# Crosscutting Research & Analysis Program Innovative Energy Concepts Project Portfolio

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U.S. DEPARTMENT OF ENERGY | the ENERGY lab
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# Introduction

The Crosscutting Research and Analysis Program develops a range of innovative and enabling technologies that are key to improving existing power systems and essential for accelerating the development of a new generation of highly efficient environmentally benign fossil fuel-based power systems. The mission space is focused on bridging the gap between fundamental and applied research and development (R&D) efforts. Technologies that successfully bridge this gap are intended to offer viable step-change improvements in power system efficiency, reliability, costs, and environmental impacts.

The Crosscutting Research and Analysis Program executes R&D efforts by partnering and collaborating with research institutions and the power generation industry throughout the United States and in select international locations. The Program also sponsors one of the longest running and most important university training and research programs to reinforce the research-based education of students at U.S. universities and colleges with emphasis on fossil energy science. The major objective for this program is to produce tools, techniques, and technologies that map to the Clean Coal Research Program efforts.

The Program comprises three technology areas: Coal Utilization Sciences, Plant Optimization Technologies, and University Training and Research. A general description of each of these technology areas is detailed below:

**Coal Utilization Sciences:** The Coal Utilization Sciences technology area research effort is conducted to develop modeling and simulation technologies leading to a suite of products capable of designing and simulating the operation of next-generation near-zero-emissions power systems such as gasification and oxy-combustion. These products are based on validated models and highly detailed representations of equipment and processes. Multinational laboratory efforts are being coordinated through the National Risk Assessment Partnership (NRAP) and Carbon Capture Simulation Initiative (CCSI) to focus on post-combustion capture of carbon, risk assessment, and integrated multiscale physics-based simulations.

**Plant Optimization Technologies:** The Plant Optimization Technologies technology area exists to develop advanced sensors and controls, materials, and water- and emissions-related technologies. Projects within this funding area enable novel control systems to optimize operations where harsh environmental conditions are present in both current and future applications in power plants and industrial facilities.

**University Training and Research:** The University Training and Research (UTR) program awards research-based educational grants to U.S. universities and colleges in areas that benefit the Office of Fossil Energy and the Crosscutting Research and Analysis Program. UTR is the umbrella program under which the University Coal Research and Historically Black Colleges and Universities (HBCU) and Other Minority Institutions initiatives operate. These grant programs address the scientific and technical issues key to achieving Fossil Energy's goals, and build our nation's capabilities in energy science and engineering by providing hands-on research experience to future generations of scientists and engineers.

In addition to the Crosscutting Research and Analysis Program listed above, NETL uses its participation in the U.S. Department of Energy's (DOE) Office of Science **Small Business Innovation Research (SBIR) Program** to leverage funding, enhance the research portfolio, and most importantly, facilitate a pathway to commercialization. SBIR is a highly competitive program that encourages small businesses to explore technological potential and provides the incentive to profit from commercialization. By including qualified small businesses in the nation's R&D arena, high-tech innovation is stimulated and the United States gains entrepreneurial spirit to meet specific research and development needs. SBIR targets the entrepreneurial sector because that is where most innovation and innovators

thrive. By reserving a specific percentage of Federal R&D funds for small business, SBIR protects small businesses and enables competition on the same level as larger businesses. SBIR funds the critical startup and development stages and encourages the commercialization of the technology, product, or service, which, in turn, stimulates the U.S. economy. Since its inception in 1982 as part of the Small Business Innovation Development Act, SBIR has helped thousands of small businesses compete for Federal research and development awards. These contributions have enhanced the nation's defense, protected the environment, advanced health care, and improved our ability to manage information and manipulate data.

The Crosscutting Research and Analysis Program comprises these key technology areas:

- **Sensors and Controls:** The basis for this research area is to make available new classes of sensors and measurement tools that manage complexity; permit low cost, robust monitoring; and enable real-time optimization of fully integrated, highly efficient power-generation systems. Controls research centers on self-organizing information networks and distributed intelligence for process control and decision making.
- **High Performance Materials:** Materials development under the Crosscutting Research and Analysis Program focuses on structural materials that will lower the cost and improve the performance of fossil-based power-generation systems. Computational tools in predictive performance, failure mechanisms, and molecular design of materials are also under development to support highly focused efforts in material development.
- **Simulation-based Engineering:** This technology area represents a vast amount of expertise and capability to computationally represent the full range of energy science from reactive and multiphase flows up to a full-scale virtual and interactive power plant. Science-based models of the physical phenomena occurring in fossil fuel conversion processes and development of multiscale, multi-physics simulation capabilities are just some of the tools and capabilities under this technology area.
- **Innovative Energy Concepts:** Innovative Energy Concepts is concerned with the development of novel cost-effective technologies that promote efficiency, environmental performance, availability of advanced energy systems, and the development of computational tools that shorten development timelines of advanced energy systems. This area provides for fundamental and applied research in innovative concepts with a 10-25 year horizon that offers the potential for technical breakthroughs and step-change improvements in power generation and the removal of any environmental impacts from fossil energy-based power system.
- **Water Management Research and Development:** Water research encompasses the need to reduce the amount of freshwater used by power plants and to minimize any potential impacts of plant operations on water quality. The vision for this program area is to develop a 21st-century America that can count on abundant, sustainable fossil energy and water resources to achieve the flexibility, efficiency, reliability, and environmental quality essential for continued security and economic health. To accomplish this, crosscutting research is needed to lead a critical national effort directed at removing barriers to sustainable, efficient water and energy use, developing technology solutions, and enhancing understanding of the intimate relationship between energy and water resources.

# Innovative Energy Concepts

Innovative Energy Concepts (IEC) is concerned with the development of innovative, cost-effective technologies that promote efficiency, environmental performance, availability of advanced energy systems, and the development of computational tools that shorten development timelines of advanced energy systems. National Energy Technology Laboratory (NETL) is working with stakeholders to focus on two research areas:

- **Advanced Power Generation Concepts** such as direct power extraction, thermoelectric generation, and other innovative ideas have the potential to increase the efficiency and offset the penalty associated with capturing $CO_2$ from power generation from fossil fuels. Although these innovative energy systems have significant potential advantages, practical development is hindered by uncertain component performance, the need for new materials, or simply the cost of development. The goal of IEC is to utilize validated, computational simulations that can predict performance of these process technologies to identify gaps in simulations and technology and guide development and accelerate the deployment of IEC technologies.

- **Power Cycling Alternatives** such as power electronics and energetic materials research with application for grid-scale energy storage devices to improve reliability and stability of the grid; provide capacity to "peak shave or load shift," enabling peak loads to be met during periods when generation, transmission, and distribution assets cannot yet be brought online; enable the integration of large scale renewable energy plants into the grid; and provide more stable and efficient delivery of electrical power— including power generated from fossil fuel sources. This will result in more stable and efficient delivery of electrical power, while reducing overall $CO_2$ emissions.

# Innovative Energy Concepts Projects


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# Novel High Temperature Carbide and Boride Ceramics for Direct Power Extraction Electrode Applications

**Performer:** Florida International University

**Award Number:** FE0026325

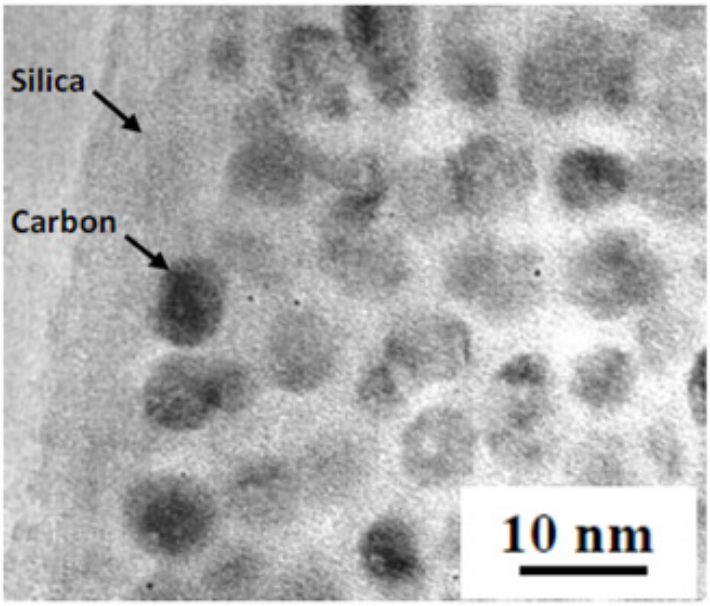
**Project Duration:** 10/1/2015 – 9/30/2018

**Total Project Value:** $ 249,970

**Technology Area:** University Training and Research

NETL is partnering with Florida International University to develop nano-carbide and boride ceramic solid solution and related composites via novel synthesis and processing and to understand the fundamental composition-processing-structure-property relationships for materials such as potential hot electrodes for direct powder extraction, e.g., magnetic hydrodynamic (MHD) systems. Basic research on new high-temperature ceramic materials, including novel means of synthesis and processing, will be performed. Fundamental knowledge will be developed and leveraged to design direct power extraction applications for cleaner and more efficient power generation using fossil fuels.

This research will provide insights into how fundamental composition-processing-structure-property relationships will support development of these materials for a broad range of applications from energy to aerospace. This research could also significantly impact the development of high- temperature MHD electrodes as well as the fields of advanced ceramics and high-temperature materials science, and could lead to dramatic reductions in the time and energy input during the materials sintering process, resulting in less costly high-temperature ceramic materials.




HRTEM image showing nm-scale local mixing of $SiO_2$ and carbon precursors obtained from solution processing and 1,100 °C pyrolysis.

# Direct Power Extraction

**Performer:** National Energy Technology Laboratory – RIC

**Collaborator(s):** West Virginia University, Oregon State University, LyTec

**Award Number:** RIC IPT FY 2016-2020 FWP, Task 4.0

**Project Duration:** 10/01/2014 – 09/30/16

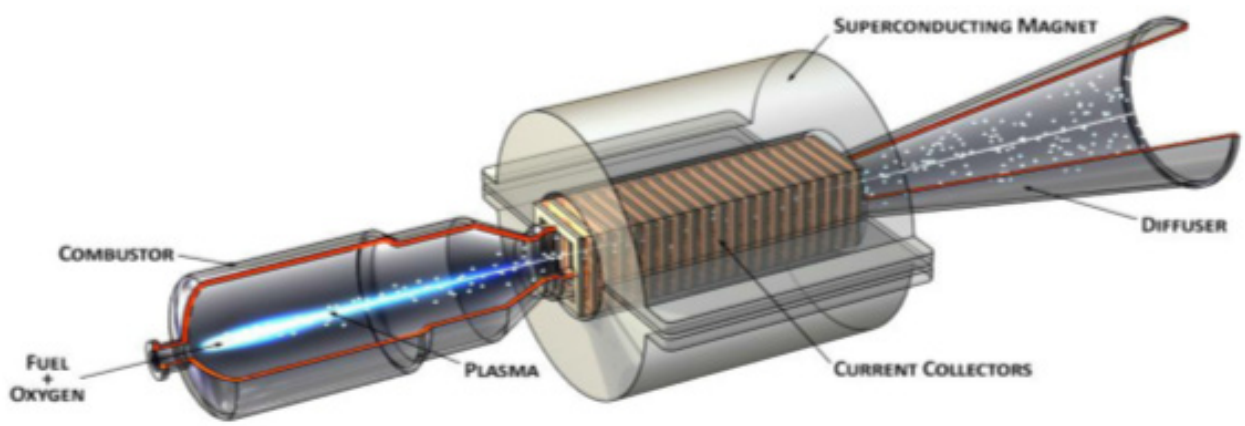
**Total Project Value:** $ 2,465,681

**Technology Area:** Innovative Energy Concepts

Direct Power Extraction (DPE) refers to the direct conversion of the thermal or kinetic energy in a fluid to useable electrical power. By avoiding an intermediate mechanical energy conversion step (e.g., the movement of turbine blades) power generation efficiencies can be extended beyond the current state of the art. This is because theoretical maximum cycle efficiencies are limited by the maximum cycle temperature in accordance with Carnot's rule, and turbine blades are one of the limiting factors in extending the temperatures of turbo-machinery.

NETL's Innovative Process Technologies (IPT) DPE task objectives are to generate useful engineering data sets, simulation tools, and materials to further the prospect of using DPE to reduce the cost of carbon capture from fossil fuel plants. A known approach for achieving DPE is through the use of a magnetohydrodynamic (MHD) generator, as shown in the figure below. The DPE task is presently focused on challenges that are unique to MHD generators and their application.

Five distinct yet integrated elements comprise this task: (1) analytical – for developing and applying analytical tools toward the evaluation of DPE; (2) computational – for developing and validating a computational fluid dynamics (CFD)-based simulation; (3) experimental – for conducting experiments capable of exposing materials of interest to realistic service conditions and for conducting validating experiments for simulation tools; (4) materials development for




An Oxy-fuel fired Open Cycle MHD Power Generator. A diffuser is used to slow the flow down prior to it entering a bottoming cycle.

DPE applications; and (5) exploration of higher risk concepts with the potential to significantly improve the reliability and performance of DPE systems.

In the task, continuous data-driven analysis is applied toward assessing and pursuing the technical viability of DPE approaches. This supports and informs the technical endeavors in the other task elements. For example, momentum transfer collisional cross-sectional data have been collected, reviewed, and summarized for use in electrical conductivity calculations of partially ionized seeded gasses. These data are applicable to the high temperatures and elevated pressures expected when using oxy-fuel, and as such, consider the multitude of species resulting from the high- temperature dissociation of the combustion products. The data analysis shows that seeded oxy-fuel combustion products can have conductivities 2–3 times greater compared to the open cycle MHD systems considered during a legacy DOE MHD program, implying that higher power densities are possible. In order to realize this, MHD generator insulators and electrodes (current collectors) would need to withstand the more aggressive conditions that will be expected.

Simulation tools for the predictive assessment of component thermodynamic and electrical performance are continually being developed as part of the task. A 1-D engineering code that considers the pertinent equations for MHD generators was developed using open source tools. This numerical code can be used to scope and assess the performance of MHD generators and is useful in channel design and system techno-economic studies. The code was utilized to specify the MHD generator in NETL's forthcoming baseline direct power extraction system techno-economic study. In addition, full 3-D simulations of high-temperature gas flows and magnetohydrodynamic interactions are being developed and deployed. The more detailed 3-D models are working toward correctly simulating the internal flows in a MHD generator. An experimental effort is primarily directed toward simulation validation and materials exposure testing. Current activity focuses on the conditions expected in oxy-fired open cycle MHD generators.

A lab-scale oxy-methane burner and Langmuir probe are being used to validate electrical conductivity predictions as a function of oxidant enrichment and potassium carbonate seeding concentration. A high velocity kerosene-oxygen combustor capable of producing nozzle exit velocities of Mach 1.8 is being used to validate system mass and heat balance predictions. The heat balances are important to predict since wall cooling can act as a significant energy sink. Initial testing of a 200 kWth system shows an approximate 20% heat balance transfer thorough the walls of a water-cooled copper combustion chamber and convergent-divergent nozzle. Planned experimental efforts include utilization of a "back-powered" MHD channel section to assess effective channel plasma conductivities and boundary layer drops. This will be followed by bench-scale MHD channel section testing in a 2 Tesla electromagnet. A particular MHD generator interest is in assessing allowable electrical stresses and current densities within a MHD channel, which is largely limited by electrical arcing. To assess this, a diagnostic that measures the induced magnetic field signatures to reconstruct the current densities (e.g., arcs) within the channel is being planned.

The task includes the selection, design, and characterization of prospective MHD channel materials. Thermo-physical, electrical, and composition evaluations are being performed to assess candidate channel materials. In particular, material interactions with seed materials are being evaluated, and it is apparent these interactions will be an important consideration for any MHD channel constructed with ceramics/refractories. Lastly, one task element will explore higher risk concepts with the potential to significantly improve the reliability and performance of DPE systems. Initial concepts being explored include the use of photo-ionization for enhanced conductivity and generator control, realization of an inductive "electrode-less" MHD generator, and investigation into the replacement of traditional alkali metal seed with a "dusty" plasma.

Although prior efforts have established the basic principles and developed methodologies and systems for achieving MHD energy conversion, current efforts are focused on investigating new concepts and applications of the technology so that program goals are met. The task is primarily focused on the realization of a transformational technology ready for demonstration in the FY30-35 timeframe. Thus, the current effort seeks to answer the question of viability of the technology and develop the specific performance requirements and attributes. In addition, to conclusively answer the primary question of technical viability, the task will produce and transfer significant research on topics such as mass and thermal flow modeling in aggressive operating environments, functional material development for aggressive applications, and in-situ measurement techniques for reactive flow streams, among others.

# Boride Based Electrode Materials with Enhanced Stability under Extreme Conditions for MHD Direct Power Extraction

**Performer:** University of Idaho

**Award Number:** FE0022988

**Project Duration:** 7/1/2014 – 6/30/2017

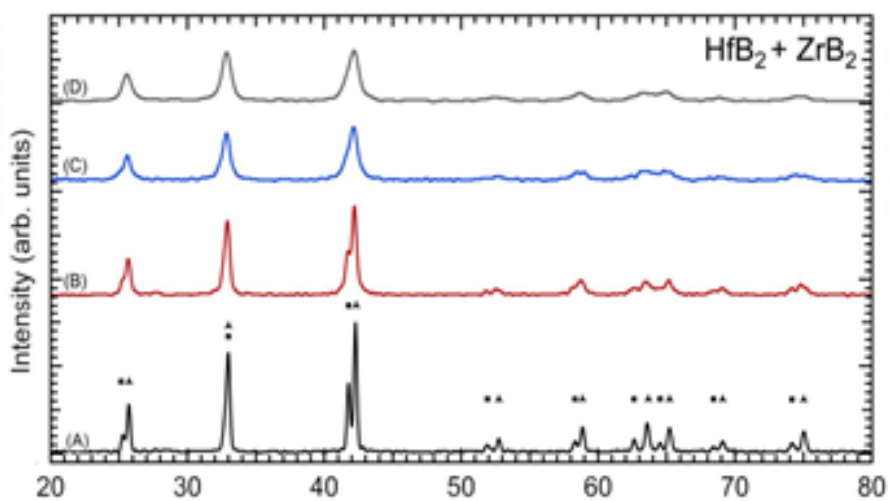
**Total Project Value:** $ 399,938

**Technology Area:** University Training and Research

NETL is partnering with the University of Idaho to develop a boride-based ultra-high temperature ceramic material that possesses all the required properties to function as sustainable electrodes in direct power extraction applications based on magnetohydrodynamics (MHD). Transition metal borides display several unique properties including high melting point, high electrical and thermal conductivities, high strength and hardness even at elevated temperatures, and chemical stability.

In MHD direct power extraction, a hot conducting combustion flame flows through a transverse magnetic field and current is directly extracted. The conductivity of the flame is increased by addition of potassium salts as seed. The operating conditions of the MHD ducts are very aggressive due to high flame temperatures (~3,000 K), high mass flow rate, and corrosive attack of the potassium salts. Oxide-based materials such as strontium-doped $LaCrO_3$ have been considered candidate materials for the current-extracting electrodes. These conventional oxide materials show high electrical resistivity, low thermal conductivity, and high volatility at MHD operating temperatures, all of which limit their functionality.

The outcome of this project will lead to a better understanding of charge and mass transport behavior of transition metal borides and their oxidation kinetics in the presence of silicon and rare earth compounds. The results obtained will help develop ultra-high temperature electrode materials for MHD direct power extraction applications, resulting in improved lifetime and performance efficiency of coal-fired power plants.




X-ray powder diffraction patterns of the products after milling a (1:1) mixture of $HfB_2$ +$ZrB_2$ powder to ball ratio (1:20): (A) 5 minute mill time, (B) 60 minute mill time, (C) 180 minute mill time, (D) 270 minute mill time ■$ZrB_2$ ▲$HfB_2$.

# Vertically-Aligned Carbon-Nanotubes Embedded in Ceramic Matrices for Hot Electrode Applications

**Performer:** University of Nebraska

**Award Number:** FE0023061

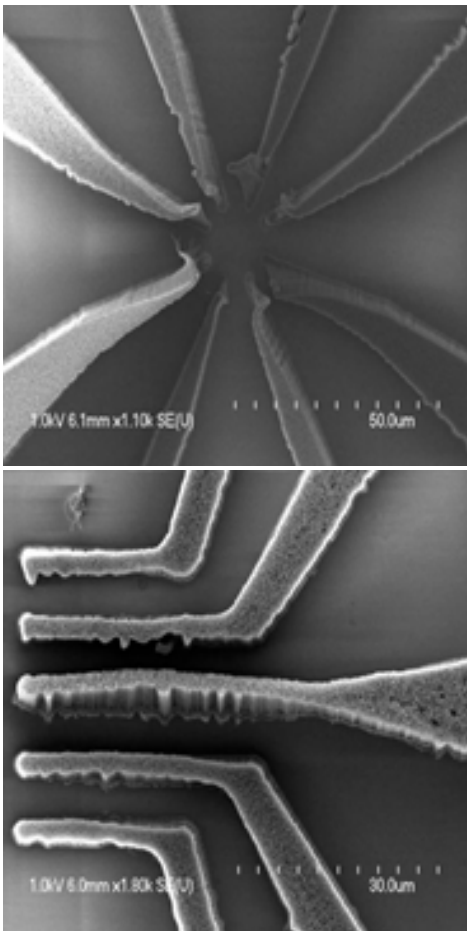
**Project Duration:** 10/1/2014 – 9/30/2017

**Total Project Value:** $ 400,000

**Technology Area:** University Training and Research

NETL is partnering with the University of Nebraska to develop carbon nanotube (CNT)-ceramic composite structures in which vertically aligned carbon nanotubes are embedded in ceramic matrices for hot electrode applications such as magnetohydrodynamic (MHD) power systems. Four objectives will be accomplished: (1) super growth of vertically aligned CNT carpets, (2) fabrication of CNT-boron nitride (BN) composite structures, (3) stability and resistance studies of the CNT-BN composite structures, and (4) thermionic emissions from the CNT-BN composite structures. The research team will grow vertically aligned carbon nanotube carpets on copper with a thickness up to 1 cm.

The successful development of the CNT-C composite structures will reduce the capital costs of the MHD power systems and establish a new family of VA-CNT-based anisotropic composite structures.




Vertically aligned CNT patterns: two potential models of the carbon.

# Developing Novel Multifunctional Materials for High-Efficiency Electrical Energy Storage

**Performer:** University of Tennessee

**Award Number:** FE0011585

**Project Duration:** 9/1/2013 – 8/31/2016

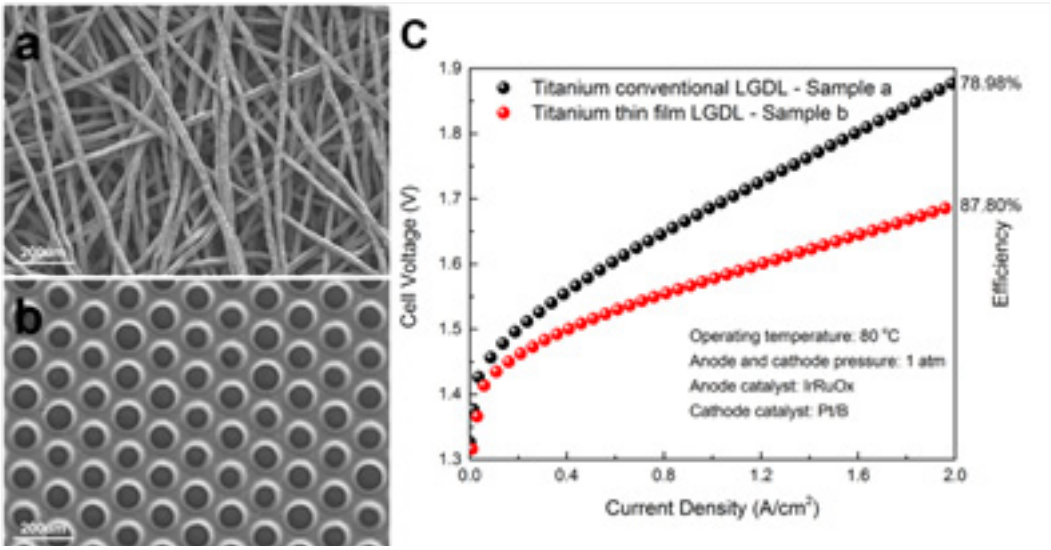
**Total Project Value:** $ 470,084

**Technology Area:** University Training and Research

NETL is partnering with the University of Tennessee to develop a thin and well-tunable multifunctional component with micro/nano fabrication for high-efficiency electrical energy storage, which is critical for the long-term utilization of coal in energy applications to provide reliable, affordable electricity, and to enable electrical grid modernization.

Novel titanium liquid/gas diffusion layers (LGDLs) with well-tunable pore morphologies were developed by employing micro/nano-manufacturing and showed significant performance improvements in proton exchange membrane electrolyzer cells (PEMECs). As shown in the figure below, the operating voltages required at a current density of 2.0 A/cm$^2$ for the LGDLs were as low as 1.69 V, and efficiency reached a reported high of nearly 88%. In addition, the reduction in LGDL thickness from the 350 µm of conventional LGDLs to 25 µm will substantially reduce the weight and volume of PEMEC stacks, which can lead to new avenues for future development of low-cost and higher-performance PEMECs. Its well-tunable features, including pore size, pore shape, pore distribution, and thus porosity and permeability, will be valuable in developing PEMEC models and validating simulations of PEMECs with optimal and repeatable performance.

This project will develop novel multifunctional materials further to promote the efficiency of energy storage technologies. Improvements to energy storage technology will promote improved utilization of power plant assets that can provide operational flexibility and result in lower capital and operating costs.




(a) Conventional felt LGDL; (b) Novel thin LGDL; (c) Performance comparisons in the PEME

# Combustion Synthesis of Boride-Based Electrode Materials for Magnetohydrodynamic (MHD) Direct Power Extraction

**Performer:** University of Texas at El Paso

**Award Number:** FE0026333

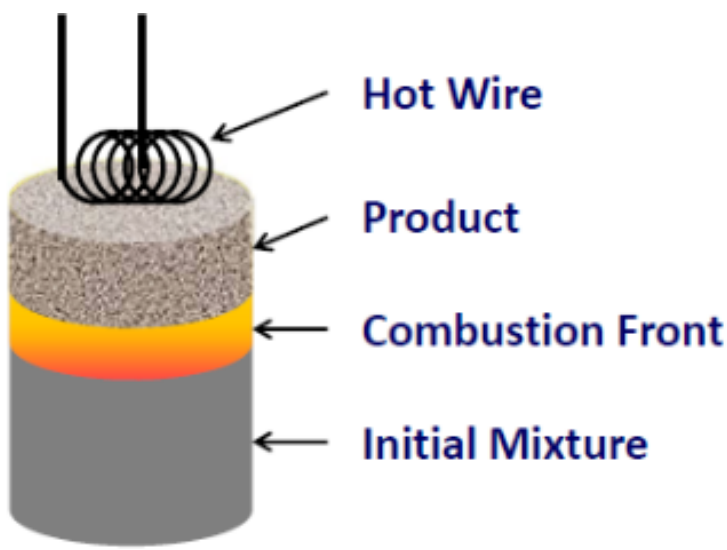
**Project Duration:** 10/1/2015 – 9/30/2018

**Total Project Value:** $ 250,000

**Technology Area:** University Training and Research

NETL is partnering with the University of Texas at El Paso to develop a novel technology for advanced, low-cost manufacturing of boride-based ultra-high-temperature ceramics (UHTCs) for direct power extraction applications. The project will determine optimal conditions of mechanical activation, self-propagating high-temperature synthesis (SHS), and pressureless sintering for fabricating doped zirconium diboride ($ZrB_2$) and hafnium diboride ($HfB_2$) that possess all the required properties needed to function as sustainable magnetohydrodynamic electrodes. The project will also determine thermophysical, electrical, mechanical, and oxidation properties of borides obtained by mechanically activated SHS followed by pressureless sintering. This effort will focus on the use of inexpensive materials such as zirconium dioxide ($ZrO_2$), hafnium oxide ($HfO_2$), boron trioxide ($B_2O_3$), magnesium (Mg), and sodium chloride (NaCl), which could lead to significantly lower production costs compared to synthesis from elements.

The technology developed in this project will solve some problems associated with SHS, such as difficult ignition of low-exothermic mixtures and high porosity of products, while exploiting SHS advantages such as low cost, low energy consumption, and high product purity.




Schematic of SHS Process.

# High Temperature High Velocity Direct Power Extraction Using an Open Cycle Oxy- Combustion System

**Performer:** University of Texas at El Paso

**Award Number:** FE0024062

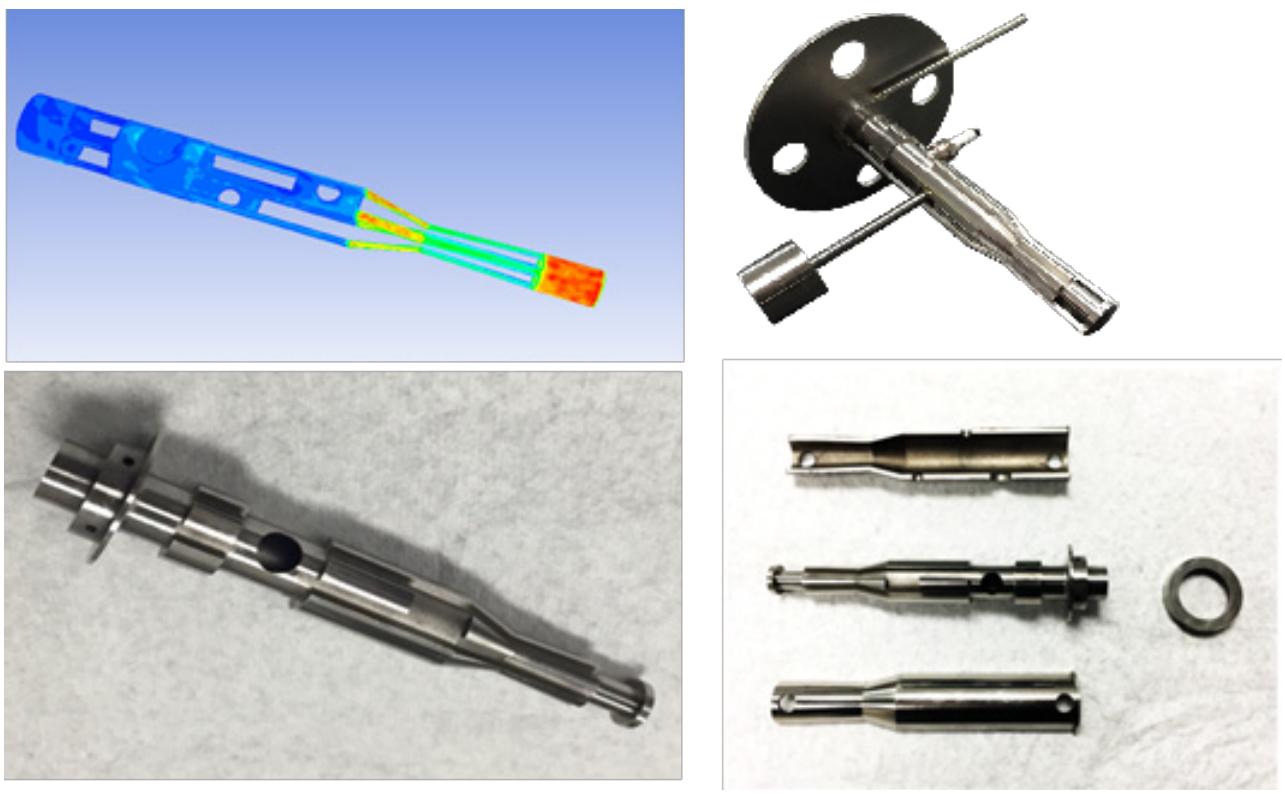
**Project Duration:** 10/1/2014 – 9/30/2016

**Total Project Value:** $ 625,000

**Technology Area:** Plant Optimization Technologies

NETL is partnering with the University of Texas at El Paso to develop high-temperature, high-velocity direct power extraction using an open-cycle oxy-combustion system. Researchers will design, optimize, and test a lab-scale high-velocity and high-temperature oxy-fuel combustor, nozzle, and injector for use in direct power extraction magnetohydrodynamic (MHD) applications. To meet this goal, a combustor will be designed and built to accommodate high-temperature and high-velocity oxy-fuel flow. Deliverables include the design, fabrication, characterization, testing, and documentation of the combustor system performance for future use in computational and system development construction of such systems.

The project will demonstrate the feasibility of MHD oxy-combustion system components for use in electrical power generation, and support the development of energy-efficient technologies that can be used in conjunction with carbon capture techniques. In addition, the outcome of the project will not only improve the fundamental understanding of oxy-fuel combustion and flame stability, it will provide critical experimental data for the validation of modeling tools.



Direct power extraction combustor designed using computational tools to operate on methane and oxygen.

# Precursor-Derived Nanostructured Silicon Carbide Based Materials for Magnetohydrodynamic Electrode Applications

**Performer:** University of Washington

**Award Number:** FE0023142

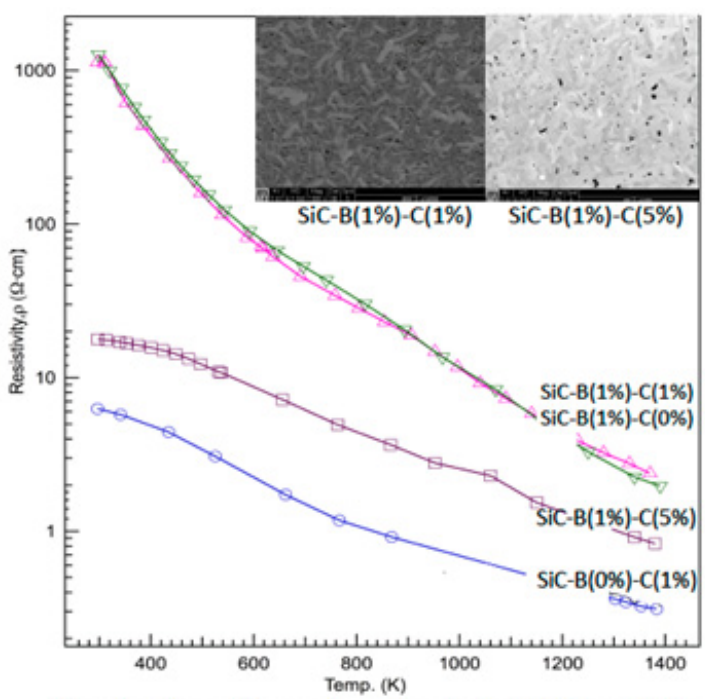
**Project Duration:** 10/1/2014 – 9/30/2017

**Total Project Value:** $ 399,989

**Technology Area:** University Training and Research

NETL is partnering with the University of Washington (UW) to develop a novel class of SiC-based ceramic composite materials through a polymer-precursor-derived route with tailored compositions for channel applications in magnetohydrodynamic (MHD) generators. UW will investigate the effect of precursor chemistry (specifically C/Si) and processing conditions (e.g., temperature) on the nanodomain structure, resultant stoichiometry, nature of the carbon phase (e.g., graphene sheets, carbon nanoparticles), and the resulting thermo-mechanical properties at elevated temperatures. A minor constituent 'X' in Si-C-X is incorporated at the precursor stage during material synthesis, and its effect on the electrical properties, including electrical conductivity, thermionic emissions, and arcing properties for use in MHD generators will be investigated. Important parameters to be investigated are the domain size, the type and distribution of carbon, and the sizes and volume fractions of crystalline SiC and the constituent X. UW will also investigate the interaction of these materials with plasma as a first step toward understanding the plasma-induced degradation process using a newly developed High Density Plasma-Materials Testing Facility that was designed and built on the UW campus.

By developing SiC-based materials with nanostructured features and tailoring their compositions, the high-temperature resistance, electrical properties, and plasma resistance of SiC will improve relative to that of SiC produced by conventional powder processing approaches such as solid state sintering. A successful outcome of this research will result in the emergence of reliable and affordable designed materials for MHD applications.




Microstructure and temperature dependent electrical resistivity of SiC-based ceramics synthesized through precursor-derived route.

# Abbreviations

$B_2O_3$ ..... Boron trioxide

BN..... Boron nitrate

C ..... Carbon

CFD ..... Computational Fluid Dynamics

CNT .....Carbon Nanotubes

CCSI ..... Carbon Capture Simulation Initiative

$CO_2$ ..... Carbon dioxide

D ..... dimensional

DOE ..... Department of Energy

DPE.....Direct Power Extraction

EPA.....Environmental Protection Agency

HBCU/OMI .....Historically Black Colleges and Universities and Other Minority Institutions (NETL program)

$HfB_2$ .....Hafnium diboride

$HfO_2$ .....Hafnium oxide

IEC .....Innovative Energy Concepts

IPT ..... Innovative Process Technologies

K ..... Kelvin

LGDL .....Liquid Gas Diffusion Layers

MASHS ..... Mechanically Activated Self-Propagating High Temperature Synthesis

MHD .....Magnetohydrodynamic

Mg .....Magnesium

NaCl..... Sodium chloride

NETL .....National Energy Technology Laboratory

NRAP ..... National Risk Assessment Partnership

PEMEC..... Proton Exchange Membrane Electrolyzer Cells

RAM.....Reliability, Availability, Maintainability

R&D .....Research and Development

RIC ..... Research & Innovation Center

SBIR ..... Small Business Innovation Research

SHS..... Self-Propagating High Temperature Synthesis

SiC .....Silicon carbide

TRL.....Technology Readiness Level

UCR .....University Coal Research (NETL program)

UHTC..... Ultra-High Temperature Ceramics

UTR ..... University Training and Research (NETL program)

UW ..... University of Washington

VA..... vertically aligned

$ZrO_2$ ..... Zirconium dioxide

# Contacts

**Robert Romanosky**
Acting Portfolio Manager
304-285-4721
Robert.Romanosky@netl.doe.gov

**Patricia Rawls**
Supervisor
Enabling Technologies and Partnerships Team
412-386-5882
Patricia.Rawls@netl.doe.gov

## Websites:

http://energy.gov/fe/coal-utilization-science

http://www.netl.doe.gov/research/coal/crosscutting/innovative-energy-concept

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**National Energy Technology Laboratory**

www.netl.doe.gov

National Energy
Technology Laboratory

1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

420 L Street, Suite 305
Anchorage, AK 99501
907-271-3618

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

13131 Dairy Ashford Road, Suite 225
Sugar Land, TX 77478
281-494-2516

WEBSITE: **www.netl.doe.gov**

CUSTOMER SERVICE: **1-800-553-7681**

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