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Applied Energy Tri-Laboratory Consortium Workshop Report

Materials Challenges and Opportunities for Energy Generation, Conversion, Delivery, and Storage

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Materials Challenges and Opportunities for Energy Generation, Conversion, Delivery, and Storage

**Co-Authored by Idaho National Laboratory,
National Energy Technology Laboratory,
and National Renewable Energy Laboratory**

**Prepared for the
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EXECUTIVE SUMMARY

This report documents the outcomes of the Applied Energy Tri-Laboratory Consortium Workshop on Material Challenges and Opportunities that was held July 31 and August 1, 2019, to begin addressing the needs, opportunities, and challenges associated with the development, fabrication, and testing of the needed materials and components for integrated hybrid energy systems (i.e., incorporating nuclear, fossil, and renewables for electric and thermal applications). This was accomplished by assembling the research program leads and principal investigators who support the research and development of new energy system technologies and system integration tools and components at the U.S. Department of Energy's (DOE's) applied national laboratories, Idaho National Laboratory (INL), National Energy Technology Laboratory (NETL), and National Renewable Energy Laboratory (NREL), and partner national laboratories. The team then identified and prioritized key materials development needs. This effort was intended to enhance communications and synergy among the applied energy Tri-Lab partners.

Advanced functional and structural materials are central to transformative energy technologies for energy production, conversion, delivery, and storage. With that in mind, the workshop focused on identifying and assessing the foundational materials research needs at both the basic and applied levels. Materials challenges include the ability to withstand harsh environments, such as high temperatures and pressures, corrosion, oxidation, or irradiation while maintaining flexible mission profiles and long service lifespans.

Advanced energy system material challenges and needs range from materials for the capture, upgrading/concentration, storage, and delivery of low-grade heat to materials for high temperature environments that involve liquid metals, molten salt, and very high temperature gas heat delivery and storage systems. Material improvements are needed for hybrid energy systems due to accelerated corrosion and stress-fatigue failure of materials and equipment, which results from increased frequency and amplitude of thermal, mechanical, and electrical cycling of systems components. Multifunctional materials are needed for high temperature electrochemical reactors and membranes that are integrated with high temperature corrosive environments. Relative to materials manufacturing, application of precise laser cutting and welding, electric-field/spark plasma sintering, and additive and subtractive methods must be understood and applied to develop both thin-layer homogenous materials and materials of graded composition. Materials modeling and machine learning will be critical to accelerate the design and production of power electronics, and nuclear reactor materials and fuel, as well as to gain an understanding of beneficial materials phenomena or deleterious microstructure evolution. There is also a need for standardized models, computational structures, data reporting protocols and modeling tools across the energy technology disciplines represented by the three laboratories. This would support the development of consistent results and analysis across multiple scales as well as support data sharing across technology areas. Combining capabilities among the three applied energy laboratories (e.g., hardware, software) would greatly increase computational capabilities and throughput and enhance opportunities for experimental validation.

The workshop identified the need to anticipate and address challenges that will emerge during scale-up. Laboratory work must connect with industry to ensure that research focuses on processes that are scalable and marketable. Industry input and perspective are essential to guide laboratory research to meet these requirements and deploy new technology in industrial demonstrations. Another aspect of scale-up is the integration of multiple systems since new challenges often arise at the subsystem interfaces. Establishing a modular scale-up manufacturing demonstration/pilot plant, potentially as an industrial user facility, would be beneficial to the laboratories and industry. Such a facility would allow researchers to find and resolve interface problems that cannot be identified by focusing only on individual parts.

Communication exchanges among the organizers and attendees and the workshop survey responses indicate that the workshop was successful in achieving its goal to identify key technology gaps and research needs. Strong positive feedback was received on the sharing of ideas, capabilities, talent, and passion to move forward on the materials-related action items.

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ACRONYMS

AMO	Advanced Manufacturing Office***
ASI	Advanced Sensor and Instrumentation
AST	Accelerated Stress Testing
C or CO_2	Carbon or Carbon Dioxide
CHP	Combined Heat and Power
COF	Covalent-Organic Frameworks
CP	Capacity
CSP	Concentrated Solar Power
CTD	Crosscutting Technology Development
DFT	Density Functional Theory
DOE	Department of Energy*
EERE	Office of Energy Efficiency and Renewable Energy**
EIL	Energy Innovation Laboratory
EMN	Energy Materials Network
FRP	Fiber-Reinforced Polymer
GEN3	Generation 3
HEATER	Highly Efficient Advanced Thermal Energy Research
HRSG	Heat Recovery Steam Generator
HTF	Heat Transfer Fluid
HYPER	Hybrid Performance Project
ICME	Integrated Computational Materials Engineering
IES	Integrated Energy System
INL	Idaho National Laboratory
IPH	Industrial Process Heat
LOHC	Liquid Organic Hydrogen Carriers
MFC	Materials and Fuels Complex
MOF	Metal-Organic Frameworks
NASA	National Aeronautics and Space Administration*

NDE	Non-Destructive Examination
NE	Office of Nuclear Energy**
NETL	National Energy Technology Laboratory
NEUP	Nuclear Energy University Programs
NG	Natural Gas
NGCC	Natural Gas Combined Cycle
NGNP	Next-Generation Nuclear Plant
NREL	National Renewable Energy Laboratory
PGM	Platinum Group Metal
PNNL	Pacific Northwest National Laboratory
PV	Photovoltaic
QTR	Quarterly Technology Review
R&D	Research and Development
ReACT	Reaction Analysis and Chemical Transformation
REE	Rare Earth Elements
RNG	Renewable Natural Gas
RTES	Renewable Thermal Energy Systems
SETO	Solar Energy Technologies Office***
SPS	Spark Plasma Sintering
TES	Thermal Energy Storage
TRL	Technology-Readiness-Level
U.S.	United States

*Agencies within the Federal government of the United States

**DOE Office

***EERE Office

WORKSHOP OVERVIEW

Background

Idaho National Laboratory (INL), National Energy Technology Laboratory (NETL), and National Renewable Energy Laboratory (NREL) jointly sponsored and led the Applied Energy Tri-Laboratory Consortium Workshop on Material Challenges and Opportunities from July 31 to August 1, 2019. The workshop was held at INL. INL, NETL, and NREL (Tri-Lab) are referred to as the U.S. Department of Energy's (DOE's) applied national laboratories and are, therefore, leads for the development needs of energy systems and infrastructure of the country.

The meeting focused on materials challenges associated with energy production, conversion, and delivery technologies that are being developed for integrated energy systems (IESs).[1] The participants considered tightly coupled and coordinated energy systems that would incorporate two or more energy generators (e.g., nuclear, fossil, renewables) to support electric and thermal applications.

Advanced functional and structural materials are central to transformative energy technologies for energy generation, conversion, delivery, and storage. The workshop focused on identifying and assessing the needs for foundational materials research, at both the basic and applied levels, that are necessary to advance the five research and demonstration projects proposed as an outcome of the Tri-Lab Workshop on R&D Pathways for Future Energy Systems [1], which was held July 24–25, 2019. These five projects, which center around thermal energy storage (TES) and utilization, integrated systems for hydrogen generation, carbon or carbon dioxide (C or CO_2) utilization, and new processes for coal-based materials, are as follows:

1. Energy System Efficiency Improvements through TES, Transport, and Utilization
2. Energy System Efficiency Improvements through Low Temperature Thermal Energy Utilization
3. First-of-a-Kind IES Supporting Renewables, Nuclear, and Fossil Generation and Supplying Hydrogen Markets in the Upper Midwest
4. Low-Carbon-Energy Powered CO_2 Utilization for Fuels and Products in the Texas Gulf Coast Region
5. First-of-a-Kind IES Supporting Hybrid[2] Carbon Conversion using Clean Energy Sources in Coal-Producing States.

The material R&D needs, drivers, and gaps for the targeted technologies were identified to support the development of a tactical and strategic course of action. Potential funding sources were identified along with a time-sensitive plan to optimize the synergy of funding approaches employed by multiple governmental funding agencies (e.g., DOE Office of Energy Efficiency and Renewable Energy, Office of Fossil Energy, Office of Nuclear Energy, Department of Defense, and NASA). The workshop participants discussed challenges and opportunities associated with the five proposed projects and related topics in which materials play a vital role. The challenges and opportunities are grouped in the following three areas:

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[1] Integrated Energy Systems are defined here as any system that involves at least two energy sources that are combined to supply a system that has variable demands. The main objective of a well-designed IES is optimization of the energy services provided relative to reliability, resiliency, affordability, environmental sustainability, security, and affordability. Technology and system flexibility and scalability are additional attributes that enable the system to apply technology advances and to adapt to changes in energy services demands.

[2] A hybrid process is one type of integrated energy systems that either combines two cooperating energy inputs and/or dynamically produces two more energy products or services depending on the temporal attributes of the energy sources and the temporal value of the energy services.

1. Ability to withstand harsh environments (e.g., high temperatures and pressures, corrosion, oxidation, or irradiation that enable material and equipment stability for flexible mission profiles and long service lifespans)
2. Cost, efficiency, selectivity, and durability of catalytic processes
3. Advanced materials processing and manufacturing gaps with continuous process improvement.

An open session was also held during the workshop to discuss new opportunities for materials, research, and ways to cooperate and leverage resources and expertise.

Purpose

The primary purpose of the workshop was to address the science and technology challenges and opportunities associated with the design, development, and deployment of new and advanced materials for components that will enable hybrid IESs.

Participants

The workshop brought together materials experts from the three applied DOE national laboratories—INL, NETL, and NREL—to identify and prioritize materials grand challenges and the associated research and development (R&D) needed to advance the five proposed IES projects. Other national laboratories, industry, and academic centers of excellence were invited to join the workshop based on their distinct capabilities, areas of expertise, and leadership in the selected research areas.

Sessions

Plenary Sessions

The workshop began with overarching presentations that defined the materials grand challenges and highlighted key capabilities of the three participating applied national laboratories.

Breakout Working Sessions

The bulk of the workshop was comprised of breakout working sessions, focused on identifying synergistic research topics to address these grand challenges.

Report

This workshop report documents the outcomes, recommendations, and path forward to address the identified materials R&D needs.

BREAKOUT WORKING SESSIONS

Breakout A: Materials Challenges for Energy Generation, Conversion, Delivery, and Storage

The initial set of breakout sessions were tasked with determining the materials development, manufacturing, and qualification/codification approaches relative to energy sources and technological advancements. Breakout sessions were divided into discussion groups covering the five project proposals, which were provided to the meeting attendees.

Topic 1: Improving Energy System Efficiency through TES

The focus of this session was to determine opportunities for one or more demonstration projects that integrate TES systems. TES systems coupled to thermal power plants may be for seasonal use or used for short durations (weeks or months) to reduce the impacts of cycling and/or enable extracted heat to be delivered to markets, improve resilience, reduce constraints on natural gas and electricity infrastructure, reduce stressors on thermal plants, and reduce energy costs. Installation of TES was targeted at current large-scale power plants and within energy systems that support small-scale municipalities or business parks. An example TES concept is illustrated in Figure 1.

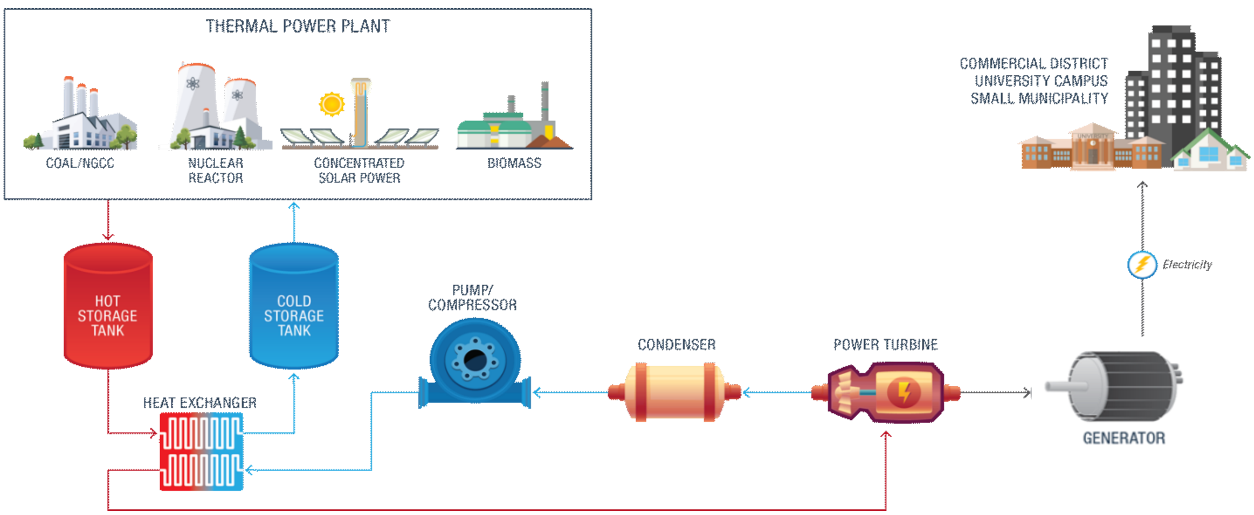

Figure 1. Example TES system coupled with a generator, increasing value to thermal power plants such as coal/natural gas combined cycle (NGCC), nuclear, concentrating solar power (CSP), and bioenergy.

Background

Thermal energy produced by a nuclear plant is traditionally directed to a coupled plant to produce electricity. Other thermal generators, such as coal and natural gas-fired units, in many instances, are deployed to provide direct support to industrial processes, but this requires co-location with the industrial plants to minimize thermal losses. Efficient thermal energy transport over long distances and long-duration TES is challenging but could enable much greater use of both nuclear energy sources and other thermal generation technologies for a wide range of industrial thermal processes. If this thermal energy is supplied by an IES, such an operation may also enable greater flexibility and dispatchability to support improved grid stability and resilience. Some benefits of TES are as follows:

1. Provide dispatchable and flexible electricity generation for the grid
2. Support stabilization of energy costs (i.e., levelized and/or reduce energy costs)
3. Reduce the carbon footprint of the industrial sector

4. Reduce the impact of flexible operations on nuclear reactor core operations or other thermal generator operations
5. Reduce the energy system impact on water resources.

Impact

TES enables the efficient use of resources and can reduce strains on energy infrastructure during peak usage periods, weather events, and other outages, which ultimately improves resilience and reduces costs.

Outcome and Objectives

To reduce the impacts of cycling and/or enable extracted heat to be delivered to markets from baseload thermal power plants (i.e., nuclear and coal), it is important to design, construct, and operate one or more demonstration projects that integrate TES systems with baseload thermal power plants. The resulting systems should improve resilience, reduce constraints on natural gas and electricity infrastructure (in winter and summer, respectively), reduce stressors on thermal plants, and reduce energy costs.

TES integrated into current power plants and small-scale plants at a municipality or business park-scale are identified as having the greatest value at this time. Locations with great advantage for this integration are those with high space heating or cooling loads, high energy prices due to peak loads or infrastructure constraints, or high levels of variable renewable generation, such as photovoltaic (PV) that present curtailment risks. Small-scale integrated TES and usage projects should provide resilience, reduce the impact of infrastructure constraints, and enable the storage of energy that might otherwise be curtailed. Project selection shall be based on energy prices or resilience concerns resulting from infrastructure constraints.

The development of engineering designs and safety analyses for the TES unit integrated into the energy provider and small-scale integrated TES in utilization projects will be based on relative benefits to the location, ability to inform R&D, and reproducibility in other locations.

Objectives for this brainstorming session included the following:

- Identify one or more demonstration projects at baseline power plants to integrate and operate a TES; identify two or more usage projects at the municipality or business park-scale to integrate a small-scale TES
- Identify the benefits to the power plant (e.g., fuel savings, reduced maintenance costs, increased output at peak times), the cost of plant modifications for heat extraction and TES (i.e., the cost of this thermal “product”), and the R&D needs to drive down storage costs while increasing storage efficiency
- Identify the TES value considering response time (i.e., seconds, minutes, hourly, daily, and seasonal), technoeconomic analyses, and the process of enabling resilience and integrated energy sources.

Targeted Benefits

The targeted benefits of improving energy production efficiency through TES integration include a significant reduction in greenhouse gas emissions, enhanced plant reliability, grid resilience, grid flexibility, energy security, and plant scalability. Reliability includes reduction of failures and impacts of thermal cycling on power plant equipment, thus reducing the need for unscheduled maintenance. Grid resilience supports the economic viability of dispatchable, baseload generators. TES provides flexibility and reliability to the grid by storing energy during periods of reduced demand or high renewable energy output. This energy can then (1) be accessed to generate electricity during peak demand, thus providing an on-demand, dispatchable resource and (2) create additional revenue streams for baseload generation.

Crosscutting Needs

Because TES systems are enabled by high density thermal storage, heat harvesting and conversion technologies, efficient heat transfer and exchange, effective thermal utilization, and durable containment materials and systems, R&D in these areas is needed to allow cost-effective integration of TES systems into baseload plants.

TES Materials Challenges and Opportunities

Advances in materials technologies are required to support the development and deployment of TES in a variety of applications. Key materials challenges for TES were identified in preparation for the workshop to guide the breakout discussions. Anticipated challenges and opportunities include the following:

- Advanced cost-effective alloys are needed to handle TES harsh operating conditions, such as very high temperature, high pressure, and corrosive working fluids.
- Advanced computational capabilities are required for materials discovery.
- Reliable materials properties and characteristics are needed for design purposes, but available data are insufficient. Properties and characteristics include (1) critical thermal properties, such as heat capacity, latent heat (phase-change materials), and thermal conductivity; (2) process/reaction reversibility characteristics; and (3) environmental impact.
- Limited data are available for materials degradation and durability under conditions of interest. Chemical compatibility between thermal carriers and containment materials are needed for design purposes, operation and maintenance, and lifetime duration determination based on expected failure mechanisms.
- Because limited data are available for thermal carriers' thermal conductivity and heat transfer correlation for non-traditional thermal fluids (e.g., liquid metals, molten salts, and supercritical gases), performance evaluation for design optimization, including insulative and thermally conductive materials, is challenging.
- Because of the early-stage knowledge of materials discovery, synthesis, and characterization, difficulties occur when understanding the scalability of TES technologies from laboratory to pilot to industrial scale.

Current DOE-Funded Efforts

To help address identified challenges and opportunities to enable TES integration feasibility, several laboratory-led research programs currently support TES technology maturation via DOE programmatic funding. Examples of projects or programs that conduct research to reduce the impact of flexible operations on nuclear reactor core operations are briefly summarized as follows:

- The Nuclear Energy University Programs (NEUP) supports the development of phase-change materials R&D aimed at developing the container materials and materials configurations for efficient heat transport and recovery from various phase-change media.
- The Highly Efficient Advanced Thermal Energy Research (HEATER) Big Idea focuses on understanding the conversion, storage, transmission, and utilization of thermal energy using a "science-to-systems" approach to help transform research in the areas of control and optimization of hybrid energy systems.
- A project funded by DOE Energy Efficiency and Renewable Energy (EERE) Solar Energy Technologies Office (SETO) is investigating Generation 3 (GEN3) Concentrating Solar Power (CSP) plants, which will use a supercritical CO_2 Brayton power cycle to drive the turbine and produce electricity. In this project, for example, solar energy receptor materials and heat transfer component materials that can withstand high temperatures are needed.

- The DOE SunShot project hopes to reduce costs to meet the 2030 cost target of \$0.05/kilowatt hour electric (kWh_e) for "baseload" CSP plants (with ≥12 hours of TES) and \$0.10/kWh_e for "peaker" (i.e., provides power during peak demand) CSP plants (with ≤6 hours of TES), allowing them to generate economical baseload power and use TES to generate electricity for up to 12 hours when the sun is not shining.
- The DOE-EERE-SETO Industrial Process Heat (IPH) project relies on national analysis of the potential for solar technologies (i.e., PV, solar thermal, and hybrid approaches that produce electricity and/or heat) to power a wide range of manufacturing IPH end uses, explicitly accounting for load-reduction potential from energy efficiency measures and load-balancing potential from energy storage. The industrial processes range from those requiring hot water at 70°C to those melting steel scrap at 1,800°C.

Select industrial players could be prime targets for technology adoption and demonstration. (The industrial sector accounts for about one-third of all the U.S. primary energy use [32 quads]. IPH accounts for the following three factors: ~7.5 quads as process steam duties, ~6.5 as process heating, and the balance for onsite power generation [often comprised of combined heat and power generation].)

- The DOE Office of Nuclear Energy (NE) program on IESs, which is managed under the Crosscutting Technology Development (CTD) subprogram, focuses on the integration of nuclear and renewable energy generation technologies to support various energy end users. Various means of energy storage (i.e., thermal, electrical, and/or chemical) are investigated as potentially enabling technologies for these systems; hence, energy storage is included in system design and optimization analyses.

Discussion on Gaps/Challenges/Opportunities

To reach targeted benefits, evaluation metrics are needed, such as levelized cost of electricity, including the value obtained from TES implementation. Lessons can be learned through CSP efforts to support TES applications for nuclear and fossil fuels. In application of TES to the broader category of IESs, researchers must ensure that technoeconomic analysis capabilities and established performance requirements are included. Nuclear, fossil, and CSP applications share some common operating temperature conditions. If hybrid energy systems are of interest, experimental results may be needed for creep and fatigue of various materials that are incorporated into a single storage system that derives thermal input from multiple sources.

Because of high temperature materials limitations, the short-, mid-, and long-term approaches to system design will require the capability to be at system temperatures below 750°C. After validating candidate TES at these more modest temperatures, the operating temperature can be increased. EERE's SETO is evaluating approaches at 750°C for application to CSP with three different pathways, including liquid, gas, and solids, based on the thermal carrier used as the working fluid at the solar receiver. In evaluating approaches for TES, the SETO-led research is evaluating the Rankine and Brayton power cycles to determine how thermal fluids and thermal storage media allows flexibility for CSP plants. When TES operating conditions exceed 750°C, significant materials and component design challenges are introduced, and various sensors are required to ensure knowledge of system conditions. These become more challenging under higher temperature conditions. The optimal storage temperature for cycling is not yet known, nor have researchers answered the question of whether energy must be stored at the maximum operating temperatures. The optimal temperature could depend on both storage requirements and the materials that are used for components and sensors. Other requirements, based on operating conditions of the different technologies, must be established to determine the target temperature.

Different material applications and heat sources used in IES can be described through modeling. Modeling and simulation can be used to determine target operating temperatures, pressures, etc., which will guide the R&D associated with technology development. Fossil-fuel power plants aim to reduce variance in thermal cycling not only for its impact on energy production but also because some containment materials have reduced lifetimes resulting from thermal cycling events. The ideal TES based on current thermal technology has yet to be determined.

The potential heat carriers for TES systems require that investigators identify components and fluids with low corrosivity and enhanced thermal properties for storage and transfer. Critical needs include high energy density, the amount of energy required for economical operations, storage in the form of sensible versus latent heat, and even thermochemical forms. Different thermal carriers have been considered, such as liquid sodium, molten salts, fluidized ceramic particles, and supercritical fluids (e.g., water, carbon dioxide [CO_2]).

Supercritical gas properties must be determined for storage and transfer, but challenges exist. Thermal and chemical compatibility characterization must include corrosive power, heat transfer properties, degradation of heat transfer based on travel distance of the heat transfer fluid (HTF), and storage properties. Issues exist, for example, in CSP with a low heat capacity (Cp) for sensible TES systems. If Cp is lower than 1.4 J/g.K (as currently is true for solar salt), then tanks must increase in size. This increases the fluid inventory as well as in amount of containment materials' requirements to maintain the same storage duration. This is a limitation for TES designs. Development of new HTFs and TES media needs to be focused on understanding the operational parameters to address the requirements for the thermal medium.

Challenges also exist within measurements in extreme conditions (i.e., high temperature, high pressure, frequent thermal cycling) under expected regular operating and failure modes. The research focus should be on materials for harsh environments (i.e., corrosive, erosive, creep), challenges with heat transfer materials, and high-computation throughput. Alloys, welding, and their manufacturing processes should be considered when examining the challenges to determine their effect on thermomechanical behavior of containment materials. Sensors and controls must be researched and selected to support an ideal design. Embedded sensors may cause failure points due to material changes induced by placement of the sensors.

The overarching outcome of the proposed TES project is to have a pilot-scale demonstration with spin-offs for research, but because gaps exist between laboratory to pilot- and industrial-scale, diversity and interaction between national laboratories are key to solving these challenges. The goal now is to determine the top priority for the Tri-Lab team to pursue for thermal energy approaches. The following questions can help determine the priority:

- What are the current gaps that the Tri-Lab team can address?
- What can the Tri-Lab team demonstrate within a reasonable timeframe? (Parameters of the timeframe include current technology and load cost balance.)
- Because of limited materials availability, should a Tri-Lab project demonstrate at a lab scale or at commercial scale, potentially in partnership with industry?

A demonstration of TES with a commercial-scale nuclear reactor could be prohibited due to the required permits and costs. However, the laboratories could perform a pilot demonstration for thermal storage with micro small modular reactors, which would allow for scaling over time.

The focus of TES in fossil-based thermal generators is to reduce cycling, which can cause excessive wear and thermal stress on systems, especially the boiler. Due to the high temperatures involved, especially in the case of advanced ultra-supercritical coal-generating units, the requirements of the TES may be different from current state-of-the-art technologies under development for other applications. For example, the TES system could theoretically store heat before the steam generation, but it would be difficult because of the current design of the boiler tubes.

Some discussion topics that arose during the breakout were whether two loops could be used with heat exchangers through thermal storage and steam to transfer heat between different heat transfer and working fluids. One need identified was to quantify the benefits of TES when ramping a coal plant to reduce stress on boiler components. More generally, there was a need identified to assess how different TES technologies could be used in different types of fossil power plants.

In the case of nuclear and CSP, TES media, such as molten salts, could have different chemistries but may display similar thermal phenomena. Thermal storage, with respect to nuclear generation, must be contained well outside of the radioactive area. CSP and nuclear thermal plants share common operating conditions, but fossil-fuel plants may be significantly different. It is important to identify the location of the TES component for effectively controlling charge/discharge efficiency. Optimal approaches could consider the use of small modular nuclear reactors and determine optimal location of the TES component. Small modular nuclear reactors have already been demonstrated globally, but plant operation security and safety need to be addressed. To advance the integration of TES into small modular nuclear reactors at a pilot scale, needed actions include targeting a relatively low temperature (possibly 500°C), performing containment materials' characterization, and performing experiments at a laboratory scale.

Research opportunities should be focused on the capabilities and expertise of the Tri-Lab working as a consortium, possibly with each lab emphasizing a particular node capability. For example, NREL could focus on chemical compatibility and thermal properties, NETL could focus on modeling, and INL could focus on thermomechanical behaviors, such as creep and fatigue. Other capabilities may be shared or leveraged under the consortium. Shared capabilities may include foundational understanding of stress relaxation cracking of weldments, ASME code qualification for use of alloys above their current ratings, and integrated molecular dynamics modeling and materials testing.) The idea is to adopt the practice established by EERE, which is to establish an Energy Materials Network (EMN) among the Tri-Lab.

Topic 2: Energy System Efficiency Improvements through Low Temperature Thermal Energy Utilization

The Tri-Lab team has identified low temperature thermal energy use as a key area for energy system improvement in the U.S. and globally. The breakout sessions for this topic first considered materials research needs for low temperature waste heat use. The end goal is to demonstrate that the heat rejected from thermal electricity generation facilities can be harnessed, stored, transported, and utilized in an economically viable manner. For this workshop, the Tri-Lab leads decided the threshold for low temperature thermal energy use is to be 200°C.

Background

Low temperature thermal energy utilization is important because a relatively large portion of the energy used in the U.S. can be provided with a heat transport and delivery system below 200°C. Those familiar with the Sankey diagram for U.S. energy utilization [2] can recognize that about two-thirds (or 67.5 quads) of the energy used for the residential, commercial, industrial, and transportation sectors is rejected to the environment as waste heat. The transportation sector is the least efficient with almost 80% of the energy content of combustible fuels lost. The heat loss from bulk electricity generation in the U.S. is only slightly better, with 78% of the energy produced by our combined nuclear, fossil, biomass, and geothermal power generation sources rejected. On the other hand, approximately 40% of residential and commercial energy use (or about 8.5 quad) is for space heating [3, 4]. Currently, less than 3% of residential and commercial heating is supplied with district heating in the U.S.

A list of several examples of industrial process heating applications is shown in Table 1[2]. With only a couple of exceptions, the heat duty of these process operations is under 200°C. These sources account for about one-fourth of the total industrial process energy (or about 8.0 quads). Similar tabulations of high temperature heat duties have been developed by the Tri-Lab, and these are now being refined and will be published in the near future.

The laws of physics limit efficient heat transfer at low temperatures. Heat transfer mechanisms depend on the temperature gradient, material thermal conductivities and high emissivity, surface properties that interact with fluid motion beginning in the boundary layer, and the geometry of the system. The temperature of an HTF (typically using a gas) can be increased using heat pump concepts, where the external heating source can be the waste heat that is currently rejected. Organic Rankine power cycles and thermal-electric generators can also convert low-grade heat into electricity, although the economics of these options remain a challenge. Another opportunity for low-grade heat is a thermal hydraulic fluid with a high heat capacity that can store the heat in adiabatic containers or transport systems for delivery to the end user. Various phase-change materials are being tested for this purpose.

Table 1. Temperature requirements for low temperature industrial process loads. (Source: Berkel, Rene Van. *Solar Heat for Industrial Processes*. Presented at Renewable Energy Invest 2018, New Delhi, India, October).

Industrial Sector	Unit Operation	Temperature Range (°C)
Food	Drying	30-90
	Washing	60-90
	Pasteurizing	60-80
	Boiling	95-105
	Sterilizing	110-120
	Heat Treatment	40-60
Beverages	Washing	60-80
	Sterilizing	60-90
	Pasteurizing	60-70
Paper Industry	Cooking and Drying	60-80
	Boiler Feed Water	60-90
	Bleaching	130-150
Metal Surface Treatment	Treatment, Electro-painting	30-80
Bricks and Blocks	Curing	60-140
Textile Industry	Bleaching	60-100
	Dyeing	70-90
	Drying, De-greasing	100-130
	Washing	40-80
	Fixing	160-180
	Pressing	80-100
Chemical Industry	Soaps	200-260
	Synthetic Rubber	150-200
	Processing Heat	120-180
	Pre-heating Water	60-90
Plastic Industry	Preparation	120-140
	Distillation	140-150
	Separation	200-220
	Extension	140-160
	Drying	180-200
	Blending	120-140
Flour By-Products	Sterilizing	60-90

All Industrial Sectors	Pre-heating Water	30-100
	Industrial Solar Cooling	55-180
	Heating of Factory Buildings	30-180

Impact

Cost-effective and efficient extraction and sale of low-grade thermal energy to industrial or other uses could improve the competitiveness of thermal power generation units as well as industries, which currently are discarding waste heat for want of high quality heat that is readily produced with low cost fossil fuels, biomass residues, and waste solids that are available in the U.S. However, if cost-effective methods could be developed to direct low-grade heat to district heating and industrial use, this would have a large impact on the emissions associated with natural gas and oil-fired furnaces currently used for home and residential building heating as well as district heating and university campuses.

The use of low-grade heat could provide additional revenue to thermal power plants. It could improve the efficiency of industrial processes and have a large impact on reducing the carbon footprint of this energy sector. Coupling thermal energy extraction with industrial or other sector processes can limit the need to turn thermal generators off during periods of low electricity demand, thereby reducing maintenance costs. Integration into industrial processes, such as drying equipment (for feeds and products), desalination, and water treatment would thereby improve efficiency and/or reduce costs.

Outcome and Objectives

Topic Area 2 was chosen to support the design, development, testing, and pilot-scale demonstration of low temperature heat transfer and temperature boosting to optimize the efficiency of the U.S. energy infrastructure. The Tri-Lab effort focuses on the thermal-electrical power generation units and on better usage of process heat that is currently rejected because of technical or cost barriers. The main cost barrier is that presently heat generation with natural gas and combustible process by-products is inexpensive. In many cases, combustion is the preferred way to eliminate tail gases or orphan solid waste streams. If pollutant emissions were not a concern, there would be little incentive to stop burning process waste by-products. Electrical heating is also relatively inexpensive. Excess electricity generation can be converted to high temperature heat that can be stored and used for low temperature heat duties. Although process heating and district heating with nuclear reactors is not practiced in the U.S., this may soon change with the advent of small modular or microreactors that are tailored to industry’s combined heat and power needs. Even the heat from existing nuclear plants could be used for future district heating. In summary, low-grade heat capture and use must be economically competitive, and this generally implies that low cost materials that can effectively concentrate, upgrade, and store low-grade heat are needed.

Before a demonstration project can begin, a small number of thermal electricity generation sites will be identified for analysis and demonstration of thermal energy use opportunities. At least one is expected to be a nuclear power plant (probably in the Midwest), and at least one other is expected to be a coal or NGCC power plant (probably in the Southwest). Other potential options include geothermal, CSP, and biomass combustion power plants. Key selection criteria include the need to increase energy producer revenue, the proximity of potential thermal energy users, and the potential for integration into the current steam cycle (i.e., ability to extract thermal energy at the facility without negatively impacting reliability and normal plant operation).

The first objective of the workshop was to identify leading process applications for low-grade heat use. Options that were discussed in the workshop include biomass feedstock drying or mild torrefaction, coal drying and detoxification, plastics melting, zero-liquid discharge wastewater treating, and low temperature ethanol distillation. A second option was to use waste heat for geothermal power systems enhancement by depositing heat into the geothermal reservoir or supplementing the power systems with an organic Rankine cycle. A third option was to demonstrate a more effective district heating system or perhaps a single building heating application. A fourth option is to boost the temperature of the low-grade heat source—a concept that only make sense if there is synergy between the low-grade heat form, the energy required to amplify the low-grade heat, and the end user. Simply put, the end user must ultimately include a temperature outlet that is lower than the low-grade heat source harvested.

The second objective of this workshop was to focus on the heat transfer fluids and heat exchanger materials/design that could effectively collect and transfer low-grade heat, and to store or concentrate and boost the temperature of the low-grade heat in a thermodynamically efficient and effective manner. The objective was not to focus on the development of the associated processes.

One example would be a membrane reactor that continuously separates the product of an electrochemical process. The objective would be the development of the materials and ways to manufacture the complex geometries that may transport heat, ionic or molecular species, and electrical current to sustain a reaction process, such as water-splitting or alkane deprotonation.

A third objective was getting a handle on the proper use of integrated computational materials engineering (ICME) with associated experimentation to develop custom materials and materials coatings. This have been proven useful to tailor the development of materials and their fabrication methods to new applications and new, harsh environments. This technique is especially useful to conduct accelerated stress testing (AST) that otherwise might require years, if not decades, to measure.

Targeted Benefits

The principal driver for IES was economics, which was to increase the revenue for the associated partners while maintaining affordability to the consumer. The second objective was to reduce pollutant emissions, including CO_2 emissions, by making full use of the energy released from thermal generators (e.g., fossil fuels, nuclear, and CSP), thereby reducing the level of consumption of fossil fuels. Additional benefits of systems integration through waste heat recovery and use systems are listed in Table 2 in accordance with the chief figures of merit that were established by the Tri-Lab team.

Table 2. System characteristic and associated benefits of waste heat recovery.

Energy System Characteristics	Benefits
Reliability	Provides an additional revenue stream for baseload generation; this project will improve the economics of those systems and the probability that they continue to provide baseload power. Successful implementation of this concept will reduce the negative impacts of thermal cycling on power plant equipment, reducing failure rates and the need for unscheduled maintenance.
Resilience	Increases the diversity of thermal energy supplies and, thus, increases energy resilience.
Flexibility	Establishes alternative sources of heat to meet key demands and could enable flexible power generation at baseload plants by diverting thermal energy to other products during periods of reduced demand or high renewable energy output.
Sustainability	Reduces emissions and improves economics by increasing the energy and economic efficiency of thermal-electrical generation.
Affordability	Reduces the consumer electricity price required for a generator to be viable and allows lower electricity costs to the customer by creating an additional revenue streams for nuclear and coal/NGCC power plants via low-grade heat recovery.
Security	Reduces the amount of wasted energy and reduces the amount of resources required, thus saving domestic resources for future use.

Scalability	Provides an example for power plants and industries across the country. (Hundreds of power plants could be refitted to improve their economics and achieve an energy savings.)

Crosscutting Needs

From an applications perspective, thermal energy losses from power plants is not just an issue for large fossil-fired and nuclear plants. Combined heat and power (CHP) systems used by industry include recovery boilers in the pulp and paper industry. Therefore, the opportunities and needs for low temperature heat recovery and utilization should be shared broadly with DOE programs. Not only does it reject heat impact energy utilization efficiency, but it also indirectly impacts CO_2 emissions and water withdrawals for cooling and process water, which impact the environment.

Programmatic crosscutting needs include materials discovery and screening using atomistic and molecular dynamics modeling. To parameterize these models, materials testing should be supported with materials fabrication and testing in conjunction with in-operando analysis using advanced electron microscopy. The approach of "model, make, measure" can be accelerated with ICME that applies machine learning to materials testing. The combined assets and capabilities of the national labs can be considered one "super capability."

While it is plausible to assume the materials used for low temperature applications will not undergo severe microstructural evolution, it will nonetheless be important to take advantage of the techniques and approaches invoked for high temperature materials development. Understanding surface and structural properties will be equally important to developing materials that transfer low-quality heat to a convenient transport media or to effectively gather or transmit long-wave infrared radiation.

Another need within the area of the crosscutting program is the development of effective, low cost heat delivery or heat recovery from emergent electrocatalytic, microbial, or enzymatic processes. The methods of heat transfer and deposition to these different types of processes can be a shared program goal.

Low Temperature Heat Recovery and Utilization Materials Challenges and Opportunities

The workshop participants recognized several materials challenges and opportunities for low temperature heat recovery and utilization. The main barriers are quality of heat (i.e., thermodynamics), cost, geographical location of low-grade heat generators versus consumers, the scale of low-grade heat, and the timing of heat availability. Additional technical challenges include manufacturing of the materials and modeling materials behavior.

Energy systems integration looks to overcome the cost and geographic challenges by developing systems that can collect, store, and transport low temperature heat. The technical challenges can be addressed with the combined capabilities of the Tri-Lab, including high performance computing, materials synthesis, fabrication and testing, and various advanced instruments for microscopy, X-ray diffraction, and nuclear magnetic resonance.

While INL has an established lab initiative for advanced manufacturing of materials for harsh environments, the Tri-Lab will still need to partner with some of the science labs to take advantage of advanced manufacturing techniques that are developing.

Phase-change materials can be difficult to obtain in large quantities needed for demonstration projects. For example, if a new phase-change material is developed by the Tri-Lab, then a commercial partner may be needed to produce a large batch of this material for the first pilot-plant prototype. Quality assurance/quality control will be imperative.

Current DOE-Funded Efforts

Efforts to reduce waste heat rejection and to increase utilization of waste heat have been a high priority of the DOE, led by the Advanced Manufacturing Office (AMO). Estimating the value that advanced, flexible CHP systems could provide to bulk power grid analysis is done by comparing the system costs for grid operations with and without a potential CHP resource. In addition to helping identify the electronics necessary to connect a CHP system to the grid for the myriad of prime movers and grid connection options, this project will also help establish current costs to accomplish each connection and determine the associated barriers.

AMO has also investigated opportunities for industrial waste heat recovery and utilization, identifying barriers, limitations, and R&D opportunities, which have been published most recently in the 2015 *Quadrennial Technology Review* (QTR) [5].

The DOE EERE Office of Strategic Programs' Thermal Energy Futures Project aims to determine the technical feasibility, barriers, and opportunities for renewable thermal energy systems (RTES) in stand-alone or hybrid configurations with fossil or renewable fuels (RTES/hybrids) for buildings and industrial thermal applications as well as to evaluate their potential net economic and environmental impacts. Meanwhile, the EERE-SETO Solar for IPH Project will develop the first national analysis of the potential for solar technologies (i.e., PV, solar thermal, and hybrid approaches that produce electricity and/or heat) to power a wide range of manufacturing IPH end uses, explicitly accounting for the load-reduction potential from energy efficiency measures and load-balancing potential from energy storage technologies.

Motivated by DOE to develop "Big Ideas" for crosscutting research addressing national needs, the national labs came up with a concept for research of HEATER in 2017. Led by Pacific Northwest National Laboratory (PNNL) and in partnership with several other national labs, this Big Idea aims to transform conversion, storage, transmission, and use of thermal energy using a "science-to-systems" approach, advancing molecular sciences that control thermal phenomena and developing new materials, chemistry, and technologies with high reliability. This effort provides a basis for the present Tri-Lab effort, which may draw PNNL into the Tri-Lab R&D effort.

Discussion on Gaps/Opportunities

Effective and affordable low-grade heat transfer requires advances in materials to achieve economical heat transfer, heat concentration, and upgrading using mechanical and chemical heat pumps. Low-grade heat is often transferred to the environment using cooling towers that discard the heat to the atmosphere or once-through cooling loops that discard the heat to surface waters or rivers. First, materials that can more efficiently transfer this heat to a second media that has a higher energy density are needed. Graphite is a common material for heat exchangers. Other carbon materials, such as diamond or pyrolytic graphite, are excellent performers and can be five times better for heat transfer than copper. There has been research to improve the thermal conduction of glass fiber composite by adding graphene. Low cost materials that exhibit a high thermal conductivity are needed. Also, previous attempts have been made to change the surface properties of materials to alter the emissivity in order to enhance radiative heat transfer (either as a receptor of low-grade heat or as a transmitter at low temperature). This may be a means of enhancing thermoelectric generators that so far have been too expensive to deploy on heat pipes for waste heat.

Research is warranted to develop materials that can improve the performance of bottoming cycles, such as organic Rankine power cycles. The challenge is cost, as the laws of thermodynamics (expressed in Carnot Efficiency) imply lower efficiencies are attainable for bottoming power cycles regardless of the working fluid. The Tri-Lab team may investigate alternatives, such as the use of electricity, to boost the high temperature of the power cycle. Direct heating of organic fluids could be accomplished in the exhaust of a gas turbine rather than recuperation of the heat in a heat recovery steam generator (HRSG). This could have two advantages: (1) avoid such a significant heat loss given that organic materials generally have a lower point of condensation than steam and (2) avoid the water losses that are associated with a standard cooling water tower.

Because of the issue of heat loss along pipe runs or from energy storage vessels, R&D focused on materials that can better insulate thermal energy. This can be approached by developing better, low cost insulation or coatings that minimize radiative losses. Weight and volume may be a concern if the goal/opportunity is to transfer thermal energy via containers to thermal energy users. However, many light-weight insulators lack structural rigidity, which can be engineered into the insulation.

Heat pumps are very common for residential and commercial heating; thus, even on an industrial scale, materials development is not a high priority for these concepts. However, in cases where a heat reservoir is used to accumulate the waste heat, then it would be valuable to focus on phase-change materials that will functionally store low-grade heat for diurnal or weekly power generation cycles. It could also be economical to develop high density or phase-change heat storage materials that can be used to transfer low-grade waste heat to an industrial process, which can use this waste heat for pre-heating feedstock or drying and concentrating liquid streams or for use in residential and commercial building heating.

Much discussion on catalytic membrane reactors applies to low temperature operations because the purpose of the membrane is to separate the product to maintain the forward reaction at its maximum rate. While only a few endothermic reactions operate below 200°C, some of these may be microbial or enzymatic processes that can benefit from removing the product or any by-product contaminants, which can harm the organism or enzymes. Material development needs in this area include advanced manufacturing or chemical process development, such as a sol-gel crystallization that produces a physical/electronic charge that can remove either the product or the deleterious solids, gases, or ions.

Research Opportunities

The workshop participants covered a wide range of opportunities under Topic Area 2. Many of those listed in Table 2 were discussed previously in this report. However, for the purposes of a demonstration project, the following priorities struck the workshop attendees as important:

- Custom building/district heating delivery and heat exchange systems (especially with storage technologies)
- Custom building cooling systems (via absorption technologies)
- Data center cooling (via absorption technologies)
- Desalination/recovery of produced water
- Low temperature demands/pre-heating for food industry (e.g., pre-heating, wash water, pasteurization, steeping in corn mills)
- Greenhouse heating
- Drying (e.g., food processors, industrial products, corn mills)
- Thermal storage media (e.g., concrete) that can be used for air/oxygen/boiling water preheat.

Based on the preceding priorities, key research topics were identified as important priorities for early R&D:

- Identify possible heat transfer media (e.g., hot water, steam, heat exchange fluids)
- Identify possible hybridization opportunities where upgrading the heat from the thermal power plant could make it usable by increasing the temperature
- Develop a method of comparing possible options that includes requirements, such as heat quality (temperature, quantity), distance from the thermal power plant, and system cost
- Develop a method to score the options and prioritize heat users (include possible synergies between different demands in the scoring methodology) and use it to select opportunities
- Develop an implementation sequence for thermal energy uses near each of the two thermal power plants

- Identify R&D needs for alternatives that could not be implemented today. Possibilities listed in the QTR include:
    - Condensing heat exchangers for gases containing high moisture levels with particulates, as discharged from paper machines, food drying ovens, or other sources
    - Nonmetallic materials (polymers) that can withstand condensed water from combustion products containing acidic gases
    - High efficiency liquid-gas heat exchangers for low temperature flue gases or exhaust air from dryers
    - Liquid-to-liquid heat exchangers for heat recovery from low temperature heat sources.

Topic 3: First-of-a-Kind IES Supporting Renewables, Nuclear, and Fossil Generation and Supplying Hydrogen Markets in the Upper Midwest

Background

The upper Midwest region of the U.S. provides an attractive venue for energy systems integrating variable renewable energy sources with a constant source like a nuclear plant. Part of the attractiveness is derived from the fact that the upper Midwest has a significant energy demand from manufacturing, which is concentrated in this area. The area also undergoes significant temperature changes between the winter and summer seasons, which results in variation in demand for electricity needed for heating and cooling. All things considered, the region would benefit from a more balanced electric power supply and demand. Since demand is difficult to manipulate, an emphasis on developing a flexible energy supply and attendant storage strategy is warranted.

An approach would be to develop and implement an IES that functions in concert with existing electric power generation plants, which broadly includes nuclear, fossil, and renewable energy sources. An existing plant that can serve as a vehicle for the development of this approach is the Davis-Besse Nuclear power plant outside of Toledo, Ohio. The plant experiences periods where electric power capacity exceeds demand, and it also generates significant waste heat. These are resources that could be directed toward production of hydrogen. This poses the potential for the efficient generation and storage of energy as well as an evaluation of the viability of hydrogen production for alternative uses like chemical feedstocks.

The region has a need for carbon-free energy generation to begin to mitigate the effects of atmospheric pollution and climate change. Surface waters in particular have been adversely affected as a result of acidification caused by acid rain, rising water levels in the Great Lakes, declining fisheries, and fertilizer and pesticide run-off caused by agricultural activity that has resulted in eutrophication and harmful algal blooms.

Impact

The impact of an IES would be to stabilize the electric power supply for the grid in the northwest Ohio region. Hydrogen generated during periods of excess capacity would be available for conversion to electric power using fuel cell technology. In addition, there may be increased economic value in the operation of the Davis-Besse power plant, realized from opportunities for improved economics for manufacturing industries that use hydrogen. The impact would also include the demonstration of a true IES that involves a nuclear power plant operating at scale, taking advantage of excess heat and electric power generation. The research would provide a template for scaling up high temperature electrolysis systems.

On a more basic science level, the topic would provide motivation for the identification of materials issues that affect water electrolysis when operated on an industrial scale and for hydrogen storage technology implemented in concert with an IES.

Targeted Benefits, Electrolysis

The materials that comprise high temperature electrolysis systems are subjected to harsh conditions characterized by high temperatures (~800°C) and oxidizing or reducing atmospheres. The consequences of these conditions are that material morphologies and compositions will change over the course of operation. Research suggests that upon initiation of operation, quickly occurring changes in morphology and composition can result in materials properties that are compatible with electrolysis function. However, continued changes in morphology and composition will eventually compromise the function of the electrolysis units.

It is worth noting that cells and stacks account for a significant fraction of the life-cycle cost of the electrolysis units. Stack replacement is expensive, both in terms of the cost of the components, and in terms of unit downtime for maintenance, so improving device durability is a high priority.

Targeted benefits of research on these topics would result in electrodes that are resistant to changes in composition, specifically that resist alteration arising from elemental migration. For example, at high temperature, a deleterious phenomenon is the migration of nickel (Ni) from nickel-yttria-stabilized zirconia (Ni-YSZ) electrodes into neighboring materials. In addition, the gadolinium (Gd) in the gadolinium cerium oxide spacers also migrates, and importantly, so does chromium (Cr). Cr is a constituent in the materials that comprise the interconnects used in the stacks and is responsible for poisoned catalyst materials. In addition to catalyst poisoning, elemental migration can contribute to the formation of new ceramic phases; the effect of the new phases is likely variable, in some instances, favoring the function of the electrolysis cell, while in other cases, it can result in the formation of new materials with significantly different thermal expansion characteristics. This can result in a mismatch with neighboring layers in the cells and can lead to cell cracking. Cracking may also result from oxygen build-up in voids that are formed in the cells. The development of materials that would not be susceptible to these phenomena would present opportunity for the emergence of electrolysis cells with better performance and durability, and with improved economics.

The development of materials that are resistant to elemental migration at temperature and atmosphere would be of high value not only to the local hydrogen economics but also to the national hydrogen effort.

The kinetics of ion diffusion processes occurring in the electrolyte also represent an area of targeted benefit. The ability to produce thinner electrolyte layers in the electrolysis cells is a combined materials and manufacturing challenge; however, research conducted in this area is expected to result in substantial improvements in electrolyte performance. Similarly, the kinetics of the redox reactions occurring at the anode and cathode surfaces are also expected to benefit from a continued research emphasis, particularly in catalysts that are incorporated into the electrodes.

Another targeted benefit will likely be the identification of operating conditions that enable electrolysis at lower temperatures. Elemental migration, adventitious formation of new phases, and consequent mismatches in thermal expansion properties will all be mitigated to some degree by operation at lower temperatures. Notably, hydrogen production kinetics will also be slower, and thus, identifying trade-offs between the stability and lifetime of electrolyzer components and the hydrogen production rate and efficiency will be an important outcome.

The problem with Cr migration and poisoning can likely be addressed by improved coatings that inhibit elemental migration. Multiple groups are currently active in this research area, yet significant problems remain, and further progress would afford excellent potential for solving the problems that impede large-scale deployment of water-splitting electrolysis technology.

Hydrogen Storage

A major barrier for the global transition from the current hydrocarbon economy to the future hydrogen economy lies in the lack of cost-affordable hydrogen storage methods [6,7]. The main technological problem of a viable hydrogen economy is its storage; so far, finding a cost-effective method of storing hydrogen remains an indomitable challenge [7]. DOE has suggested that the gravimetric density should reach 9 wt% and that the volumetric capacity should be 81 grams of hydrogen per liter (g of H_2/L) by 2015 [7]. Sreedhar evaluated approaches for hydrogen storage in a 2018 review, with respect to DOE's targets of a minimum storage capacity of 5.5 wt% and 40 g/L with a 5-minute filling time [8]. They concluded that while hydrogen has excellent energy density by weight, its energy density by volume is very poor compared to hydrocarbons, making it difficult to store and transport [9]. Accordingly, DOE's 2015 targets remain challenging goals.

Compression

Hydrogen compression is volumetrically and gravimetrically inefficient [7, 10]; however, smaller compressors are conceivable and could approach some level of affordability. Hydrogen density is very low regardless of whether it is stored as a compressed gas or as condensed liquid. As a gas at 700 bar, the density is only 0.024 (kg H_2/L) [6]. Hence, ultra-highly pressurized tanks have been proposed. However, these require assembled materials with super-high compressive strength, and even when these are used, there are safety risks and significant energy consumption during compression [6]. At pressures above 700 bar, the gas deviates from ideal behavior, and volume reduction is more limited with increasing pressure. Increased wall strength is needed, without commensurate volume reduction.

Compressed hydrogen storage can be achieved using a variety of vessels, which can tolerate up to 1,000 bar for fully composite materials, but the cost is high and with unresolved reliability uncertainties [11].

Liquefaction

As a liquid at 20 K, the density only increases to 0.071kg H_2/L. For hydrogen liquefaction, significant losses of hydrogen resulting from heat transfer and large energy requirements severely impede practical application, despite the advantages of higher volumetric density [6]. The density of liquefied hydrogen is much higher compared to compressed hydrogen, but it has the second lowest critical temperature at 33 K, so cryogenic-compressed approaches store hydrogen as a supercritical fluid, which enjoys higher storage density [12] and storage capacity (~5x greater). Hydrogen liquefaction is energy intensive and time consuming, with lost energy content as high as 40%, whereas with compressed gas, it is only 10% [3]. Thus, liquefaction requires a huge amount of energy, accounting for 20 to 50% of the heating value of the hydrogen. Generally, cryogenic storage has a poor energy efficiency, and compressed storage requires large volumes due to the low density of hydrogen [11]).

Hydrogen liquefaction requires a large capital investment [12, 7]. High costs are, in part, due to the need for specialized storage, driven by the demanding requirements imposed by liquid hydrogen. At atmospheric pressure, liquid hydrogen exists at 20 K, and the tanks used need be well insulated. The need for composite tank materials, to reduce losses due to hydrogen boil-off, and the current high costs of tanks are impediments to implementation [7]. An insulating pressure vessel is required to do this (H_2 condenses at -253°C, or 20 K), and currently, liquid hydrogen can only be stored in an open system. Alternatively, cryo-compressed storage of supercritical hydrogen can minimize boil-off, thereby maintaining its high energy density; however, the cost of pressurization and cryotanks is high, and there is a safety concern regarding their operation.

Currently, there is no infrastructure to support hydrogen storage using these approaches. Composite storage vessel reliability needs further research, including better understanding of damage mechanisms and identification of inspection and maintenance approaches [11].

Physisorption Media

Alternatively to physical approaches, hydrogen can be stored using materials that function by either physisorption or chemisorption [6]. Hydrogen can be stored using physisorption that uses carbon materials, metal-organic frameworks (MOFs) [11], covalent-organic frameworks (COFs), zeolites, or other types of metal-organic complexes [7]. Additional candidates include a variety of carbon types (e.g., fullerenes, nanotubes, graphene) [10], hyper-crosslinked polymers, capillary arrays, and glass microspheres [8]. An example of materials that act by physisorption are MOFs, which have surface areas as high as 2,000 m^2/g. The MOFs are most effective at hydrogen uptake at cryogenic temperatures, and "pillared layer" structures have shown large surface areas and good hydrogen storage capacity at liquid nitrogen temperature (-196°C) [9]. However, storage capacity is <2 mass% at ambient temperatures, so these types of materials must function at cryogenic temperatures because of weak interactions that bind hydrogen to their surfaces. The low hydrogen binding energy can result in fast charge and discharge kinetics, which are operationally beneficial. The cost of materials to support this work is decreasing; however, to date, only small-scale experiments have been conducted because the hydrogen capacity and operating pressure temperatures are less than desired. In general, these materials display intriguing properties but do not meet DOE's storage targets.

Metal Hydride Chemisorption Media

A variety of metal hydride materials have been identified that function to bind hydrogen by chemisorption. These materials combine with atomic or ionic H via metallic, covalent, or ionic bonding to achieve solid hydrogen storage. More typical metal hydrides absorb hydrogen with up to 5 to 7 wt% capacity but need to be heated to 2,500°C or higher in order to affect formation [7, 10]. The bound hydrogen is fairly tightly held, so the release of hydrogen requires 120 to 200°C. Good hydrogen storage density, storage volume, safety, purity, and reversibility can be achieved.

Historically, materials, such as lanthanum nickel hydride ($LaNi_5H_6$) or titanium iron hydride ($TiFeH_2$), are representative of early-generation compositions that were capable of up to 2 wt% H_2. Currently, the focus has shifted to light metal materials containing lithium, beryllium, boron, carbon, nitrogen, sodium, magnesium, and/or aluminum in their hydride forms. These materials have high hydrogen storage capacity and are normally inexpensive. Catalysts can be added, which reduce the energy needed for hydride release as hydrogen. Hydrides are reactive, which does pose a safety risk to be mitigated, but the risk is significantly lower compared to that posed by other forms of storage. In general, the light metal hydrides are safe.

Magnesium (Mg) hydrides or complex hydrides that contain borohydrides (BH_4^-) or alanates (AlH_4^-) are attractive because they can bind significant weight percentages of hydrogen [8, 11]. For example, Mg can store 7.6 wt% of hydrogen while lithium borohydride ($LiBH_4$) can bind 18.6 wt%. There are a lot of other alloy compositions that have received consideration, but in most cases the gravimetric storage density is too low. Materials containing ammonia, borane, and borohydrides (containing boron tetrahydride, BH_4^-), particularly as compounded with low-atomic weight lithium, have been considered for hydrogen storage [9], and a variety of substances can achieve the 9 wt% DOE goal.

Implementation of hydride compounds as hydrogen storage media has been hindered by either unfavorable kinetic barriers or the stable thermodynamics of the compounds, which can result in poor reversibility. The kinetic barriers principally result from the fact that hydrogen has to diffuse through the metal hydride solid for both hydrogen uptake and release [12]. Consequently, the binding and release kinetics are unacceptably slow, and the hydrogen adsorption coefficient is not favorable [9]. To get around this, metal hydrides have been formulated as particles, which can range down to the nanometer scale. However, this approach does not overcome the thermodynamic limitations that stem from the strong bond of hydrogen in the metal hydrides, which results in a large energy input requirement for hydrogen release.

The thermodynamic impediment, to some extent, can be ameliorated by incorporating a catalyst in the metal hydride to reduce desorption temperatures [12]. This approach has also been combined with attempts to improve storage capacity using doping and nanoconfinement approaches. These are attractive strategies, although they increase the system complexity in a significant way, suggesting the need for meaningful, fundamental research to increase our ability to rationalize, predict, and control behavior. Recent advances in nano-structuring and catalyst doping [6] suggest that a workable storage technology may emerge from these areas. For example, inclusion of Ti catalysts on MgH_2 resulted in a reduction of desorption temperature from 278 to 185°C, and $NaAlH_4$ doped with Ti have displayed enhanced hydrogen adsorption storage capacity [7]. However, other research has encountered problems, for example, sodium borohydride will slowly hydrolyze to generate sodium borate and hydrogen, but, in general, a platinum group metal catalyst is needed. Unfortunately, the metal catalyst nanoparticles tend to aggregate [9].

It is also noted that while the stability of the metal hydrides is detrimental to their utility as hydrogen storage media, it brings several advantages. First, it allows storing hydrogen at ambient temperatures and pressures without losses during the storage period. Second, flammability and explosion risks are significantly lowered, reducing safety risks.

Non-Metal Hydride Chemisorption Storage Media

A variety of hydrogen storage approaches that are not based on metal hydrides have been developed. For example, ammonia has been considered as a hydrogen storage medium, which can be reformed to generate hydrogen with no CO_2 emission [7]. Formic acid is also a potential hydrogen storage material—reaction with H_2O over a catalyst will release hydrogen and CO_2. It has a gravimetric hydrogen storage density of 4.3 wt% at room temperature and pressure [7]. Similarly, carbohydrates are considered potential hydrogen storage media, capable of releasing 12 moles of hydrogen and 6 moles of CO_2 per mole of sugar.

Liquid organic hydrogen carriers (LOHCs) include compounds like toluene, which can be combined with hydrogen to make methylcyclohexane [12]. A disadvantage of the LOHCs is that they have a vapor pressure, so there are impurities when the hydrogen is released. PGM catalysts and temperatures of 200 to 300°C are needed for initial hydrogenation, although hydrogen release requires slightly lower temperatures. LOHCs include compounds like cyclohexane and decalin, which can be dehydrogenated to the corresponding aromatics, and simple derivatives of these compounds are easier to dehydrogenate compared to the base compounds. N-heterocycles are also used, including boron nitride compounds. These technologies can be low cost and low weight and operating temperature; although, unwanted gases can be formed in the process. While most of these are solids, LOHCs are attractive; hydrogen is chemically bound to hydrogen-lean compounds and released by catalytic dehydrogenation. The limitation of the LOHCs is its modest storage capacity.

Large-Scale Hydrogen Storage

Large-scale hydrogen storage poses commensurately large capacity challenges. Approaches include salt caverns, which are being used in Germany, Texas, and the UK [11]. Typical volume is $7x10^5$ m^3, and a maximum operation pressure is 20 MPa (197 atm). These are attractive attributes, but the effects on the environment have not been established.

Hydrogen delivery also poses challenges toward eventually achieving a hydrogen economy [11]. Delivery can be accomplished in three general fashions: gaseous, liquid, and material-based hydrogen carriers. Gaseous delivery is achieved using pipelines or tube trailers that operate at 250 bar (25 MPa) and have a capacity of ~600 kg. However, gas pressure variations and leakage are common phenomena. Liquid hydrogen delivery is considered economical and compatible with the capacity of eight liquefaction plants in North America, which can generate 5 to 10 tons per day (metric). Hydrogen carriers can provide higher safety levels because storage pressure is lower, and they have good density compared to gaseous storage. However, they are not suited for high demand. There is inadequate data for almost all storage and delivery technologies relevant to the hydrogen infrastructure, which hinders the evaluation of implementation potential [7, 11].

Materials-Related Challenges and Opportunities

Hydrogen embrittlement is an important concern for steel materials [11], resulting in loss of ductility and fracture resistance. An alternative approach is to use fiber-reinforced polymer (FRP); research on this material was funded at Savannah River National Laboratory by DOE.

Composite tanks and piping are susceptible to rupture, delamination, and matrix cracking. Ensuring robustness against flammability is a concern for polymeric and composite materials. At the present time, there is a lack of degradation and failure data and a lack of detailed probability models for hydrogen gas ignition.

Materials-based storage methods are in early development and need more research.

Specific Applications Related Activity

Topic Area 3 covered three main areas: hydrogen production, storage and transportation, and hydrogen utilization. The following are common themes and needs that emerged:

- Materials degradation in harsh environments
- Materials discovery guided by modeling and simulation
- Sensors to support control of corrosion and materials degradation
- Material reduction costs by improving process kinetics. (Note: Reduction slows kinetics/rates and leads to higher material costs.)

Hydrogen production material challenges focused on low, intermediate, and high temperature electrolysis and thermochemical water-splitting cycles. These challenges are compared in Table 3.

Implementation Considerations

Hydrogen storage challenges identified include materials strength, degradation, and high cost (e.g., compression or cryogenic cost). Use challenges include the interfaces with other energy sources, brittleness, and creep issues. Transportation and infrastructure challenges include stress corrosion and hydrogen embrittlement, environmentally induced cracking, corrosion protection/coatings, and stresses and mechanical failures (crack origination and propagation).

Items for consideration:

- Retrofitting existing pipelines
- Compressors.

Hydrogen utilization challenges:

- Interface with other energy sources
- Brittleness and creep issue.

Table 3. Hydrogen production material challenges identified with low, intermediate, and high temperature water-splitting cycles.

High/Low Temperature Electrolysis
Integration of materials not understood Crossover challenges other areas: pressure/temperature stability, cost of materials, catalysis durability Material issues (porosity issue, pore structure, transport issues) Electrolysis cells: electrochemically unstable interfaces Degradation mechanisms accelerated when modes are switched from adsorption to desorption, other degradation mechanisms are activated; microstructure analysis is a need Fundamental scale: time scale issues, no fundamental science that consistently explains the macroscopic experimental studies.
Intermediate Temperature Electrolysis
Catalysis stability and kinetics Modeling and computation needs and their coupling to machine learning/data analysis applications Solid-solid interface challenge and interconnect corrosion issue.
Thermochemical Cycles
Catalysis stability Material of construction issues.

Topic 4: Low-Carbon-Energy Powered CO_2 Use for Fuels and Products in the Texas Gulf Coast Region

The CO_2 utilization project proposes to leverage a combination of renewables, nuclear energy, and CO_2 captured from a fossil energy source to produce value-added chemicals and fuels that will sustain a robust and diverse energy grid and industrial ecosystem, enhance America's energy independence, and ensure sustainable use of fossil-fuel resources.

Background

Texas leads the U.S. in wind power generation with wind farms in the south region of the state where significant solar potential exists. The South Texas Nuclear Generating Stations are licensed through 2047/2048 and may have potential for expansion. Southeast Texas currently hosts the only U.S.-based, full-scale, carbon-capture facility, Petra Nova, at a coal-fired power plant site. This regional combination of energy resources, industrial demands, and technical experience in all three energy types makes Texas a potential research site for integrated application for low-carbon fuels and products.

Impact

Leveraging the integration of carbon-free electricity from renewable sources (i.e., solar and wind) and nuclear sources with excess carbon-free heat from nuclear sources to convert CO_2 captured from a fossil energy source (i.e., coal-fired power plant) to produce value-added chemical and fuels. Such integration would monetize waste CO_2 streams, allow more effective use of renewable electricity generation, and maximize energy output from nuclear plants.

Outcome and Objectives

The overall objective is to demonstrate the design and integration of technologies for producing carbon-neutral industrial materials and processes from CO_2 captured from fossil energy systems while using low-carbon electrons. The proposed project will have two primary efforts: (1) systems integration and optimization R&D and (2) development and demonstration of advanced CO_2 conversion technologies.

An important aspect of this project will be conducting systems integration and optimization R&D, which includes the following:

- Dynamically couple and operate non-emitting generators (i.e., renewables and advanced nuclear) with CO_2 capture from fossil energy systems as a hybrid IES
- Capture and purify CO_2 from existing industry, including oil and gas production, power plants, chemical production, and other industrial processes
- Conduct research on CO_2 combined-capture/use chemistry that enables synergies of an integrated approach and is applicable to lower-concentration CO_2 sources
- Develop and demonstrate electrochemical, catalytic, and/or biological C1-processes[3] (utilizing CO_2, CO, and CH_4 as feedstocks) to generate higher valued carbon products
- Design and demonstrate complex control systems for tightly coupled hybrid CO_2 use concepts
- Estimate potential impacts of varying levels of CO_2 purity and effect of trace contaminants
- The R&D portion of this project would consider three options for converting CO_2, including (1) the use of electrolytic generated hydrogen within a gas fermentation biomethanation reactor to generate renewable methane; (2) the combination of renewable electricity to drive a microwave reactor, augmented with thermal energy to convert methane and CO_2 to hydrogen and carbon monoxide (CO) via dry reforming; and (3) the electrochemical reduction of CO_2 to CO.

Biomethanation: This involves the direct conversion of CO_2 and H_2 to methane (i.e., renewable natural gas [RNG]) via a whole-cell biocatalyst (microbial catalyst). The biocatalyst has high specificity and can tolerate impurities in the input gas stream like O_2, CO, and H_2S. The process is continuous but can be operated variably and can cycle on and off to follow available low-carbon electrons. The process is exothermic, but it operates at a very manageable 65°C. A 50,000-liter bioreactor working volume will produce between 25 million and 43 million liters of 98% pure methane for injection into the natural gas network. A first-of-its-kind in the United States pressurized bioreactor system to produce RNG is being commissioned at the NREL with partners Southern California Gas Company and Electrochaea GmbH. The project aims to demonstrate improved integration and efficiency between a 250-kilowatt electrolyzer and 700-liter bioreactor. Aspects of the biomethanation technology that require further development have TRLs around 4–5 while the scale of demonstrations of this technology overall has a TRL of 6.

[3] C1 refers to any molecule stoichiometry that is has only a single carbon atom.

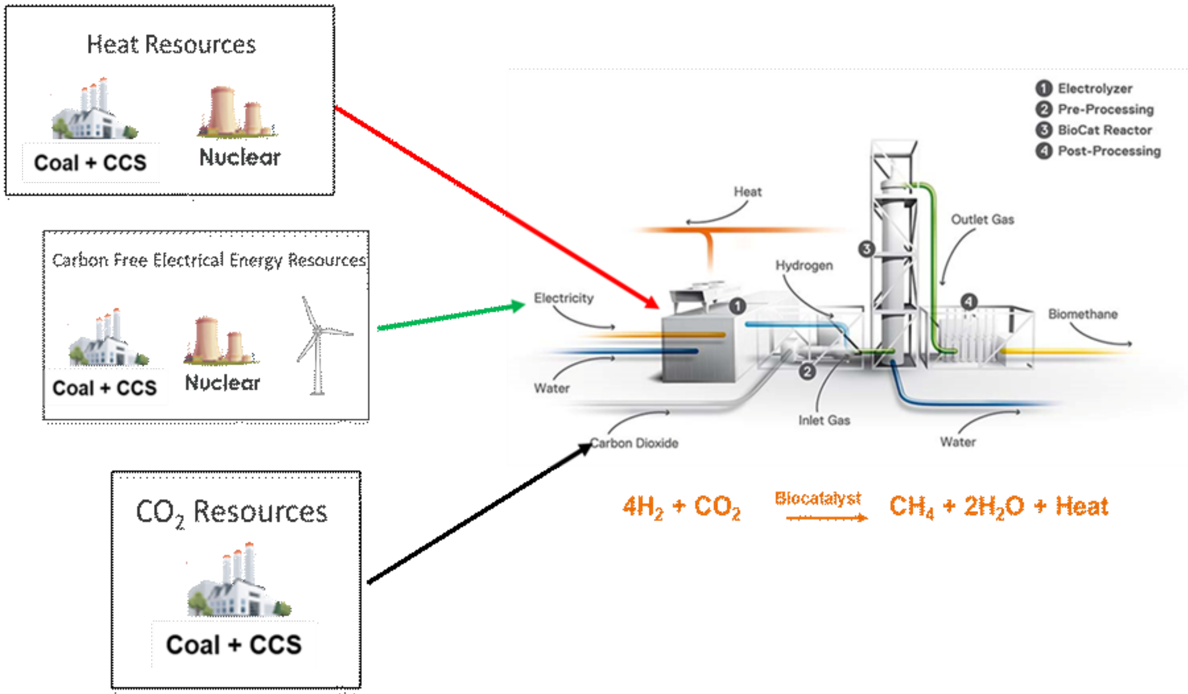

Figure 2. Generation of methane from captured CO_2 and carbon-free electricity using biomethanation.

- **Dry reforming:** This process has been under investigation for decades but has not reached commercial sustainability. It considers the reaction of CO_2 with CH_4 to produce syngas. Dry reforming methane by developing an intensified modular catalytic process technology that utilizes heat from a coupled nuclear reactor would be novel. Developing a modular and intensified process might be challenging but offers an excellent opportunity to reduce two of the most dangerous greenhouse gas (GHG) compounds and facilitates integration to the distributed system. It also provides a mechanism for utilizing part of the methane formed in the bioreactor (described below). Dry reforming produces a syngas with a H_2/CO ratio of 1, which is ideal for acetic acid production, while it is a ratio of 2 for methanol and 3 for hydrocarbons production. The combination of a dry reformer with H_2 derived from water electrolyzers will widen the product options.
- **Electrochemical syngas formation and upgrading:** This approach will produce a saleable industrial feedstock that reduces the carbon footprint of fossil-fuel-powered processes and offsets CO_2 capture costs. Carbon-free electricity derived from nuclear, wind, solar, etc. can be used to electrochemically convert CO_2 and water into syngas ($CO + H_2$) at ambient temperatures [15]. Energy requirements increase with product complexity. Direct electrochemical formation of larger hydrocarbons and alcohols becomes impractical, as indicated in a recent technoeconomic analysis that identified the production of syngas ($CO + H_2$) as the most practical target because electricity costs associated with direct electrochemical production of hydrocarbons or alcohols could exceed their market value [16]. Electrocatalysts and process conditions have been identified for tuning the H_2/CO ratio, and large-scale water electrolysis has been demonstrated for efficient H_2 production. CO_2-derived syngas can be thermally upgraded into methanol using existing mature catalytic process technologies. Our proposal is to use waste heat from nuclear reactors. Coupling these two concepts will allow high-volume production of a carbon-neutral, value-added commodity chemical that can be used in the plastics industry as a direct fuel source or for upgrading to gasoline.

Crosscutting Needs

From an applications perspective, hybrid approaches are required to effectively use renewable electricity and nuclear-based electricity and heat to convert CO_2 from fossil fuel-based sources such as coal-fired power plants. Such approaches may combine biotic and abiotic technologies. For example, the generation of renewable methane is currently being developed and demonstrated using electrolytic generated hydrogen from water and CO_2 via gas fermentation (shown in Figure 2). Building on the expertise of electrolytic generation of hydrogen, the electrochemical conversion of CO_2 to a range of commodity chemicals and fuels is an active area of research in academia, national labs, and industry. This initiative is building capabilities to investigate electrocatalysts, membranes, electrode/cell configuration, electrolyte composition, and applied potential/current. Besides conducting research, these capabilities can be used to develop and scale electrochemical systems not only for CO_2 reduction, but the electrochemical processing of a variety of feedstocks (N_2, alcohols, biomass-derived compounds). In the longer term, technologies outside of electrochemistry that used electricity as an energy source for manufacturing are also of interest. Such technologies include the use of artificial light-driven reactors, plasma and non-thermal plasma reactors, microwave-driven reactors, electricity-driven separations, metal reduction, and plastic deconstruction.

Targeted Benefits

This CO_2 utilization project, which integrates renewables with nuclear to generate value-added products, will provide sustainable benefits to the energy grid and industrial ecosystem via the following:

- Reduced carbon footprint of fossil-fuel powered systems
- Use of captured CO_2 and carbon-free electricity to create valuable products (e.g., alcohol/fine chemicals)
- Reduced curtailment of clean energy generation (i.e., nuclear power, while enabling future development of low-carbon electricity sources).

RNG from the biomethanation process will require very little clean-up before injection into the natural gas (NG) network. The vast NG storage network provides a means to store low-carbon and low cost electricity from days to months to seasons. There is significant potential to recycle CO_2 with the biomethanation process. For example, a small 10-megawatt electrolyzer system feeding a bioreactor will recycle 7,500 tons of CO_2 per year.

Materials-Related Challenges

While there are many potential technologies that could be integrated to convert CO_2 to fuel and materials using available carbon-free electrons and heat, this workshop focused on the use of renewable hydrogen combined with gas fermentation to generate methane from CO_2 (biomethanation), novel reactor schemes for the dry reforming of methane with CO_2, and the direct electrochemical conversion of CO_2 to generate CO, hydrocarbons, and alcohols. Each process has several unit operations with different materials needs. Presented below are summaries about material needs for each of the technologies discussed.

Generation of Renewable Methane via Gas Fermentation

NREL has built and is now operating a demonstration unit that uses electrolytic hydrogen with a gas fermentation reactor to generate methane. While this is a working demonstration, materials and technology challenges were identified around the bioreactor (see Figure 2).

Material challenges include channels and/or packing to improve mixing for hydrogen absorption, materials that are necessary within the bioreactor that promote and maintain microbe growth, materials that are necessary for sterilization, improved reactor design for mass transfer, and scaling of the bioreactor.

Figure 2 shows that the generation of the renewable methane via gas fermentation has two process steps: (1) carbon-free hydrogen generation and (2) methane generation via gas fermentation. Material challenges for the generation of hydrogen from a variety of sources, including electrolytic hydrogen generation, have been outlined in Table 3 under Topic 3. NREL has built and is now operating a demonstration unit that uses electrolytic hydrogen with a gas fermentation reactor to generate methane. While this is a working demonstration, materials and technology challenges were identified around the bioreactor, including the following:

1. Design of channels and/or packing to improve mixing for hydrogen absorption
2. Materials of construction of channels, packing, and bioreactor shell that promote and maintain microbe growth
3. Materials of construction necessary to allow sterilization of packing and bioreactor shell
4. Improved bioreactor design for mass transfer of feed H_2, CO_2 as well as product methane
5. Scaling of the bioreactor.

Generation of Syngas via Dry Reforming Using a Microwave Reactor

NETL is investigating the use of microwave reactors to convert methane and CO_2 to hydrogen and CO via dry reforming. The advantages of such a reactor system include quick responses to the availability of the intermittent electricity supply typical of renewable electricity generation, such as wind power and solar power. Additionally, such systems could use high temperature heat to drive the reaction thermally or use low temperature heat from either a nuclear or coal plant to keep a microwave-driven reactor in stand-by mode (See Figure 3).

Material challenges include microwave reactor design, microwave compatible materials (such as ceramic or plastic), and microchannel reactor systems.

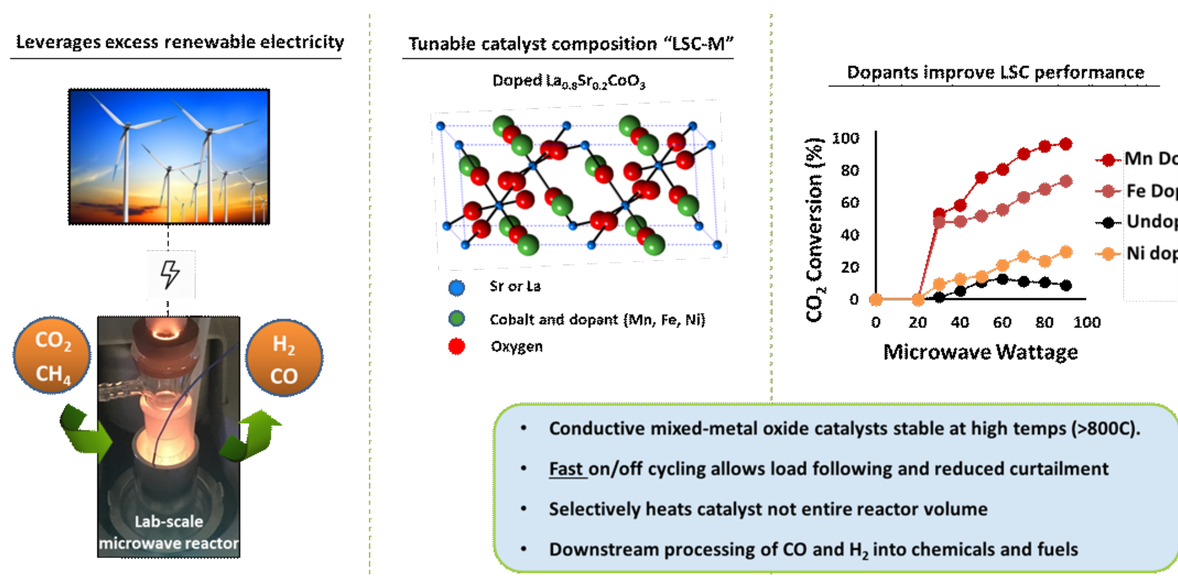

Figure 3. Material challenges for microwave-driven dry reforming. (LSC is any stoichiometry of La, Sr, Co; M designates it is a matrix of metal oxides.)

Material challenges include:

1. Microwave reactor design

2. Microwave compatible materials (such as ceramic or plastic)
3. Microchannel reactor systems.

Generation of CO via the Electrochemical Reduction of CO_2

NREL is leveraging the experience they have gained from electrolytic hydrogen generation to develop pathways for electrochemically reducing CO_2 to products. Initially, the generation of CO is desirable as it can be combined with electrolytic hydrogen as a syngas feedstock for commercial technologies, such as methanol synthesis or Fischer-Tropsch synthesis.

Material challenges include developing gas diffusion electrodes to improve current densities from mA/cm^2 to A/cm^2, developing a bipolar membrane to allow water oxidation in alkaline electrolyte, developing new cathode electrode architectures to manage reactants and multi-phase products, and proving the effectiveness and reliability of membranes, catalysts, and electrodes (see Figure 4). This is important because the effective surface-specific production rates as a function of current density determine the size of the electrochemical cell.

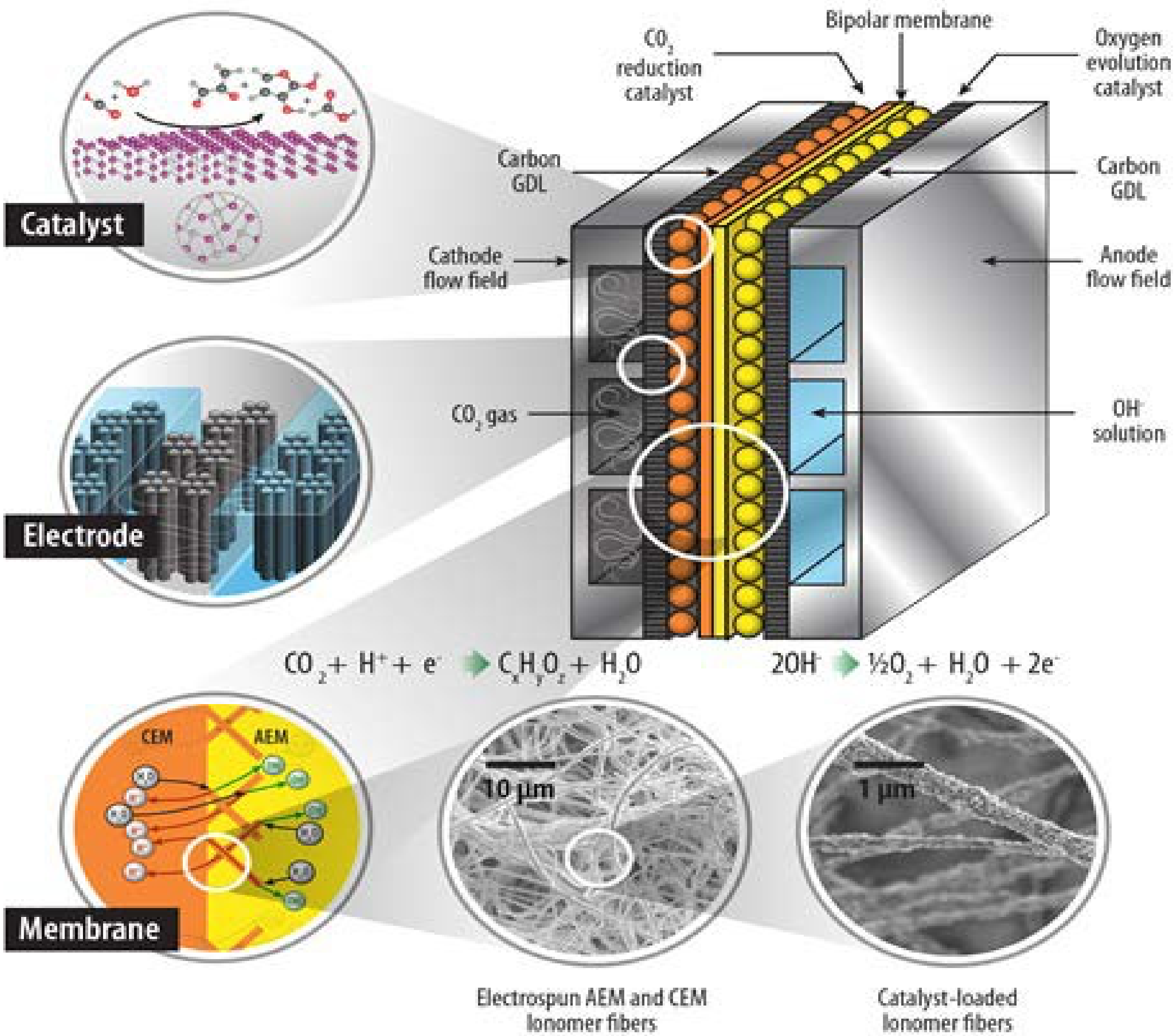

Figure 4. Material challenges for the direct electrochemical reduction of CO_2, where GDL is a gas diffusion layer, AEM is alkaline-exchange membrane; CEM is a cation-exchange membrane.

Material challenges (see Figure 4) include the following:

1. Development of gas diffusion electrodes to improve current densities from mA/cm^2 to A/cm
2. Development of a bipolar membrane to allow water oxidation in alkaline electrolyte
3. Development of new cathode electrode architectures to manage reactants and multi-phase products
4. Proving the effectiveness and reliability of membranes, catalysts, and electrodes.

Topic 5: First-of-a-Kind IES Supporting Hybrid Carbon Conversion Using Clean Energy Sources in Coal-Producing States

The focus of Topic 5 is an evaluation of the potential for conversion of the country's abundant coal resources into high value materials, chemicals, and fuels through new, efficient carbon conversion methods that use cost-competitive, clean energy inputs. Achieving these targets would help reestablish economic stability in coal-producing states and bolster national security.

Topic 5 discussions covered three main areas within the broad field of hybrid carbon conversion using clean energy sources: (1) coal-to-fuels/chemicals via gasification, (2) coal-to-high-value carbon materials, and (3) extraction of strategically important rare earth elements (REEs) from coal.

Achieving breakthroughs in these areas will require advances in materials, advanced manufacturing for component fabrication, and modeling, computational science and data analytics.

Background

Historically, coal has been a significant contributor to the nation's energy supply. However, consumption of coal for energy production has become increasingly disfavored because of the release of carbon to the atmosphere. Coal production in the U.S. peaked between 2005 and 2010, at about 1,200 million short tons (MMst), but has since declined (to 774.6 MMst in 2017, 5, left). As a result, declining coal production in eastern and western states has severely impacted local economies, especially rural West Virginia, Wyoming, New Mexico/Arizona (specifically, the Navajo Nation), and Utah where alternate jobs are not available. In the future, energy production using coal combustion may be phased out of the energy portfolio.

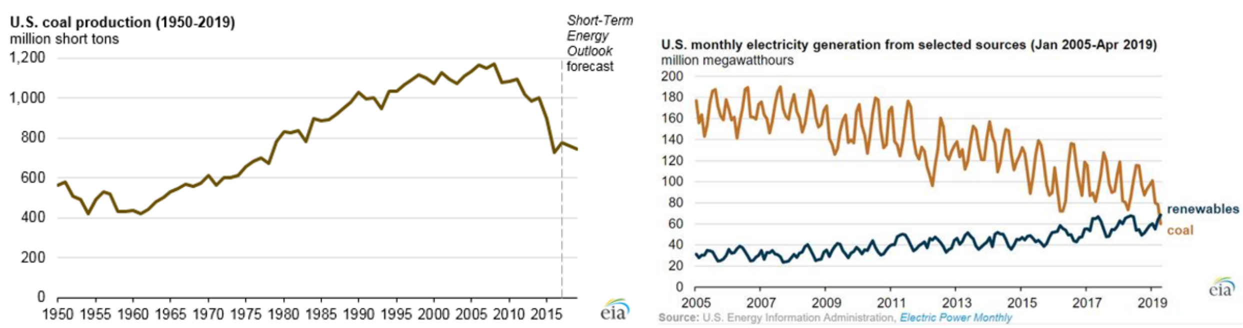

Figure 5. Left, U.S. coal production from 1950 to 2019. Right, U.S. monthly electricity generation from January 2005 to April 2019. The brown trace is coal and blue trace is renewables. Source: U. S. Energy Information Administration, Electric Power Monthly, https://www.eia.gov/.

The decline of coal has been hastened by the historically low cost of NG, causing coal production to significantly decrease in eastern and western states. Increased penetration of variable renewable energy, particularly wind and solar photovoltaics, is impacting traditionally baseload power plants (i.e., coal and nuclear), reducing potential revenue, and potentially increasing maintenance costs due to increased thermal and mechanical cycling.

Similarly, the monthly electricity generation from coal has declined from 160 to 170 million megawatt hours in 2005 to around 80 million MWh in 2019. Electricity generation from renewables surpassed coal for the first time in 2019 (See Figure 5, right).

In addition to the negative impact on the economies of coal-producing states, the phase-out of coal production will eliminate a valuable manufacturing feedstock, that has the potential to supply industrial production of value-added carbon materials. Continued processing of coal also enables industrial recovery of REEs, which is a goal increasing in national importance.

Yet, coal has other uses and is currently converted into a wide range of products via direct or indirect pathways. Between 300 and 400 million tons/year of coal are consumed globally for non-power uses (excluding coal consumed for metallurgical coke making and in calcining of cement). The products range from specialty chemicals to energy sources (e.g., transportation fuels) and include carbon fiber, silicon carbide (SiC), and other carbon-based products. It is likely that a much-expanded utilization of coal could be realized if better processing systems become available. Expanded coal use is envisioned through new IESs capable of cleanly converting coal to fuel or to value-added chemicals and materials. The development of new IES technology capable of carbon conversion using clean energy holds the promise of efficient use of the carbon feedstock represented by coal, spurring manufacturing while at the same time offsetting the economic effects resulting from the phase-out of coal as an energy source. However, realization of the potential of new IESs will be largely dependent on the development of new IES technology, specifically, materials capable of functioning under harsh conditions, which frequently will be used for processes with improved efficiency.

In considering the materials issues related to IES technologies, five common themes emerged in the context of the carbon conversion concept:

- Materials that are compatible with applications in harsh environments and with flexible operations imposed by cycling units. For instance, materials are needed that can tolerate extreme temperatures (>700°C) to transfer heat from nuclear power plants at high efficiency and that can function as insulation, imparting improved safety and reliability. Examples include materials with enhanced mechanical and structural properties that are compatible with harsh environments (i.e., thin sheet materials with improved fatigue resistance at high temperatures) and materials specifically designed for flexible operations that will tolerate the frequent cycling in power plants
- Materials capable of supporting improved efficiency and economics of existing coal-to-products processes. Examples include high performance and robust catalysts for coal-to-fuels and chemicals production and new membrane materials to replace energy-intensive thermal separation processes
- Materials generated from large-scale use of coal-derived carbon products
- Materials production approaches using advanced manufacturing approaches for producing functional materials that cannot be made with conventional processes and for manufacturing parts with complex geometries
- Modeling and simulation approaches for guiding materials discovery. (An additional computational need is the establishment of an updated/modernized coal database.)

Topic 5 focused on three aspects of carbon conversion: coal-to-fuels, chemicals, and high value carbon materials. Achieving breakthroughs in these areas will require advances in materials, advanced manufacturing, modeling, computational science, and data analytics.

Opportunities

There are numerous potential opportunities for the development of alternative uses for coal (beyond the production of electricity). Coal can be converted into a wide range of products either directly, via pathways, such as pyrolysis, or by indirect means, such as gasification. Products include specialty chemicals (e.g., benzene, fuel additives), construction materials (e.g., asphalt and heavy tars used for road construction and roofing materials), and energy sources (e.g., transportation fuels, gases for use in electricity generation). Coal's high-carbon concentration lends itself to conversion or purification to carbon-based materials, such as carbon fibers, SiC, and other carbon-based components.

Coal conversion opportunities include Fischer-Tropsch conversion of syngas to paraffins, syngas to methanol, syngas to glycol, ammonia production, methanol to olefins, and synthetic NG production [13]. These approaches are widely practiced in China but have not been widely adopted in the U.S. [14].

The challenge in realizing these opportunities has been in improving the economics and environmental impacts of coal refining processes. IESs represent a highly attractive alternative for improvement in that they utilize clean energy sources with enhanced efficiency and sustainability. For example, coal conversion in a refinery can be driven by nuclear heat, operating at higher temperatures with enhanced process efficiency.

From a compositional perspective, coal feedstock can be highly variable. While this represents a processing challenge, it is also an opportunity, since the production of a variety of different carbon materials with distinct properties for different applications can be facilitated by using different feedstocks. This may legitimately include the integration of hybrid energy systems for coal-to-carbon materials production. Proper characterization and quality control of carbon products derived from different coal feedstocks grow from documented understanding of coal feedstocks. For this, an updated, modernized coal database would be most valuable. The database would be able to correlate variable coal sources with production of high-carbon content products such as the following:

- Pigments, dyes, and optical brighteners
- Graphene composites
- Energy storage materials
- Electronics, touch panels, and displays
- Membranes
- Additives for polymers and construction materials
- 3D printing materials
- Carbon fiber materials.

From an economic perspective, coal-to-carbon materials have the potential for significant value-added carbon products, opening the way for new economic opportunities [13]. It is estimated that carbon fiber and structural composites value is $100,000/ton, 3D printing materials are $70,000,000/ton, and carbon nanomaterials are valued at $100,000,000/ton.

Process economics can be further enhanced by extraction of strategically important REEs from coal and coal by-products. Fly ash can have ~400 ppm REE, while coal has 60 ppm. The strata above and below coal seams (shales and clays) can have ~180ppm. Acid mine drainage water and drainage solids have 5 ppb and 500 ppb, respectively.

Development of applications in these areas would leverage ongoing research at NETL that is focused on conversion of domestic coal to low cost graphene inks and fluids, carbon quantum dots, graphene-enhanced cement, and engineered plastics.

Challenges and Opportunities

The development of IES technologies will encounter technical barriers that will have to be surmounted if the promise of IES-focused coal-to-carbon products is to be realized. Barriers include identification and development of materials for applications in harsh environments and for flexible operations (repeated operational cycling). An additional barrier is the need for development of new materials to improve efficiency and lower the cost of existing coal-to-products processes that are vitally important and that allow large-scale use of coal-derived carbon products. Another barrier is the implementation of advanced manufacturing, for the manufacturing of parts with complex geometries, and for producing functional materials that cannot be made with conventional processes.

Materials-Related Challenges

Development of new coal-to-fuels and coal-to-chemicals processes that significantly drive down processing and conversion costs will require materials innovation to enable exploration of hybrid energy systems with improved efficiency and sustainability. Particular interests include the development of high performance catalysts, next-generation membrane materials/separation technology, advanced manufacturing for modular reactors, and the utilization of cost-effective, clean energy inputs to improve these processes.

Specifically, materials are needed that are tolerant of extreme temperatures (>700°C), which would enable utilization of high-grade heat from nuclear sources. A salient example would be the development of thin sheet materials with enhanced mechanical/structural properties and excellent fatigue resistance at high temperature, which are capable of transferring heat from nuclear power plants while limiting efficiency losses. In addition, materials with extreme heat resilience are required for insulation. High reliability is required to ensure safety envelopes.

Hybrid energy systems will be compatible with the development of new coal-to-fuels/chemicals processes that significantly drive down processing and conversion costs and improve efficiency and sustainability. However, they are likely to function in a fashion characterized by frequent process cycling caused by variations in demand and generation, which imposes challenging operational environments on materials. Accordingly, materials specifically designed for flexible operations that can tolerate the frequent cycling in power plants are needed, specifically for electronics, composites, and membrane applications.

High performance, robust catalyst materials will be needed for coal-to-fuels and coal-to-chemicals processes. Catalysts capable of operating over ranges of temperature and feedstock composition will be required, which are tolerant of variability in concentrations of constituents that will poison catalyst activity.

It is likely that highly efficient membrane separations will replace energy-intensive thermal separation processes; however, this evolution will also result in needs for new membrane materials capable of functioning at high temperatures and with variable feed streams.

REE Extraction from Coal Challenges and Opportunities

Recovering the significant REEs from coal and fly ash presents significant processing, concentration, and separation challenges. Initial separation may involve high temperature processing, although recent efforts have involved electrochemical approaches conducted at near-ambient temperatures. Variations in the feedstock, and the potential for electrode poisoning suggest needs for robust materials that can function as electrodes in processes that enrich low concentrations of REEs derived from coal and coal by-products. In addition, development of separations processes for the individual REEs capable of functioning with extractant matrices is expected to be an ongoing challenge.

Advanced Manufacturing

The evolution of IESs for coal-to-fuels and coal-to-chemicals conversion will pose significant challenges that can be addressed via advanced manufacturing approaches. The materials that will be needed to function in extreme environments may be challenging or impossible to produce using conventional materials production methods. Particularly challenging objectives are composite materials and materials with complex geometries. Furthermore, it is likely that next-generation, modular reactors in particular may pose significant manufacturing challenges stemming from the need to fabricate unique shapes and sizes starting from the new material compositions. Scale-up represents another challenge, and identification of gaps between laboratory scale and industrial scale is needed for coal-to-products processes. In fact, optimal process scale has not been determined. It may be possible to leverage lessons learned from previous unsuccessful gasification projects to settle on an optimal scale, and the commensurate plant design.

It was noted that it would be highly advantageous to generate carbon materials from different coal feedstocks on a large scale. This observation points to additional challenges for advanced manufacturing processes for converting coal-to-high-value carbon materials that are derived from the fact that the composition of coal feedstock can be highly variable. However, it is possible that this might be leveraged to tailor different feed compositions to the production of specific materials. An additional challenge emerging from these considerations is the need to characterize the coal process feed, in order to inform the materials manufacturing process to be used.

Modeling/Computational Science/Data Analytics

Materials discovery will be guided by modeling and simulation. An overarching objective is to develop approaches for rational design of materials, enabling structure-property relationships. This represents a crosscutting issue common to many areas beyond Topic 5. One specific challenge is the need for a coal database that can inform coal-to-materials processes, which may require updated or modernized versions of existing coal databases or perhaps the evolution of new databases tailored to the needs of advanced manufacturing processes.

Approaches

New Materials Development

Research campaigns for identifying desired materials properties followed by synthesis and characterization are needed. Properties must be identified based on manufacturing environments that will be encountered. Rationalization and control of materials behavior under harsh environments will involve deep understanding of materials at the microstructural level, particularly at interfaces, so research that ranges from the fundamental level to applications space is needed. Materials research should be guided by computational approaches.

Rare Earth Element Extraction

The recovery of strategically important REEs from coal feedstocks has received significant attention at NETL, where boiler and baghouse/electrostatic precipitator operations are combined with selective catalytic reduction to optimize production of mixed rare earth concentrates. Multiple recovery techniques and optimum feed materials have been identified. These research efforts provide the basis for advanced REE extraction/recovery research, where compatibility with carbon materials synthesis and process optimization need to be emphasized.

Advanced Manufacturing

Advanced manufacturing research is needed to establish economically competitive, scalable processes that use coal feedstocks for producing high value products, particularly carbon materials and strategically important REEs. Processes identified will inform materials research, so that manufacturing processes that span a range of operating environments can be considered, including those performed under harsh or chemically aggressive environments.

Hybrid energy systems for gasification-based coal-to-fuels and coal-to-chemicals production should be investigated because if economical IESs are identified, scalable processes for generating high value carbon materials that are economically competitive with improved sustainability may result.

Impact

The emergence of coal-derived carbon products at a very large scale is necessary for the nation to fully use its abundant coal resources. Conceptually, the development of an economically viable coal value chain is achievable, given the emergence of processes capable of converting carbon materials to commercial applications (See Figure 6). Improving the economics of conversion of domestic feedstocks to carbon materials poses an ongoing set of challenges, but it is likely that these can be surmounted with focused R&D investment. Achieving this goal will reinvigorate the coal industry in a sustainable fashion compatible with protection of the environment and will avail the U.S. of a carbon source critical for development of next-generation materials and advanced manufacturing processes.

Finally, REEs can be extracted profitably from coal, if challenges can be met, for example, enrichment of low concentration of REEs in coal and coal by-products and efficient REE separation processes.

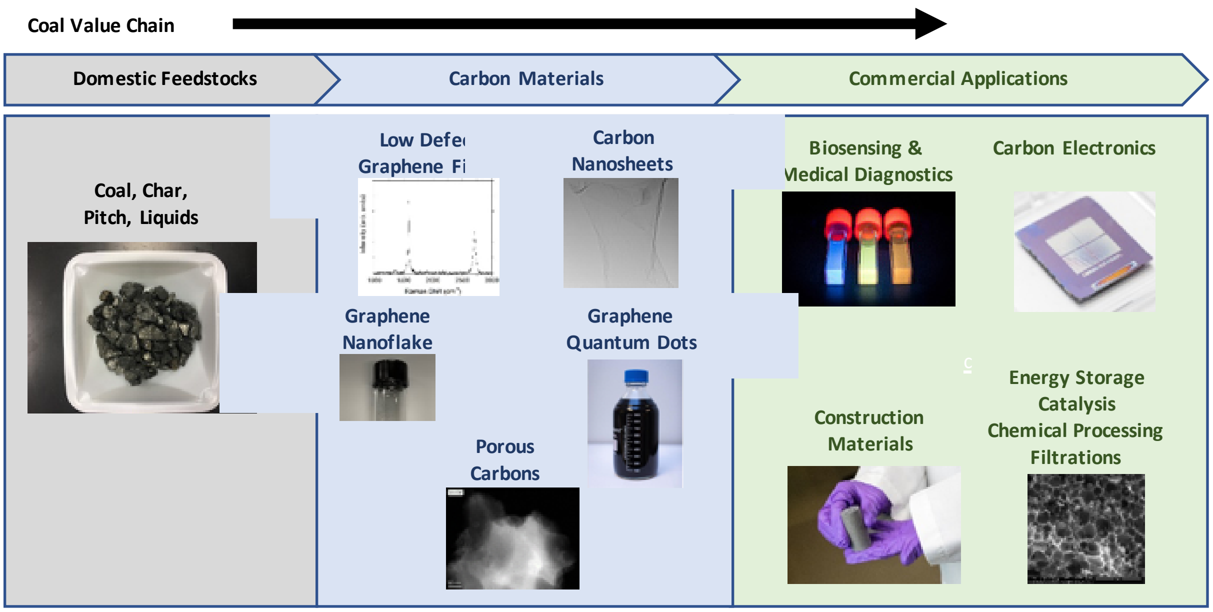

Figure 6. Representation of coal value chain to make carbon-based materials leading to high value commercial applications (Source: NETL).

Breakout B: Materials Research Needs/Gaps

While the objective of the first day was to discuss materials development needs relative to the five use cases, the second day Breakout B sessions were focused on relevant R&D gaps pertinent to these use cases. The workshop was divided into groups to discuss and list the gaps. Subsequently, the workshop participants grouped the R&D needs into common themes—or subjects—in order to align the needs with lab capabilities. The intent was to provide the lab and DOE Program Offices with a better understanding of how the Tri-Lab can address the technical development challenges to accelerate technology development, validation, and demonstration.

Group Questions

To begin Day 2, the participants formulated a set of questions to consider during the group discussions. The following significant comments were captured:

- How can the Tri-Lab use or transfer ongoing materials development and apply it to the use cases?
- How is materials development applied to manufacturing, whereas laboratory research generally focuses on grams (maybe up to kilograms) but materials for practical uses and manufacturing are performed on the scale of tons of material?
- How should developers and end users be involved in resolving material gaps?
- Given the wide range of R&D needs, what are the highest priorities?
- What capabilities might need to be established to address the highest priorities?
- How can sensors be applied to manufacturing as well as materials health monitoring to prolong the life of materials used in harsh environments?

As an example, the DOE STEP (DOE-FE Supercritical Transformational Electric Power) project was a multi-program use case. Several of the capabilities of this program were noted as being transferable to the five use cases.

Next, the workshop affirmed or formulated consensus around the common research needs as follows for materials manufacturing:

- Development of materials for harsh environments, addressing materials durability, and multifunctional materials
- Manufacturing/qualification should be divided into three main categories, namely near-term, mid-term, and long-term, with three temperature ranges for each category: low (<200°C), medium (<600°C), and high (>800°C)
- Application of artificial intelligence through integrated computation materials engineering to support materials scale-up
- Scale-up of manufacturing pilot plants can serve as a focal point for each project; integrated materials inspection and rapid analysis techniques can help increase manufacturing rates
- Development and use of sensors for harsh environments for materials health monitoring as well as process conditions monitoring.

Scale-Up

As noted, the workshop identified a strong need in materials manufacturing and scale-up. The theme is addressed in detail here to capture the comments and input provided during the workshop.

Scale-up can enable a foundational understanding of the manufacturing challenges in all five topical areas. Many materials that are developed using manual steps in a laboratory eventually must be transferred to mechanized equipment to produce large-sized components that are mass manufactured.

Hence, a scale-up manufacturing pilot plant can serve as the focal point for each project; integrated materials inspection and rapid analysis techniques can help increase manufacturing rates.

Laboratories need to anticipate and address problems that will occur during scale-up; however, this is difficult because the problems can be hard to foresee. Laboratory work must connect with industry and must ensure that research focuses on processes that are scalable and marketable. Industry input and perspective are essential to guide research to meet these requirements and to deploy new technology in industrial demonstrations. Establishing a scale-up manufacturing demonstration/pilot plant, such as an industrial user facility, would be beneficial to the laboratories and industry. Prototypes of complete systems would demonstrate to customers the interactions between system components. Such systems should be modular so that the prototypes can test multiple options (e.g., swap new membranes in and out). In addition to materials aspects (e.g., metals, ceramics, and polymers), a scale-up manufacturing facility could include testing new instrumentation to better monitor operations and processes. A critical aspect of scale-up is integrating multiple systems, and new challenges often arise at the subsystem interfaces. A modular scale-up manufacturing demonstration/pilot plant would allow researchers to find and resolve interface problems that cannot be identified by focusing only on individual parts. Scale-up further allows for qualification procedures to be examined (such as non-destructive examination [NDE] methods).

Funding levels from DOE and industry would determine the scope of the scale-up. If funds are limited, laboratories would likely limit R&D to metals, which are universally useful to all energy industries. Key items that are important for all materials (e.g., metals, ceramics, and polymers) include automation, instrumentation, qualification, and cybersecurity (see Figure 7).

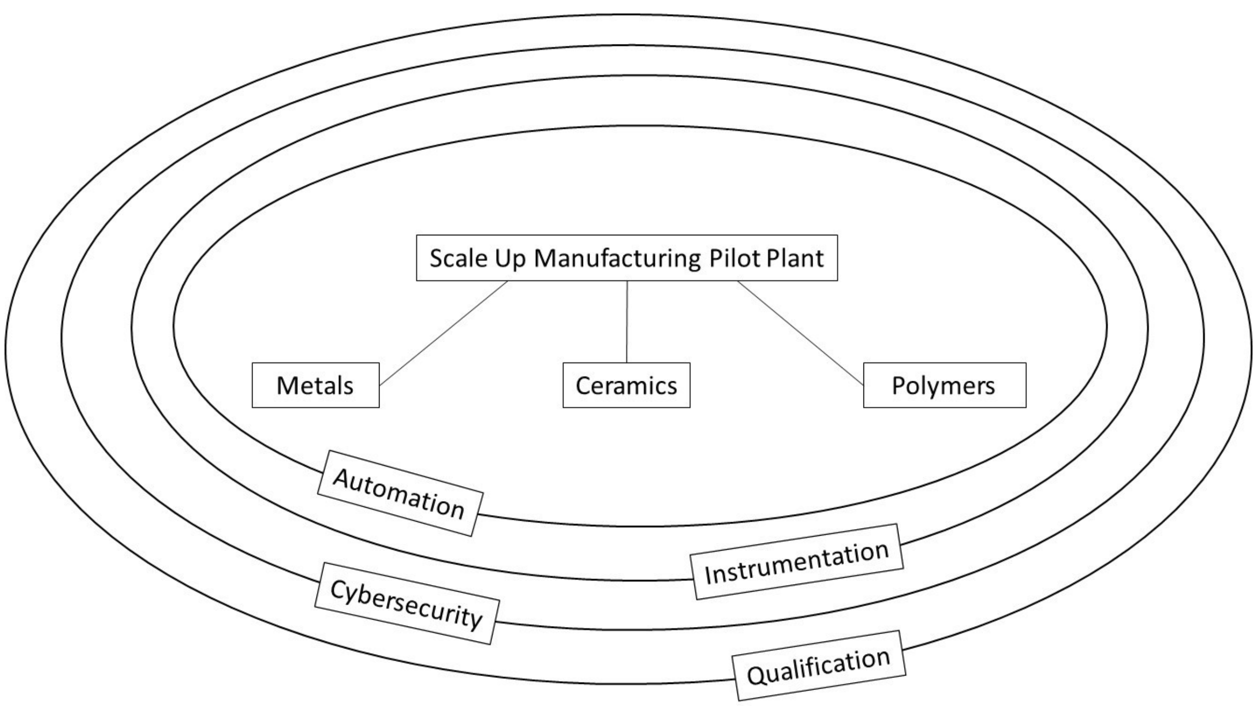

Figure 7. Key items that are important for all materials (e.g., metals, ceramics, and polymers).

Instrumentation/Sensors

Given the relevance of the development of instrumentation for integration with materials, the following section captures workshop comments and descriptions of lab capabilities that are applicable to this subject.

INL has in-pile testing and demonstration capabilities as a part of the DOE-NE Advanced Sensor and Instrumentation (ASI) program, which evaluates a variety of sensors/instrumentation for harsh environments (nuclear test reactors). ASI considers both passive and active sensors, falling into both traditional and novel sensors designs. Capabilities include melt wires, thermocouples, dosimeters, strain gauges, optical (laser based) measurements, and ultrasonic measurements. The following is a look at some of the resident advanced manufacturing techniques at each of the Labs:

NETL is working to develop in-situ measurements such as chemical measurements through optical (laser) methods. NETL is also working to incorporate fiber optics. In addition, NETL supports DOE-FE with research on emissivity control in the design of materials (i.e., a material reflects when thermal energy is to be stored and permits waves to pass through when there is a desire to transfer heat).

NREL has experience with high temperature electronics, instrumentation, and diagnostics associated with the electric grid, solar panels, wind nacelles, and wind towers. Capable of large complex component design, NREL has extensive experience in automotive applications and design of complex flow paths. These approaches pursued by NREL typically work on a small scale, particularly for additive parts. ARPA-E work at NREL consists of working with a company to scale-up microwave processes.

Printed sensors are of interest to all three laboratories. INL is working in this arena; NETL is pursuing laser sintering, and NREL is using microwave sintering and inkjet printing. INL is currently working to develop larger scale systems (new Spark Plasma Sintering [SPS] system is coming, and possibly some work in wire-fed additive processes).

Materials Testing Research Platforms

The workshop discussed the importance of clarifying industry needs; however, from a research perspective, it was decided that it may be best to build a prototype for industry and have them come test the prototype designs. These research platforms allow the materials to be tested under realistic conditions that include high temperature thermohydraulic conditions, reacting chemical environments, and duty cycles. It is beyond the scope of this workshop report to describe these facilities. Only a cursory description is given here to underscore the capabilities relative to the needs of materials manufacturing, scale-up and testing in real-time, harsh environments, and IESs:

- NETL HyPer Laboratory—dedicated to testing fuel cells, gas turbines, and hybrid fuel cell/gas turbines and reversible fuel cells/electrolysis cells
- NETL Reaction Analysis and Chemical Transformation (ReACT) Facility—applicable to direct and indirect heating and conversion of carbonaceous fuels and feedstocks to higher value carbon fuels
- The Carbon Materials Manufacturing Facility (CaMMF)—applicable to develop manufacturing processes to convert carbon materials (coal, natural gas, biomass, and plastic consumer waste into high value carbon materials)
- NETL Advanced Alloy Development Laboratory and Severe Environment Corrosion and Erosion Research Facility (SECERF)—dedicated to the development of affordable and durable alloys for harsh environments
- NREL ARIES Campus—inclusive of the Energy Systems Integration Facility for testing materials used in concentrating solar operations, hydrogen production, and dispensation/distribution
- NREL Biomass Conversion Laboratory—applicable to testing materials used in hybrid carbon conversion unit operations
- INL IES Laboratory—dedicated to the development and testing of thermal energy generation, storage, distribution, and application, including high temperature steam electrolysis

- INL Advanced Manufacturing of materials—applicable for harsh environments, including an industrial-scale Electrical Field/SPS.

Specific Materials Research Needs and Gaps

Detailed materials research needs and gaps were developed by breakout sessions participants with subject-matter leads attending the workshop. The goal was to identify materials needs for these five predetermined use cases. Participants were encouraged to consider (1) the specific materials needs; (2) the environments in which the materials are expected to be used, including temperature ranges, pressure, chemical environment, and pressure as well as any cost constraints; and (3) function(s) of the materials for interest, whether structural or functional. The main outcomes of these group meetings are tabulated below (see Tables 4 through 8).

Table 4. Materials needs for TES for Topic 1: Transport and carbon utilization.

Materials Functions	Heat carrier: Low cost, high energy density, high heat Capacity (Cp), ΔH latent, reversibility, high materials stability, good thermal conductivity (K), and good thermal, and chemical stability Containment materials: Good heat transfer properties, good structural properties, good corrosion resistance properties, good thermomechanical degradation resistance, >750°C, ability to withstand thermal cycling Operating window of room pressure: 30 MPa, Ni-based material
Operating Temperature	>300°C; >750°C
Containment Materials	Types of materials: Alloys, ceramic, heat transfer needs (insulative, conductive), chemical degradation-stress corrosion cracking, thermomechanical degradation, P, T, ΔT, ΔP-creep, fatigue, stress relaxation resistance above 700°C- extent of thermal cycling, pressure stress-rating of 25–30 MPa, cost, size of TES-amount of material needed (T >300°C, TES), corrosion resistant erosion resistance, high energy density (P, Cp, ΔH), low/affordable cost, high thermal conductivity (K), stability cyclability (charge/discharge), chemical stability Material Environments: Operation includes liquid gases and solids (molten salts, Na, sCO_2, particle oxides) as well as thermal and chemical stability.

Table 5. Materials needs for Topic 2: Low temperature thermal energy carbon utilization.

Operating Temperature	20–200°C
Pressure	Low pressure

Specific Materials Characteristics	Efficient heat transfer of metallic and alloy material, coating materials, degradation, and corrosion resistant/easy manufacturing/design/modeling, low cost Heat upgrading pump: metal, metal oxides, catalyst performance Phase-change materials (20–200°C) Thermal-electrical materials (e.g., semiconductors, conductive polymers).

Table 6. Materials needs for Topic 3: Supporting renewables, nuclear, fossil generation, and supplying hydrogen markets.

Operating Temperature	Low Temperature Environment: 60–90°C, acid-base, high E >1.8V
Catalyst Materials	High selectivity, high durability, catalyst support materials, cost (low loading and PGM-free), conductivity, durability, crossover, membrane (acid and base) Porous transfer layer/GDL-carbon (Pt-Ti), low cost, high durability interfaces Material integration: deposition method, scalable
Operating Temperature	High temperature environment: 700°C–1000°C
Operating Conditions	High temperature electrolysis (one-way and reversible) Fuel side hydrogen, steam (H_2O), Oxygen/air side
Material Types Needs	Oxides, metals
Anticipated Material problems	Degradation at interfaces, interconnects, corrosion Balance of plant (heat exchangers, blowers, fuel cleaning, contaminants) sulfur
Solutions/Approaches	Modeling of degradation, increased material/cell stability, in-operando analysis, improved post-mortem analysis.

Table 7. Materials needs for Topic 4: Low-carbon-energy powered CO_2 utilization for fuels and products.

Operating Temperature	Seals for low temperature (60°C) and high temperature (800–1000°C)
Applications	Microbes-bio electrochemical compatibility, bioreactor materials, mass transfer limits (note: when CO_2 is converted to C-C bonds, then product separation) Example reaction mechanism: CO_2 + hydrogen + e- » CH_i » -C-C-
Materials Needs	Membrane development-electrochemical, structural (printed circuit boards).

Table 8. Materials needs for Topic 5: Supporting hybrid carbon conversion.

Operating Temperature	High temperature (plasma process; >1000°C) thermal transfer from nuclear reactor to drive process
Operating Environment	High temperature processing >700°C, materials that function at, coal gasification/hydrogenation, manufacturing, qualification Dealing with contamination-coal specific (by-products from gasification): gaseous and solid-catalyst deactivation Separation of downstream products, process specific.

Second Categorization Results

At the conclusion of this breakout meeting, participants were asked to further define materials development needs based on material types envisaged for the identified research needs listed in the first categorization session, operating temperature ranges, media the materials and components will operate in, type of material(s) that will resist and how material(s) performance will be evaluated, what materials performance verification is required, type of innovation is required to develop this material, and capabilities of each laboratory to contribute to materials development, performance, and verification. Tables 9, 10, and 11 capture the main points noted during the breakout sessions. These tables list possible materials of interest, but they should not be considered comprehensive or even priorities.

Notably missing is the temperature range of 200-300°C. This range simply does not fall within the five use cases of the workshop.

In most cases, candidate materials are already available for high temperature service applications. However, they may not be code-qualified for IES applications. For example, codification of alloys for the very high temperature of a helium gas cooled reactor under the Next-Generation Nuclear Plant (NGNP) focused on Alloy 617, a nickel-chromium-cobalt-molybdenum alloy having an exceptional combination of high temperature strength and oxidation resistance. DOE invested about $15 million at INL, Oak Ridge National Laboratory, and Argonne National Laboratory over the span of 12 years to prove Alloy 617 is suitable for high temperature advanced reactor concepts. The concerted effort showed Alloy 617 can withstand operating temperatures of 950°C—nearly 200°C hotter than the next best material. The American Society of Mechanical Engineers subsequently added this alloy to its Boiler and Pressure Vessel Code—the first to be added in 30 years. The question that now arises is whether this alloy is suitable for the molten salts being developed for high temperature nuclear reactors and TES. If not, then the Tri-Lab may reconstitute the type of capabilities put to work under the NGNP program.

The Tri-Lab can collectively examine thermophysical properties of metals and ceramics. They are equipped to address metal fatigue cycles and creep behavior, microstructural evolution, and corrosion phenomena. Under existing and developing advanced manufacturing capabilities, the Tri-Lab can also lead both traditional metals-oxide materials tape-casting and additive manufacturing methods as well as the testing of heat treating and joining procedures.

Table 9. High temperature materials (1,000°C Class) needs.

Materials Type Desired	1. High Nickel alloys (e.g., Ni/Cr in stoichiometries with Mo, Co, Nb) Besides Alloy 617 (qualified for use up to 950°C for helium gas), Nickel Inconel 718 (melting temperature of

	1260-1336°C) is used for a wide range of applications, such as liquid-fueled rockets, rings, casings, various formed sheet metal parts for aircraft and land-based gas turbine engines, cryogenic tankage, and for fasteners and instrumentation parts. 2. Tungsten-based alloys, in stoichiometries Ni, Fe, Cu; as tungsten-carbide; and tungsten titanium-carbide composites Tungsten is becoming an important element in future alloys. Whether tungsten alloys can be extended to very high temperature applications is unknown. Newer tungsten titanium-carbide composites are becoming available, which have increased hardness and high temperature strength compared to traditional carbides. There is also current research on creating radiation-proof alloys, and there has been some success with a tungsten-tantalum-vanadium-chromium alloy. Tungsten nickel iron alloys have a low expansion coefficient useful for glass-to-metal seals and possess high moduli of elasticity, which makes them resistant to elastic deformation. These alloys are perfect for radiation shielding, as its high density matched with its radiation resistance are ideal for protective components. 3. Ceramic Material, including alumina compounds, silicon compounds and zirconia compounds, alumina compounds, and metals carbides Alumina (Al_2O_3) provides the basic structure for most high temperature, high refractory service requirements. It is resistant to molten slag at temperatures over 1300°C for use in lime kilns and coal gasifiers. It can be toughened with aluminum and zirconium as a composite ceramic material with zirconia grains in the alumina matrix. Silicon carbide (SiC) offers increased operating temperatures for use in combustion systems as ignitors for pilot lights, as bayonet tube process heaters, for heat treatment of metals, float glass production, and production of ceramics and electronics components, among other applications. SiC is a primary ingredient of TRISO-coated nuclear fuel particles. It helps provide structural support of the fuel particles and serves as the main diffusion barrier. SiC heating elements are rates to temperature as high as 1600°C. Silicon nitride (Si_3N_4) is another ceramic that is commonly used for air heating elements, given its resistance to oxidation, high thermal shock resistance,

	high electric insulation, and thermal conductivity. It has a maximum application temperature of 1200°C in air. Because it is resistant to both acid and alkali corrosion, it may be a good candidate for emersion in molten salts and high temperature gas mixtures. It is currently used widely in petrochemical industry fired-heaters and electrical heaters. 4. Ultra-high temperature ceramics, including stoichiometries of SiC, zirconium carbide, zirconium boride, and Hafnium nitride The development of high temperature materials by the aerospace industry remains largely untapped for high temperature energy applications. Though systematic investigation of the refractory properties of binary ceramics, the Air Force Materials Laboratory discovered that early transition metal carbides, borides, and nitrides have exceptionally high thermal conductivity, resistance to oxidation, and good mechanical strength. One key is matching the thermal expansion properties to metallic equipment pieces and vessels. For example, of these, ZrC, ZrB_2, HfB_2, in composites containing approximately 20 percent volume SiC were found to be the best performing. All of these ceramics are stable and exhibit melting points ranging from 2800 to 3400°C. 5. Cerium/cerium oxide is used for two-step thermochemical production of hydrogen. For the first step, cerium (IV) oxide is thermally dissociated in an inert gas atmosphere at 2,000°C (3,630°F) into cerium (III) oxide and oxygen.
Operating Environment/Media	Combustion environments, particulate-bearing, high pressure, hot gases, low-volatile molten salts, and molten metals Glass and refractory manufacturing Advanced nuclear fuels fabrication Temperature boosting of thermal hydraulic fluids for heat storage and transfer Thermochemical water-splitting hydrogen production
Materials Characterization/Performance Requirements	Photon transfer: Thermochemical resistance/stability, thermal conductivity, CTE mismatch minimization, chemical resistance, corrosion resistance, high strength, fracture toughness, excellent thermal properties, microstructural stability, scalability

Materials Verification/Materials Innovation Required	Cost analyses, creep/creep fatigue testing capabilities, mechanical testing, corrosion testing (high temperature accelerated) Materials fabrication by additive and subtractive manufacturing.

Table 10. High temperature materials (500 to 1000°C Class) needs.

Operating Temperature	500–600°C, 700–1,000°C
Materials Type Desired	Ceramics, composites, steel, membranes, catalysts 1. Most of the high temperature alloy materials presented in Table 9 have relevance to the 500–1,000°C range. This temperature range shares the requirements of corrosion resistance, and materials strength uses with molten salts, hot gases, and supercritical steam as well as ultra-supercritical equipment, vessels, and power cycles. Power systems and heat transport in the range of 500–600°C may not require high nickel alloys but may require special alloys to manage corrosion, thermal cycling, and high pressure boundaries. 2. Solid-oxide zirconium oxides with stabilized yttrium, scandium, and lanthanum stoichiometries as well as barium oxides and lanthanum oxides stabilized with cerium and yttria and gadolinium. Solid-oxide fuel cell and electrolysis cell electrodes and electrolytes that formulated to the multi-physics of catalysis, ion transport, and electrical and thermal conductance. 3. Perovskite is a class of compounds having a crystal structure such as $CaTiO_3$. Many different cations can be embedded in this structure, allowing the development of diverse engineered materials. Besides its use in photovoltaics as superconductors, zirconium and titanate perovskite can be applied to ceramics for radioactive waste immobilization. 4. High temperature inorganic membranes for chemicals separation at reactor conditions above continues to be a frontier for IESs. Early research has focused on alumina membranes at temperatures up to about 600°C. Now, zeolite membranes for

	applications in water-gas shift membrane reactors are under development. 5. Catalysts for high temperature and harsh environments continued to be pursued for unit operations such as the water-gas-shift reactions, steam cracking of hydrocarbons, catalytic combustion, and acid gas dissociation. Catalytic combustion that can be carried out over a wide range of fuel concentrations in air and at low temperatures (as an alternative to conventional thermal combustion) has received considerable attention during the past decade. Research efforts have been promoted by the need to use energy sources more efficiently and to control pollutant formation that occurs at high temperature. Perovskites, cerium-oxides, nickel, and alumina-based catalyst remain as contenders for catalytic combustion. Many of the thermochemical looping reactions used to produce hydrogen involve the dissociation of an acid at temperatures above 500°C. Low pH environments include sulphuric and hydrochloric conditions.
Operating Environment/Media	Steam, molten salts, liquid metals, high temperature gases used in TES H_2 and O_2 production and compression Solid-oxide fuel cells and electrolysis cells Catalytic combustion and product separations
Materials Characterization/Performance Requirements	Contamination resistant, corrosion resistance, degradation synergy resistant, optimum surface reactivity, gas tight, hydrogen embrittlement resistant, oxygen resistant Mechanical strength, thermal cycling, and creep tolerance Low microstructure evolution and low element migration
Materials Verification/Materials Innovation Required	Thermal properties enhancement for media and material discovery (e.g., data mining/analytics, design/modifications, aging studies) Materials fabrication by additive and subtractive manufacturing.

Table 11. Low temperature materials (200°C Class) needs.

Operating Temperature	Low temperature (< 200°C)
Materials Type Classes	Polymeric, membranes, catalysts, PGMs, Ni, Fe, MOFs, catalyst supports
Operating Environment/Media	Aqueous, organics, ionic liquids, salt hydrates, solids, PCMs Electrochemistry, pH variation, 1,000 pounds per square inch (psi)
Specific Materials Characteristics Required	e-conductive.

The Tri-Lab is well positioned to address the R&D needs that were identified. In particular, the current capabilities (not an exhaustive list) are in place to investigate the following materials development challenges:

- Alloy development (ingot metallurgy to 300-pound ingots)
- 3D printing and SPS for nuclear fuels and solid-oxide composite layers
- Roll-to-roll manufacturing (NREL is a member of the EERE R2R Consortium)
- Thermal-mechanical processing capabilities for producing experimental and custom alloys
- Measurement of thermophysical properties, thermomechanical behavior, and microstructural changes
- Performance assessment capabilities (e.g., creep, fatigue, fracture mechanics, corrosion, and electrochemistry)
- Membrane design fabrication and evaluation in simulated service environments
- Catalysts design, testing and up-scaling
- Materials modeling and simulation capabilities (atomic level through continuum level; e.g., ab-initio, Phase-Field, and Density Functional Theory)
- Metabolic engineering and synthetic biology.

Integrated Computational/Materials Engineering

Breakout Session B, Topic 3 covered the perceived needs and opportunities related to computational modeling across a wide range of materials development and performance parameters. Referred to as ICME, this research approach combines multi-scale materials modeling with fabrication and testing outcomes to optimize the composition and fabrication methods of materials to achieve specific materials performance objectives.

Common themes that emerged were a uniform need across projects for additional computational work at multiple scales (e.g., atomistic, device/component, and systems-level models). The session participants identified five specific needs/opportunities: (1) increased computational throughput without losing accuracy, (2) computational materials performance, (3) cross-scale integration, (4) shared computational tools and protocols, and (5) examples of near- and long-term incorporation of computational models with near- and long-term outcomes that have important impacts.

Possible suggestions for addressing increased computational throughput without losing accuracy included coupling DFT with molecular dynamics simulations as well as neural networks and machine learning approaches. The ability to model and predict materials performance includes structural evolution over time (corrosion/degradation [micro and bulk], tightly coupled experimental validation, and lifetime prediction) and lifetime predictions (in years). Computational models need to be validated with experimental data as a third area needing improvement. These models include synthesizing and characterizing model structures, accelerated degradation testing, and structural and chemical properties. Finally, a shared dataset for data mining/machine learning was identified as a key need regarding both computational modeling and experimental validation.

The ability to combine models between micro (atomic) and macro scales was identified as a critical need. This would provide the ability to extend atomic level DFT calculations to device/component and even to systems level. For example, predicting the performance of a system based on fundamental surface processes:

- "Data Fusion"
- Device/component level up to systems-level efforts are needed for consensus analysis between scales
- Iterative process where data from different modeling scales informs/revises/improves calculations at the other scales
- Coupled with Item 2 to identify operational environments/conditions that allow realistic computational materials performance modeling/testing.

Another critical area identified was the need for standardized models, computational structures, data reporting protocols, and modeling tools across all three laboratories. This would allow consistent results, analysis, and data sharing. Additionally, combining computational capabilities between the three laboratories (viz., high performance computational resources and laboratory-developed multi-physics solvers) would greatly increase computational capabilities and throughput. Examples of near- and long-term incorporation of computational modeling with near- and long-term impacts are detailed in Table 12.

Table 12. Examples of near- and long-term outcomes of ICME.

Research Need	Near-Term	Long-Term
Improving energy systems efficiency through thermal energy storage	Materials design, selection, and fabrication methods for corrosion mitigation for harsh environments Identified gaps lead to longer-term R&D (mid to long range) AST and code-qualified materials	New materials and manufacturing methods available and being used in pilot demonstration projects Materials for high temperature gas heat transfer; for example, CO_2, He, and H_2
Improving H_2 production and storage materials longevity, costs, and safety	Modeling results for environmentally induced embrittlement and stress cracking in H_2 transport and storage materials	Understanding long-term corrosion costs on an H_2 economy
Low temperature heat capture and concentration	Low cost materials, surface conditioning, coatings, and media for more efficient heat transfer and concentration	Enhanced low temperature heat recuperation Radiative energy concentration and photovoltaic technology enhancement

Concluding Remarks

The information generated by this workshop is considered preliminary and is far from being comprehensive. As such, it identifies both general gaps and specific research activities in material development, testing, and IES applications that need to be addressed beyond typical industry applications. New process innovations in electrochemistry, chemical looping reaction, thermal energy delivery and storage, hydrogen production/transport/storage, and radiation-induced chemical reactions are some emerging energy conversion and use technologies that require materials development, fabrication, and manufacturing scale-up. Multifunctionality of materials is often required. Understanding thermal, electrical, and mass transport in these media is essential to the development and optimization of these materials. Understanding microstructure evolution over time requires AST, which can be accomplished through integrated computational/experimental materials development.

Tri-Lab is in a good position to tackle the materials development and testing challenges of IES that will advance materials requirements. The labs, collectively, are well-grounded in materials development, testing, and manufacturing across the spectrum of needs identified in the workshop. Additionally, the labs have appropriate testing capabilities to qualify the materials under real-time conditions.

Heat transfer and chemical reaction applications with harsh environments above present needs and opportunities for crosscutting DOE program materials development, testing, and code qualification. High nickel alloys, advanced refractories, and hybrid or composite materials need to be developed. Research that is currently in progress by Tri-Lab can be leveraged to address these needs. High throughput materials fabrication and materials joining also need to be addressed for the new materials.

At the bottom end of the spectrum, there is an opportunity to harvest and utilize low temperature heat through the develop of materials and systems that can cost-effectively capture and possibly concentrate or amplify this heat.

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APPENDIX A—WORKSHOP AGENDA

Optional Tours: Wednesday, July 31, 7:30 a.m. – 12:00 p.m. Materials & Fuels Complex Facilities
Transportation to be provided by meeting organizers.
Thursday, August 1, 3:00 p.m. – 5:30 p.m. INL Research Center
Energy Systems Laboratory, Systems Integration Energy Innovation Labs

Day One: Wednesday, July 31, 2019		
Optional Tour of Materials & Fuels Complex Facilities		
Willow Creek Building (WCB) | 1955 Fremont Ave | Idaho Falls, ID		
6:45 AM	Badging (for those participating in MFC tours)	Jeff Aguiar, INL
7:00 AM	Depart for MFC	Jeff Aguiar & Seongtae Kwon, INL
Materials & Fuels Complex (MFC)		
8:00 AM	MFC Entry and Dosimetry Briefing – Till Conference Room	Jordan Mclaughlin, INL Doug Crawford, INL
8:20 AM	Brief MFC Overview – Till Conference Room	
 8:30 AM 9:30 AM 10:15 AM	Group One: Hot Fuels Examination Facility Irradiated Materials Characterization Laboratory Advanced Fuels Facility	Jesse Bean, INL Brandon Miller, INL Tim Hyde, INL Brandon Miller, INL Tim Hyde, INL Jesse Bean, INL Jeff Aguiar & Seongtae Kwon, INL
8:30 AM 9:15 AM 10:00 AM	Group Two: Irradiated Materials Characterization Laboratory Advanced Fuels Facility Hot Fuels Examination Facility	
11:00 AM	Return to WCB	
Willow Creek Building (WCB) | 1955 Fremont Ave | Idaho Falls, ID		
12:30 PM	Badging (for those who have not already badged in from MFC tours)	
Energy Innovation Laboratory (EIL) Meeting Center | 775 University Boulevard | Idaho Falls, ID		
1:00 PM	Welcome	Mark Peters, Director, INL
1:15 PM	Overview of the Tri-Laboratory Consortium	Shannon Bragg-Sitton, INL Tri-Lab Lead
1:30 PM	Review of Tri-Laboratory Project Proposals • Goals/objectives • Risk elements • Challenges, R&D needs • High-level technoeconomic assessments • Potential sponsors and advocates	Randy Cortright, Tri-Lab Leadership Team, NREL

2:00 PM	Summary of outcomes from the Tri-Lab Modeling and Analysis Workshop hosted by NETL	Peter Balash, Tri-Lab Leadership Team, NETL

2:15 PM	**Materials Perspective and Applied Laboratories' Ongoing Activities** (focus on key capabilities to support the demonstration projects); 30 minutes each • INL • NREL • NETL Highlight laboratory capabilities and expertise that can be leveraged to support materials development, characterization and testing activities for the proposed tri- laboratory projects.	Jeff Aguiar/Matthew Kerr, INL Judith Vidal/Todd Deutsch, NREL David Alman, NETL
3:55 PM	Break	
4:00 PM	Breakout A: Materials Challenges (presentations followed by breakout groups to identify challenges and R&D approaches) Determine materials development, manufacturing, and qualification/codification approaches relative to energy sources and technological advancements. Breakout Sessions will be divided into discussions covering the five project proposals	Moderators: Topic 1: Judith Vidal, NREL Topic 2: Richard Boardman, INL Topic 3: Daniel Ginosar, INL Topic 4: Randy Cortright, NREL Topic 5: Conjun Wang, NETL
5:30 PM	Close of Day 1, guidance for Day 2	
6:00 PM	No Host Dinner for Breakout Moderators/Note Takers/Facilitators	

Day Two: Wednesday Aug. 1, 2019		
EIL Meeting Center | 775 University Boulevard | Idaho Falls, ID		
8:00 AM	Continental Breakfast	
8:30 AM	Recap of Day 1 and Overview of Day 2	Shannon Bragg-Sitton, INL
8:40 AM	Out brief of Breakout Meetings and Discussion	Topic 1: Judith Vidal, NREL Topic 2: Richard Boardman, INL Topic 3: Daniel Ginosar, INL Topic 4: Randy Cortright, NREL Topic 5: Congjun Wang, NETL
9:15 AM	Framing Discussion for Breakout B Having discussed current challenges methodologies for materials research, development, production, and supply, the workshop will break down the R&D needs and gaps relevant to each proposed project. Research priorities should be determined and a general path leading to demonstrable outcomes will be developed	Anne Gaffney, INL David Alman, NETL
9:45 AM	Break	
10:00 AM	**Breakout B: Materials Research Needs/Gaps** Identified materials challenges will be grouped into overarching categories. Breakout groups will identify research gaps needed to address materials challenges and identify areas where labs can collaborate on research to mitigate these gaps. Specific breakout groups will be based on grouped challenges identified on Day 1. Possible categories could include: • Materials for harsh environments, including materials durability, multifunctional materials • Advanced manufacturing methods, materials joining • Testing and qualification; embedded sensors, quality and assurance, etc.	Moderators: Gabriel Ilevbare, INL Panos Datskos, NREL Doug Kauffman, NETL
12:00 PM	Working Lunch	
1:00 PM	Outbrief of Breakout B	Gabriel Ilevbare, INL Panos Datskos, NREL Doug Kauffman, NETL

1:30 PM	Group Discussion: Establishing a Path Forward for Materials R&D • Identify potential DOE and industrial sponsors for programmatic funding, Lab Calls, Industry FOAs • Identify specific research collaborations that will be pursued • Identify other laboratories and organizations that should be invited for project specific R&D and projects	Moderators: Richard Boardman, INL David Miller, NETL
3:00 PM	Closing/Introduction of Post-Workshop Survey	Shannon Bragg-Sitton, INL
3:15 PM	Break	

Optional Tours of In-Town Facilities		
INL Research Center (IRC) | 2351 North Boulevard | Idaho Falls, ID		
3:30 PM	Carbon Characterization Lab	Will Windes, INL
3:40 PM	The Creep and Mechanical Testing Labs	Thomas Lillo, INL
3:50 PM	The Laser Lab	Robert Schley, INL
4:00 PM	The High Temperature Environmental Testing Labs	Michael McMurtrey, INL
Energy Systems Laboratory (ESL) | 750 University Boulevard | Idaho Falls, ID		
4:15 PM	Systems Integration Laboratory	Jim O'Brien/Victor Walker, INL
Energy Innovation Laboratory (EIL) | 775 University Boulevard | Idaho Falls, ID		
4:45 PM	C111 Transient Kinetic Surface Characterization	Yixiao Wang, INL
5:00 PM	C212 Electroceramics development and testing	Dong Ding, INL
5:15 PM	B207 Human Systems Simulation Laboratory (HSSL)	Ron Boring, INL
5:30 PM	B314 Electrochemistry Lab	Tedd Lister, INL

APPENDIX B—TRI-LAB WORKSHOP ROSTER

Assigned Topics	
Alex Abboud	INL
Zia Abdullah	NREL
Harry Abernathy	NETL
Jeff Aguiar	INL
David Alman	NETL
Robert Bell	NREL
Pralhad Burli	INL
Randy Cortright	NREL
Jordan Cox	NREL
Doug Crawford	INL
Panos Datskos	NREL
Dayna Daubaras	INL
Todd Deutsch	NREL
Dong Ding	INL
Huyen Dinh	NREL
Jill Engel-Cox	NREL
Bob Fox	INL
Dan Ginosar	INL
Michael Glazoff	INL
Gregory Hackett	NETL
David Hopkinson	NETL
David Hurley	INL
Junhua Jiang	INL
Joshua Kane	INL
Douglas Kauffman	NETL
Ross Kunz	INL
Victor Kusuma	NETL
Seongtae Kwon	INL
Shiwoo Lee	NETL
Robert Leland	NREL
Boryann Liaw	INL
Thomas Lillo	INL
Daniel Maloney	NETL
Michael McMurtrey	INL
Gorakh Pawar	INL
Magdalena Ramirez-Corredores	INL
Ibrahim Reda	NREL
Mark Ruth	NREL
Debbie Sandor	NREL
Fred Stewart	INL
Bjorn Vaagensmith	INL
Isabella Van Rooyen	INL
Judith Vidal	NREL
Yixiao Wang	INL
Congjun Wang	NETL
Christina Wildfire	NETL
William Windes	INL
Keith Wipke	NREL
Richard Wright	INL
Margaret Ziomek-Moroz	NETL

Unassigned	
Douglas Arent	NREL
Peter Balash	NETL
Richard Boardman	INL
Shannon Bragg-Sitton	INL
Todd Combs	INL
Regis Conrad	DOE
Carl Friesen	DOE
Anne Gaffney	INL
Gabriel Ilevbare	INL
Susan Lesica	DOE
Linda McCoy	DOE
David Miller	NETL
Mark Peters	INL
John Yankeelov	DOE

Pinching Maness	NREL
Colin McMillan	NREL

Tour Guides	
Ron Boring	INL
Heather Chichester	INL
Tim Hyde	INL
Seongtae Kwon	INL
Tedd Lister	INL
Jordan Mclaughlin	INL
Mitch Meyer	INL
Rob Schley	INL
Victor Walker	INL