing continuous wave (cw) superconducting rf cavities with integral photocathodes operating at high acceleration gradients; (6) ~1 GHz cw polarized electron sources delivering beams of ~10 mA with longitudinal polarization of ~80%; (7) ~28 MHz cw polarized sources delivering beams of ~500 mA with ~80% polarization; (8) novel high quantum efficiency, long life photocathode materials, such as chalcopyrites, for brightness electron sources with polarizations >90%; (9) devices, systems, and sub-systems for producing high current (>200µA), variable-helicity beams of electrons with polarizations >80%, and which have very small helicity-correlated changes in beam intensity, position, angle, and emittance; (10) methods to improve high voltage stand-off and reduce field emission from high voltage electrodes in the presence of work function lowering material (i.e., cesium), and which are compatible with ultra high vacuum environments; (11) wavelength tunable (700 to 850 nm) mode-locked lasers with pulse repetition rate between 0.5 and 3 GHz and average output power >10 W; and (12) a high average power (~100 W) green laser light source, with a rf-pulse repetition rate in the range of 0.5 to 3 GHz for synchronous photoinjection of GaAs photoemission guns.

Grant applications also are sought to develop software that adds significantly to the state-of-the-art in the simulation of such physical processes as intra-beam scattering, electron cooling, beam dynamics, transport and instabilities, electron or plasma discharge in vacuum under the influence of charged beams, etc.

d. Accelerator Control and Diagnostics—Grant applications are sought for: (1) "intelligent" software and hardware to facilitate the improved control and optimization of charged particle accelerators and associated components for nuclear physics research (developments that offer generic solutions to problems in the initial choice of operation parameters and the optimization of selected beam parameters with automatic tuning are especially encouraged); (2) advanced beam diagnostics concepts and devices that provide high speed computercompatible measurement and monitoring 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 and techniques that are nondestructive to the beams being monitored); (3) beam diagnostic devices that have increased sensitivities through the use of superconducting components (for example, filters based on high T_c superconducting technology or Superconducting Quantum Interference Devices); (4) measurement devices/systems for cw beam currents in the range 0.1 to 100 μ A, with very high precision ($<10^{-4}$) and short integration times; (5) beam diagnostics for ion beams with intensities less than 10^{7} nuclei/second; (6) non-destructive beam diagnostics for stored ion beams such as at the RHIC and/or for 100 mA class electron beams; (7) devices that can perform direct 12-14 bit digitization of signals at 0.5-2 GHz and have bandwidths of 100+ kHz; (8) systems for predicting insipient failure of accelerator components through the monitoring/cataloging/scanning of real-time or logged signals; (9) devices/systems that measure the emittance of intense (>100kW) cw ion beams, such as those expected at the Rare Isotope Accelerator facility; and (10) beam halo monitor systems for ion beams.

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- * Available from Springer-Verlag New York, Inc. Telephone: 800-777-4643. Website: <u>http://www.springer-ny.com/aip/</u>

46. NUCLEAR PHYSICS PARTICLE AND RADIATION DETECTION SYSTEMS, INSTRUMENTATION AND TECHNIQUES

The Department of Energy (DOE) 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 and outside the usual scope of research and development activities at the nuclear physics national laboratories and university programs. In addition, a new suite of next-generation detectors will be needed for the proposed Rare Isotope Accelerator (RIA), the energy upgrade at

TJNAF, the proposed underground laboratory, the proposed luminosity upgrade at RHIC, and a possible future electron-ion accelerator. All grant applications must explicitly show relevance to the nuclear physics program. **Grant applications are sought only in the following subtopics:**

a. Advances in Detector and Spectrometer Technology—Nuclear physics research has a need for devices to detect, analyze, and track charged particles, and neutral particles such as neutrons, neutrinos, photons, and single atoms. These devices include: solid-state devices such as highly segmented coaxial and planar germanium detectors, and silicon strip, pixel, and silicon drift detectors; photosensitive devices such as avalanche photodiodes, hybrid photomultiplier devices, single and multiple anode photomultiplier tubes, highintensity ($\sim 10^{20}$ y/s) gamma-ray current-readout detectors (e.g. Compton Diodes), photodiodes for operation at liquid helium temperatures with a signal-to-noise ratio comparable to a photomultiplier tube, and other novel photon detectors; detectors utilizing photocathodes for Cherenkov and UV light detection, and the development of new types of large area photo-emissive materials such as solid, liquid, or gas photocathodes; micro-channel plates; gas-filled detectors such as proportional, drift, streamer, microstrip, Gas Electron Multipliers (GEMs), Micromegas and other types of micropattern detectors, straw drift tube detectors, time projection chambers, resistive plate chambers, and Cherenkov detectors; liquid argon and xenon ionization chambers and other cryogenic detectors; single-atom detectors using laser techniques and electromagnetic traps; particle polarization detectors; electromagnetic and hadronic calorimeters, including high energy neutron detectors; and detection systems for detecting the magnetization of polarized nuclei in a magnetic field (e.g., Superconducting Quantum Interference Device (SQUIDS) or cells with paramagnetic atoms that employ large pickup loops to surround the sample). Grant applications are sought to develop advancements in the technology of the above mentioned detectors.

With respect to solid state tracking devices, such as the segmented germanium detectors and the silicon drift, strip, and pixel detectors, grant applications are sought for: (1) manufacturing techniques, including interconnection technologies for high granularity, high resolution, light-weight, and radiation-hard solid state devices; (2) highly arrayed solid state detectors for neutron detection, with integrated electronics to read-out pulse height; (3) thicker (more than 1.5 mm) segmented silicon charged-particle and x-ray detectors and associated high density, high resolution electronics; and (4) cost-effective production of n-type and p-type silicon drift chambers with active areas greater than 16 cm².

With respect to position sensitive charged particle and photon tracking devices, grant applications are sought for the development of: (1) position sensitive, high resolution, germanium detectors capable of determining the position (to within a few millimeters utilizing pulse shape analysis) and energy of the individual interactions of gamma-rays (with energies up to several MeV), hence allowing for the reconstruction of the energy and path of individual gamma-rays using tracking techniques; (2) hardware and software needed for digital signal processing and gamma-ray tracking – of particular interest is the development of efficient and fast algorithms for signal decomposition and improved tracking programs; (3) alternative materials, with comparable resolution to germanium, but with significantly higher efficiency and relatively higher temperature operation (in order to overcome the costly and bulky requirement to cool germanium detectors to liquid nitrogen temperatures); (4) improvements and new developments in micropattern detectors - this would specifically include commercial and cost effective production of GEM [23] foils and other types of micropattern structures, such as fine meshes used in Micromegas [24], as well as novel approaches that could provide high resolution multidimensional readout; (5) advances in more conventional charged-particle tracking detector systems, such as drift chambers, pad chambers, time expansion chambers, and time projection chambers (areas of interest include improved gases or gas additives that resist aging, improve detector resolution, decrease flammability, and offer larger/more uniform drift velocity); (6) high-resolution, gas-filled, time-projection chambers employing CCD cameras to perform an optical readout; (7) gamma-ray detectors capable of making accurate measurements of high intensities (>10¹¹/s) with a precision of 1-2 %, as well as economical gamma-ray beam-profile monitors; (8) for the RIA, next-generation high spatial resolution focal plane detectors for magnetic spectrographs and recoil separators, for use with heavy ions in the energy range from less than 1 MeV/u to over 100 MeV/u; and

(9) a bolometer with high-Z material (e.g. W, Ta, Pb) for gamma ray detection with segmentation, capable of handling 100 -1000 gamma ray per second; (10) detectors made of more conventional materials (silicon or scintillator) capable of reconstructing multiple-Compton gamma-ray scattering with mm resolution; and (11) advances in CCD technology, particularly in areas of fast parallel, low-power readout and cross-talk control.

With respect to particle identification detectors, grant applications are sought for the development of: (1) inexpensive, large-area, high-quality Cherenkov materials; (2) inexpensive, position sensitive, large-sized photon detection devices for Cherenkov counters; (3) high resolution time-of-flight detectors; (4) affordable methods for the production of large volumes of xenon and krypton gas (which would contribute to the development of transition radiation detectors and would also have many applications in X-ray detectors); and (5) very high resolution particle detectors or bolometers based on semiconductor materials and cryogenic techniques. Of particular interest are detector technologies capable of measuring energies of alpha particles and protons with less than 5 keV resolution, allowing spectroscopy experiments using light charged particles to be performed in the same way as gamma spectroscopy.

Grant proposals also are invited for development of systems for predicting insipient failure of detector components through the monitoring/cataloging/scanning of real-time or logged signals.

Grant proposals also are invited for innovative design of high-resolution particle separators needed for the spectrometer research program associated with the Rare Isotope Accelerator project [21]. (Please contact Dr. J.A.Nolen, Jr [nolen@anl.gov] of Argonne National Laboratory for additional details).

b. Technology for Rare Particle Detection—Grant applications are sought for particle detectors and techniques that are capable of measuring very weak, rare event signals in the presence of significant backgrounds. Such detector technologies and analysis techniques are required in searches for rare events (such as double beta decay) and for applications in extending our knowledge of new nuclear isotopes produced at radioactive beam facilities. Rare decay and rare phenomenon detectors require large quantities of very clean materials, such as clean shielding materials and clean target materials. Neutrino detectors need very large quantities of ultra-clean water, for example.

Grant applications are sought to develop: (1) ultra-low background techniques of contacting, supporting, cooling, cabling, and connecting high-density arrays of germanium detector – ultrapure materials must be used in order keep the generated background rates as low as possible (goal is 1 micro-Becquerel per kg); (2) advanced germanium detector cooling techniques and associated infrastructure (high-density signal cabling, signal and high voltage interconnects, vacuum feedthroughs, front-end amplifier FET assemblies) to assure ultra-low levels of radioactive contaminants; and (3) measurement methods for the contaminant level of the ultra-clean materials.

Grant applications also are sought for new technologies to produce large quantities of separated isotopes, such as kg quantities of Ge-76 and other materials, which are needed for rare particle and rare decay searches in nuclear physics research.

c. Large Band Gap Semiconductors, New Bright Scintillators, Calorimeters, and Optical Elements— Grant applications are sought to develop new materials or advancements for photon detection. Of specific interest are: (1) large band gap semiconductors such as (CdZnTe); (2) bright, fast scintillator materials (LaBr₃:Ce, HgI₂, AlSb, etc.); (3) plastic scintillators, fibers, and wavelength shifters; (4) cryogenic liquid scintillation gamma ray detectors (LXe); (5) Cherenkov radiator materials with indices of refraction up to 1.10 or greater with good optical transparency; (6) high reflectivity VUV mirrors, which operate at wavelengths below 193 nm, especially at 157 nm and 126 nm, and which are robust with respect to radiation damage, especially synchrotron radiation; and (7) new and innovative calorimeter concepts, including new materials, higher packing densities, or innovative fiber and absorber packing schemes. **d. Nuclear Targets and High-Radiation Environment Beam Transport Components**—Grant applications are sought to develop specialized targets for the-nuclear physics program, including: (1) polarized (with nuclear spins aligned) high-density gas or solid targets; (2) frozen-spin targets; active (scintillating) targets; (3) windowless gas targets; supersonic jet targets for use with very low energy charged particle beams; (4) liquid, gaseous, and solid targets capable of high power dissipation when high intensity, low emittance charged particle beams are used; (5) high-power targets with fast release capabilities for the production of rare isotopes; and (6) thin (<few micro-g/cm²) condensed phase hydrogen targets that can be well localized (1mm in all directions). In addition, grant applications are sought to develop techniques for: (1) the production of ultra-thin films needed for targets, strippers, and detector windows – in particular, for the RIA, there is a need for stripper foils or films in the thickness range from a few micrograms per cm² to over 10 milligrams per cm², for use in the driver linac with very high power densities from uranium beams; and (2) preparation of targets of radioisotopes, with half-lives in the hours range, to be used off-line in both neutron-induced and charged-particle-induced experiments.

Grant applications also are sought for techniques and strategies needed for addressing the development of ion beam transport in the high-radiation environment anticipated at RIA [25]. Approaches of interest include: (1) simulations to characterize radiation doses to magnets and other components near the production targets and beam dumps; (2) development of appropriate containment for activated coolants such as liquid lithium and water; and (3) development of magnet design concepts that are consistent with the radiation dose, field, and aperture requirements set by optics calculations.

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- For article ordering information and to view abstract, see: <u>http://www.sciencedirect.com/science/publications/journal/physics</u>. In center of page under "Search for a title," select "Browse A-Z." Select "n" from letters of the alphabet and scroll down to journal title. Continue search using information given in citation.

PROGRAM AREA OVERVIEW OFFICE OF DEFENSE NUCLEAR NONPROLIFERATION

http://www.nnsa.doe.gov/na-20

The Office of Defense Nuclear Nonproliferation, a component of the Department of Energy's National Nuclear Security Administration (NNSA), sponsors the development of many types of sensors, data collection systems, and data analysis systems to detect and deter the proliferation of weapons of mass destruction. The scope of this mission includes technologies for nuclear explosion monitoring, detection of the production of materials for nuclear weapons, and detection technologies to support the Non-Proliferation Treaty (NPT) http://www.state.gov/www/global/arms/treaties/npt1.html#1.

47. TECHNOLOGY TO SUPPORT THE NUCLEAR AND RADIOLOGICAL NATIONAL SECURITY PROGRAM

The DOE/NNSA Office of Defense Nuclear Nonproliferation sponsors the development of many types of sensors, data collection systems, and data analysis systems to detect and deter the proliferation of weapons of mass destruction. The scope of this mission includes developing technologies to detect the production of materials for nuclear weapons, and to support the Non-Proliferation of Nuclear Weapons Treaty (NPT). The Nuclear and Radiological National Security Program (NRNSP) develops technologies for detecting the radiation and chemical signatures associated with the production of nuclear weapons and nuclear weapons materials. This topic focuses on the development of detection systems and data analysis methods to address these NRNSP missions. **Grant applications are sought only in the following subtopics:**

a. Radiation Detection Technologies—Improved, enabling technologies must be developed and demonstrated to support stand off and onsite monitoring and verification of the NPT and other international arms control agreements. In particular, research is needed to demonstrate practical methods for detecting the diversion of small quantities of nuclear materials from known production sites of highly enriched uranium. Therefore, grant applications are sought to develop: (1) new scintillator materials, other suitable materials, and enabling technologies to substantially increase the performance (in resolution, sensitivity, and range) of currently available radiation detectors; (2) new safeguard practices for the improved detection, identification, and

tracking of diverted fissile materials in transit, particularly when the materials are shielded; (3) unattended sensor systems that integrate signature analysis and alarm functions into an expandable network based on state-of-the-art communication and internet protocol systems; and (4) alternative signatures/techniques that indicate a radioactive source is present or, better yet, identify the source – this can include the use of nano-technologies, bio-sensors, or any other advanced concept for close up and long range applications.

b. Detection and Monitoring of Nuclear Facilities—The Nuclear and Radiological National Security Program continues to develop improved instrumentation for the analysis of chemical samples related to nuclear nonproliferation activities. To support this program, grant applications are sought to develop:

(1) An economical femtosecond laser source for use in laser ablation mass spectrometry analysis. The laser source must have a laser pulse duration less than or equal to 1 picosecond FWHM (full-width at half-maximum), and a UV wavelength less than or equal to 300nm. The laser should be able to produce a fluence of approximately $5J/cm^2$ at a focal spot diameter of 5μ m and a repetition rate of 1KHz. For further information or clarification of these requirements please contact Dr. Richard Russo [(510) 486-4258, rerusso@lbl.gov] at the Lawrence Berkley National Laboratory.

(2) Next-generation instrumentation for elemental/isotopic mass analysis. The new instrumentation, which would complement or replace existing instrumentation, should be based on technologies other than existing mass spectrometers or optical spectroscopy systems.

c. Algorithms for Effluent Detection and Identification—Advanced LWIR hyperspectral imaging sensors, used for effluent detection and identification, are capable of observing target areas repeatedly for time periods that span seconds, minutes, hours, days, and many months. Moreover, the targets may be observed from a variety of viewpoints: from overhead with large ground sample distances (few meters); at modest angles from overhead (say 45°); along horizontal paths viewed from mobile and fixed ground locations, with sub-meter ground sample distances; and up-looking from close in, with the sky as the background. The nature of the multi-scan data collection modes, coupled with the range of viewing conditions and the need to provide information in a timely manner, presents a challenging problem set for the effective exploitation of data. Therefore, grant applications are sought to develop algorithms that can exploit the temporally changing plume target position and/or background for improvements in target detection, chemical effluent identification, and false alarm rejection. The algorithms must be suitable for analyses by a person-in-the-loop, have full automation capability to support batch processing, and be amenable to implementation in real-time operating systems.

Phase I should be a feasibility study using existing multi-look sensor data as an initial problem set. The algorithms developed must demonstrate the capability to exploit temporal information and to provide increased performance with regard to plume detection and effluent identification. The potential for automation is important and should be demonstrated. All software code must operate in a Sun/UNIX environment, with an ultimate goal of operating in a PC/Windows environment in Phase II. Phase II would involve research for automating advanced detection and identification methods and for developing a prototype software package that implements automated algorithms. In addition, Phase II would involve a feasibility study for real-time implementation.

For further information or to clarify these requirements, please contact Dr. Randy S. Roberts [(925) 423-9255, roberts38@llnl.gov] at the Lawrence Livermore National Laboratory. Contact and discussion is recommended to avoid misunderstandings and unresponsive grant applications.

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48. RESEARCH TO SUPPORT PROLIFERATION DETECTION

The DOE Office of Defense Nuclear Nonproliferation (NA) sponsors the development of many types of sensors to help detect the proliferation of weapons of mass destruction. This topic is focused on the development of critical components that will enable or facilitate the field deployment of these sensor systems and data exploitation systems for extracting information and knowledge. **Grant applications are sought only in the following subtopics:**

a. Manufacturing Support Technologies for Information Exfiltration—Grant applications are sought to develop a method for fabricating millimeter-scale spheres, which have an optical index that varies smoothly and continuously from the center to the surface. The overall objective is to develop miniature spherical retroreflectors with reduced spherical and chromatic aberrations, thereby enabling a broad range of remote detection scenarios. The fabrication technique must be flexible enough to allow a range of index profiles to be created, and the technique must be capable of scaling to low-cost, multiple-copy production. The spheres, which can be made from either organic or inorganic materials, must be optically transparent and have a refractive index differential greater than 0.2. The optical quality of the final product must be capable of providing near diffraction-limited performance.

For further information or to clarify these requirements, please contact Dr. Charles Stevens [(925) 422-6208, stevens2@llnl.gov] at the Lawrence Livermore National Laboratory. Contact and discussion is recommended to avoid misunderstandings and unresponsive grant applications.

b. Semi-Structured System for Sharing Data (S4D)—The proliferation of sensor data and associated data exploitation applications, distributed over several national laboratories, are driving the need to effectively manage huge quantities of data, information, and knowledge for collaborative research and analysis. Semi-structured data and XML meta-data are emerging as standards for managing large data sets in multi-national-laboratory and multi-agency applications. This approach offers the benefit of information system integration without disrupting local operations. However, to realize this concept, a semi-structured information management component must be added to each individual laboratory system. Although research on various components and techniques (e.g. XML databases, optimizing XML queries, etc.) is underway, a system that can integrate the semi-structured information management components is required. System level research must be conducted in order to gain insight on how the various pieces of the system will interact and what exactly will be required from each piece.

Therefore, grant applications are sought for the research and design of a semi-structured system for sharing data (S4D). The research should address issues of storage (meta-data views) and search and retrieval (data, information, and analysis results), but not collection (which is mission specific and locally managed) or use (local applications). The S4D design goals should include: (1) minimizing the amount of structure, in order to maximize the diversity of data supported; (2) uniform handling of diverse data; (3) data modeling that maintains the semantics of the data; (4) the support of dynamic data resource discovery; (5) the prevention of direct access to the database – instead, network enabled services (e.g. Web services) should be used to provide custom views of the database; (6) allowing owners of data to set access restrictions; (7) a layered approach to query results, in order to manage network load; (8) the ability to discover if data is available, and if available, how much and

from what sources; and (9) options to retrieve meta-data only, or meta-data and a slice of data, or meta-data and full data.

The Phase I project should: (1) research the viability of using the Resource Description Framework (RDF) as the means of publishing heterogeneous meta-data; (2) investigate and recommend a means for network enabled database views, in order to retrieve data, information, and analysis results from diverse information systems. (e.g., Web services, twisted framework, etc.); (3) investigate and select a native XML database for Phase II; and (4) document trade-offs considered in the selection process and report the results of any tests that are conducted. Then, the Phase II project should: (1) develop a test bed system to explore the management and sharing of a wide variety of data; (2) model a representative data set using semi-structured techniques; (3) store the data in a semi-structured format; (4) publish meta-data information to facilitate data discovery; and (5) make meta-data and data available through a general-purpose interface that facilitates querying.

For further information or to clarify these requirements please contact Mr. John G. Burns [(505) 844-0742, jgburns@sandia.gov] at the Sandia National Laboratories. Contact and discussion is recommended to avoid misunderstandings and unresponsive grant applications.

c. Solid-State Pump Laser for Generating Non-Harmonic Ultraviolet Light—Pulsed ultraviolet (UV) lasers are required for the detection of effluents associated with proliferation. The generation of non-harmonic ultraviolet wavelengths, using, for example, optical parametric oscillators, requires pump lasers with high optical beam quality. Therefore, grant applications are sought to design and develop, and provide proof-of-concept experiments for, a diode-laser-pumped, Q-switched, ~1-micron solid-state laser (such as Nd:YAG or Nd:YLF), which can serve as the pump laser for nonlinear optical conversion to the UV (250 to 400 nm). In order to achieve efficient conversion to UV output (which usually entails pumping optical parametric and frequency mixing processes) the pump laser must operate on a single frequency and have excellent beam quality. The most desirable near field output beam shape is a slightly rounded flat-top or a second-order supergaussian intensity distribution. In addition, it is critically important that all of the energy is contained in a single lobe (i.e. no side lobes) and that the wavefront deviation is less than $\sim\lambda/4$ over 80% of the beam aperture. Furthermore, an output energy of >200 mJ/pulse, a repetition rate of 100 Hz or more, and a pulse length of between 10 to 15 ns FWHM is desired. Since the ultimate goal of the pump laser/UV conversion system is for a remote sensing system, the pump laser should be relatively compact (volume < 2ft³) and efficient (power consumption < 1 kW).

For further information or to clarify these requirements, please contact Dr. Phillip Hargis [(505) 844-2821, pjhargi@sandia.gov] or Mr. Randal Schmitt [(505) 844-9519, <u>schmitt@sandia.gov</u>] at the Sandia National Laboratories. Contact and discussion is recommended to avoid misunderstandings and unresponsive grant applications.

d. Broadly Tunable Infrared Quantum Cascade Diode Lasers Based on an External Cavity—Lasers based on quantum cascade gain media represent a powerful new tool for optical detection in the infrared spectral region. This is the result of several interesting characteristics that have been demonstrated, including high power, narrow spectral linewidth, improved reliability, and the potential for non-cryogenic operation. However, the commercialization of an infrared quantum cascade laser (QCL) capable of broad spectral tuning, which would be the key to chemical measurement applications, has not reached fruition. Currently available QCL's are constructed as distributed-feedback (DFB) or Fabry-Perot (FP) cavities. In these systems, the mirrors that define the laser cavity are intimately bonded to the semiconductor gain region, and the limited thermal expansion range of the fixed cavity limits the tuning range of the device to about 10 cm⁻¹. However, QCL's have been demonstrated that can support gain over a much broader (297 cm⁻¹) spectral bandwidth. Also, infrared diode laser products that can tune very broadly (100 cm⁻¹) now exist; in these products, the diode gain medium is inserted into an external cavity that can both select frequencies and adjust cavity length over a much broader range than DFB or FP cavities.

Therefore, grant applications are sought to develop concepts for producing and demonstrating broadly-tunable QCL's using external cavity (or other) approaches. Desirable characteristics for the laser system include: (1) operation within the 8 to 14 micron spectral region; (2) a tuning range of 50 to 100 wavenumbers (more is better); (3) a linewidth of 100 MHz or narrower; (4) power of 1 mW or more (although 0.1 to 1 mW still would be useful); and (5) non-cryogenic cooling (e.g., thermal electric cooling) – however, a cryogenic system still would be useful. Although some examples of this capability have been reported in the literature, no commercial products have resulted from the research. Moreover, the reported demonstrations have not employed the highly engineered tuning mechanisms that exist in the commercial world.

For further information or to clarify these requirements, please contact Dr. Thomas Kulp [(925) 294-3676, <u>tjkulp@sandia.gov</u>] at the Sandia National Laboratories. Contact and discussion is recommended to avoid misunderstandings and unresponsive grant applications.

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49. RESEARCH TO SUPPORT GROUND-BASED NUCLEAR EXPLOSION MONITORING

The Nuclear Explosion Monitoring Research & Engineering (NEM R&E) program is sponsored by the U.S. Department of Energy's (DOE) National Nuclear Security Administration's (NNSA) Office of Nonproliferation Research and Engineering. This program is responsible for the research and development necessary to provide the U.S. Government with capabilities for monitoring nuclear explosions. The NEM R&E program provides research products to the Air Force Technical Applications Center (AFTAC), which collects and analyzes data from a network of seismic, radionuclide, hydroacoustic, and infrasound data collection stations. Within the context of one or more of these technologies, research is sought to develop algorithms, hardware, and software for improved event detection, location, and identification at thresholds and confidence levels that meet U.S. requirements in a cost-effective manner. Grant applications responding to this topic must demonstrate how the proposed approaches would complement and be coordinated with ongoing or completed work (see list of ongoing contracts <u>https://www.nemre.nnsa.doe.gov/coordination</u>) while improving capability. In addition, grant applications must be specifically related to nuclear explosion monitoring and **must respond only to the following subtopics:**

a. Seismic Monitoring of Nuclear Explosions—Grant applications are sought to develop and field test communications hardware and software systems concepts to provide timely, high data availability for intraarray communications among seismic array elements. The separation of seismic array elements may vary from 0.5 to 10 kilometers and the separation of array elements from a central collection point may extend up to 50 kilometers.

Grant applications also are sought to develop and field test next-generation communications hardware and software systems for the transmission and management of data from near-real-time distributed seismic sensor

systems. Systems must be secure, robust (no single point of failure, high data availability), low-power, wideband (up to 2 Mbps), adaptive, low-cost, capable of operating in remote locations, and flexible enough to be used with a combination of communication systems. Approaches should seek to leverage both existing and emerging technologies under development in the commercial sector.

Finally, grant applications are sought to develop computer-based training systems, using Web technology, for systems control and troubleshooting of seismic monitoring stations around the world. Phase 1 should include a product requirements definition in coordination with potential customers; therefore, grant applications should include input from operational logistical personnel as well as level 1 maintenance operators. The training materials should be high quality, comprehensive, available on-line, and of significant value and interest to both novice and experienced users alike. The training modules should be in English only; translation to other languages would be considered only after the final training product is perfected.

b. Radionuclide Monitoring of Nuclear Explosions—The detection of alpha and beta radiation in environmental field samples would be a very useful screening measure for determining which samples must undergo additional, costly, or time consuming measurements. Therefore, grant applications are sought to develop a very-low-background alpha-particle counter with position resolution less than 5mm fwhm and low sensitivity to vibration or electromagnetic interference. Novel design ideas and modular constructs are preferred over traditional ion-chamber designs. The desired outcome is a robust, self-contained system to scan thin, flat field samples for alpha and beta contamination.

Semiconductor detectors used in the field, along with certain chemical processes, require cryogens for cooling. In the past, this has been accomplished by carrying large volumes of liquid nitrogen, or alternatively by using mechanical coolers for the detectors. Therefore, grant applications are sought to develop a more flexible and robust solution, in which a compact, portable, field-robust, and efficient device produces liquid nitrogen in a field setting at a rate no lower than 12 liters per day. Operation on world power (defined as 110V-240V and 50-60 cycles per second, see: <u>http://kropla.com/electric2.htm</u> or <u>http://www.voltageconverters.com/voltageguide.htm</u>) is highly desirable, as is a module weight of <50 lbs.

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