

LINKING TRANSFORMATIONAL MATERIALS and PROCESSING for an **ENERGY-EFFICIENT and LOW-CARBON ECONOMY:** *Creating the Vision and Accelerating Realization*

Opportunity Analysis for Materials Science and Engineering



TIMS ENERGY

energy.tms.org

*In support of DOE EERE Industrial Technologies Program
In cooperation with ASM International and The Energy Materials Initiative*

ACKNOWLEDGEMENTS

The Linking Transformational Materials and Processing for an Energy-Efficient and Low-Carbon Economy project draws on the contributions of 55 technical experts from industry, academia, and government. We thank them for their thoughtful contributions and active involvement in this work. The effort was supported by the U.S. Department of Energy's Industrial Technologies Program and Oak Ridge National Laboratory. This document was prepared by Dr. Warren H. Hunt, Jr. of The Minerals, Metals, & Materials Society (TMS); Ross Brindle of the Nexight Group, LLC; and Mallory James of Energetics Incorporated. Mauricio Justiniano, Ridah Sabouni, Melanie Seader, Jennifer Ruch, Howard Andres, and Muhammad Zafar of Energetics contributed to writing.

Notice:
This report was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or any agency thereof.

EXECUTIVE SUMMARY	III
I. INTRODUCTION	1
Energy, Carbon, and Economic Development Opportunities for the United States.....	1
The Potential Impact of Materials Science and Engineering	3
Overview and Process of the Current Study.....	3
II. MSE THEME 1: FUNCTIONAL SURFACE TECHNOLOGY	7
Product and Process Innovations.....	7
Catalysts with High Selectivity and Conversion Efficiency	9
Smart Coating/Lubricant Systems for Lightweight Alloys	10
Coatings to Inhibit Galvanic Corrosion	11
New Solar Photovoltaic Materials that Utilize a Broader Spectrum of Light	12
New Surface Treatment Processes to Rebuild or Enhance Surfaces	13
High-Flux Membranes for Selective Separation of Atmospheric Gases.....	14
III. MSE THEME 2: HIGHER-PERFORMANCE MATERIALS FOR EXTREME ENVIRONMENTS.....	15
Product and Process Innovations.....	15
High-Temperature, Phase-Stable Alloys	17
Thermoelectric Materials with High Conversion Efficiency	18
Lightweight, High-Strength Ductile Materials.....	19
Irradiation-Resistant Structural Alloys For Nuclear Applications	20
High-Pressure Hydrogen-Resistant Materials	21
Collaborative, Comprehensive Materials Database	22
Predictive Materials Performance Code	23
IV. MSE THEME 3: MULTI-MATERIALS INTEGRATION IN ENERGY SYSTEMS.....	24
Product and Process Innovations.....	24
Low-Cost Carbon Fibers and Composites Manufacturing Processes	27
Joining Process for Assembling Multi-Material Structures	28
High Energy Density, Low-Cost Battery Cathodes	29
Low-Cost Fuel Cell Catalyst	30
Integrated Computational Materials Engineering Modeling Package.....	31
V. MSE THEME 4: SUSTAINABLE MANUFACTURING OF MATERIALS.....	32
Product and Process Innovations.....	32
Net-Shape Processing of Structural Metals	35
Additive Manufacturing of Components and Systems	36
Low-Cost Processing and Energy Reduction Technology for Metals	37
Separation of Materials for Recycling	38
Real-Time Sensor Technology for Gases and Molten Metals	39
VI. NEXT STEPS	40
APPENDIX A: REFERENCES	41
APPENDIX B: ACRONYMS	42
APPENDIX C: LIST OF PARTICIPANTS.....	43

EXECUTIVE SUMMARY

The United States and the world face significant challenges in meeting their future energy needs. Increasing economic growth will require efficient and economical production, distribution, and end-use of energy. At the same time, growing concerns about global climate change are pushing companies and governments to address the challenge of significantly reducing carbon emissions. Materials and their processing have a pivotal and ubiquitous impact on meeting these national and international challenges. To effectively focus the effort of the materials science and engineering enterprise toward these challenges, a study entitled *Linking Transformational Materials and Processing for an Energy Efficient and Low-Carbon Economy: Creating the Vision and Accelerating Realization* is underway.

In the first phase of the study, published in June 2010, the Energy Materials Blue Ribbon Panel explored how materials and processing can play a vital role in addressing national energy, carbon reduction, and economic development needs. In their Vision Report, the Panel emphasized areas of energy production and use where Materials Science and Engineering (MSE) could have the greatest potential impact. Specifically they identified the highest priority near term opportunities being in industrial energy efficiency, vehicle energy efficiency, nuclear fission, and energy storage with highest priority long term opportunities in energy storage, nuclear fusion, and hydrogen and fuel cells. In addition, they identified four cross-cutting MSE themes (Functional Surface Technology, Higher Performance Materials for Extreme Environments, Multi-Materials Integration in Energy Systems, and Sustainable Manufacturing of Materials) and three foundational areas (Computational Modeling, Advanced Characterization Methods, and Integrated Process Control and Sensors) for further focus.

In this second phase, Technical Working Groups comprised of experts from the community used the MSE cross-cutting themes and foundational areas as a starting point to select product and process areas that, if successfully developed and deployed, would create significant economic impact, energy savings, and carbon emission reductions in the United States. From this group, top-priority opportunity areas were identified

with the primary criteria that they have importance across multiple energy generation or use areas and that they will have nearer term impact, defined as readiness for commercial implementation in the 5-10 year period. Particular focus was placed on those product and process innovation opportunities which were identified by more than one of the Technical Working Groups, indicating both increased recognition of the opportunity and the need for a cross-cutting approach. These selected areas align well with the highest priority near and long term application area opportunities identified by the Energy Materials Blue Ribbon Panel. While the areas outlined below represent the group's consensus on the highest impact opportunities, there are certainly other MSE-driven product and process opportunities that can have impact in selected energy application areas both now and in the longer term.

These areas are summarized below in a framework representing the type of opportunity (Performance Breakthrough or Radical Cost Reduction) and the primary focus of the innovation needed (Product Innovation or Process Innovation). A brief description of each of these six areas follows.

NEXT-GENERATION BATTERY AND FUEL CELL MATERIALS AND CONCEPTS

Next-generation battery and fuel cell materials and concepts that enable radical cost reduction through product innovation are key to further realizing the potential in this area. Battery materials with higher energy density, lower-cost, abuse tolerance, and longer cycle-life can enable transformational battery technologies for transportation and stationary applications. However, available battery materials with even moderate performance are expensive and not amenable to easy or large-scale processing. In particular, low-cost materials for large-scale energy storage and processing are not available. Greater understanding of solid electrolyte interfaces, electrolytes that offer high ionic conductivity at room temperature, and low environmental impact materials can enable improved performance. More robust and compatible electrodes and electrolytes are also needed to reduce battery material costs.

	PRODUCT INNOVATION	PROCESS INNOVATION
Radical Cost Reduction	<ul style="list-style-type: none">• Next-generation battery and fuel cell materials and concepts	<ul style="list-style-type: none">• New paradigm manufacturing processes for metallic and non-metallic materials and their composites
Performance Breakthroughs	<ul style="list-style-type: none">• Breakthrough thermoelectric materials• Next-generation structural metals for extreme environments• Catalysts for fuels and energy-intensive processes	<ul style="list-style-type: none">• Surface treatment processes for product performance and life extension

BREAKTHROUGH THERMOELECTRIC MATERIALS

Thermoelectric materials with greatly enhanced conversion efficiency would represent a breakthrough in product performance in the efficient conversion of waste heat into useful electricity. Developing thermoelectric materials with a figure of merit, or ZT, greater than 3.0 will allow these materials to become cost-effective “energy recyclers.” In addition to improved conversion efficiency, these materials also require improved mechanical performance, lower toxicity, and low cost processing methods.

NEXT-GENERATION STRUCTURAL METALS FOR EXTREME ENVIRONMENTS

Structural alloys with greater stability in adverse environments are an important family of product developments that would enable markedly enhanced performance in a number of energy application areas. Increased stability at elevated temperatures is needed to enable higher-temperature steam cycles for electricity production, higher-efficiency industrial processes, and more efficient use of nuclear fuel in power plants. Structural metals for nuclear applications also must offer stability at radiation levels of 100 displacements per atom.

CATALYSTS FOR FUELS AND ENERGY-INTENSIVE PROCESSES

Catalysts to drive chemical-to-chemical and chemical-to-power reactions represent an important technical area with cross-cutting applicability. Product performance breakthroughs in catalytic materials with higher selectivity and conversion efficiency can improve efficiency in industrial, hydrogen fuel cells, solar, and carbon management applications. For industrial applications, higher selectivity with higher conversion efficiencies would offer significant performance improvement opportunities. Reducing operating temperatures in chemical production processes would save significant amounts of energy and associated carbon emissions. In addition, replacement or extension of noble metals used in catalysts with non-noble metals will improve the cost effectiveness of resulting products. Efficient photocatalytic materials such as titanium dioxide and better alternatives, more efficient catalysts for reduction reactions, and nanostructured catalysts can enable more cost-effective hydrogen generation. Additionally, there is a need to identify more efficient catalysts for reduction reactions and nanostructured catalysts for hydrogen generation and carbon dioxide reduction. A robust catalyst for fuel conversion is a high priority to support carbon management.

NEW PARADIGM MANUFACTURING PROCESSES FOR METALLIC AND NON-METALLIC MATERIALS AND THEIR COMPOSITES

While the search for new lightweight materials and composites has received significant attention in the past, particularly for vehicles, a new focus on manufacturing process techniques, including lower-cost processes for unique product configurations via new processing paradigms that incorporate life-cycle considerations can yield new progress. By drastically reducing the cost of processing lightweight metals (aluminum, magnesium, titanium, mixed-metal structures) and non-metallic materials (plastics, composites) and their composites into final products, these high-performing materials can capture far greater use in transportation and manufacturing applications. Lower-cost primary materials processing and secondary component processing and assembly can bring specialty materials such as aerospace alloys and composites to mass market applications. In addition, combining sustainable product and process design with materials recovery and recycling will lead to new processing paradigms in which processing will not only cost far less, but will also require far less energy and a minimal carbon footprint.

SURFACE TREATMENT PROCESSES FOR PRODUCT PERFORMANCE AND LIFE EXTENSION

Surface treatment processes can extend the service life of products by addressing surface fatigue, environmental protection, and damage tolerance issues. Process innovation in this area offers the potential for performance breakthroughs in products while providing substantial energy and carbon savings. New repair and remanufacturing processes are needed for advanced materials and alloys. Promising techniques include new surface treatment processes that utilize a diffusion process as well as nanoparticles to repair damage and self-healing materials. Smart materials with the ability to detect damage are also important for improving industrial energy efficiency.

Integrated Computational Materials Engineering (ICME) is a major crosscutting set of tools underlying and in some cases enabling successful development in all opportunity areas. Key elements are not only fundamental materials and processing models informed by critical experiments and fueled by robust databases, but also predictive performance models again tuned by experimental data. Through successful integration of existing tools as well as yet-to-be-developed capabilities, ICME can accelerate and enhance the probability of successful development and commercial

implementation of product and process innovations. A significant investment in ICME will ensure that these foundational tools will offer the enabling power needed to accelerate progress, including the identification of novel technical pathways.

In summary, this Opportunity Analysis for Materials Science and Engineering provides the basis for targeted development activities to realize key product and process opportunities that address the priority areas identified by

the Energy Materials Blue Ribbon Panel. If successful, such activities can improve energy efficiency, reduce carbon emissions, and greatly accelerate the growth of clean energy industries based in the United States. A strong MSE enterprise will enable not only advances in the areas highlighted above, but also a number of important materials and process innovations in application areas such as solar energy, energy-efficient buildings, and low-energy production processes that can have longer-term impact on the competitiveness of the U.S. economy.

I. INTRODUCTION

Innovation in materials and materials processing can have a profound impact on the energy and carbon emissions profile of the United States while creating jobs and bolstering the U.S. economy. Breakthroughs in material science and engineering (MSE) can serve as powerful enablers of longer-term national and global ambitions for a more energy-efficient and low-carbon world in multiple ways. New materials and processing approaches will play an essential role in supporting large-scale deployment of cost-effective renewable energy sources and advanced non-renewable energy technologies. Further, MSE breakthroughs hold great promise to reduce the energy use and greenhouse gas emissions of large-scale material manufacturing processes themselves.

The United States can realize these advances by leveraging the strength of its world-leading universities, national research laboratories, and capital markets to create jobs, companies, and even entire industries around MSE breakthroughs. In this way, MSE innovation can also play an important role in supporting a healthy and growing U.S. economy.

Despite this great potential, MSE traditionally has not received significant national attention as a pathway to lower energy consumption and carbon emissions. The same ubiquity that makes materials and processing such an essential presence in daily life has also contributed to an underappraisal of their promise for meeting today's most urgent societal needs.

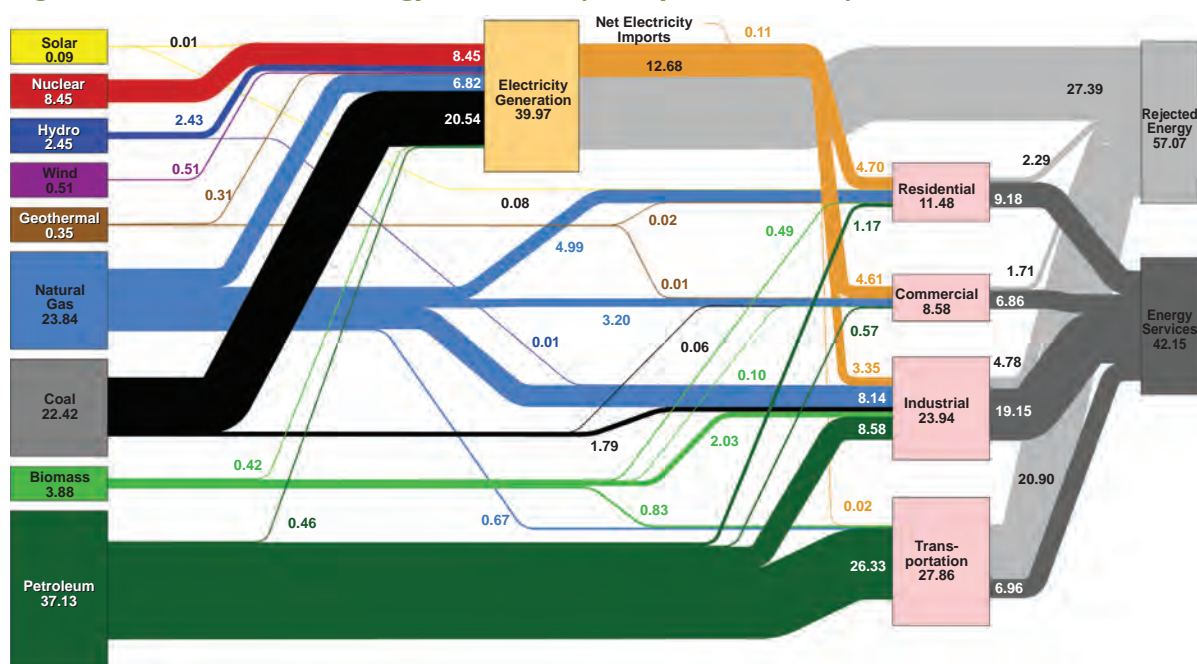
In this report, materials science and engineering (MSE) is used to represent the science and engineering of the full spectrum of materials, and includes both primary and secondary materials, manufacturing and synthesis processes, system integration, and performance.

This document aims to bring materials and processing into the forefront of energy and carbon discussions by detailing new products, processes and manufacturing methods that, if successfully developed, would have a transformational impact on national energy and carbon intensity as well as economic competitiveness.

ENERGY, CARBON, AND ECONOMIC DEVELOPMENT OPPORTUNITIES FOR THE UNITED STATES

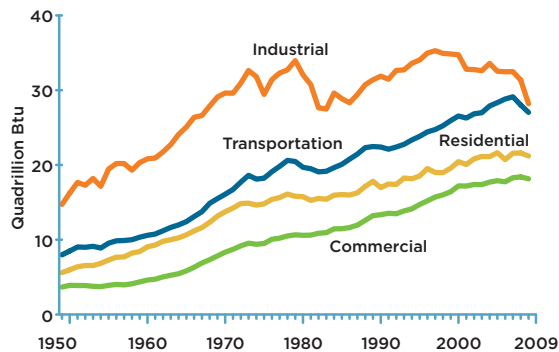
Access to affordable, reliable, and secure energy has been essential to sustaining U.S. economic leadership and the high standard of living that Americans enjoy. More than 80% of energy consumed in the United States is derived from fossil fuel sources (Figure 1), generating large quantities of carbon dioxide and other greenhouse gas emissions that are increasingly worrisome as concerns regarding climate change grow.

Figure 1. Estimated U.S. Energy Use, 2008 (99.2 quadrillion Btu)



Source: Lawrence Livermore National Laboratory;
https://flowcharts.llnl.gov/content/energy/energy_archive/energy_flow_2008/LLNL_US_EFC_20081.png

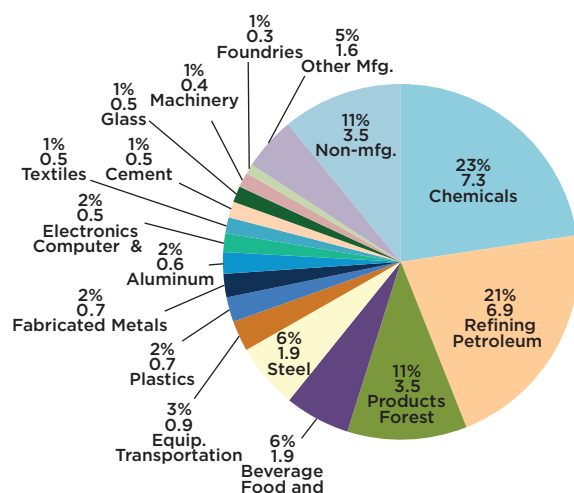
Figure 2. Total Energy Consumption by Sector (1949-2009)



Energy consumption and associated carbon dioxide emissions can be grouped into four end-use sectors: industrial, transportation, residential, and commercial. Figures 2 and 3 show that energy consumption has steadily grown in each of these sectors during the past 60 years, albeit at a rate slower than overall economic growth. Carbon dioxide emissions follow a similar pattern, with the notable exception of the industrial sector, which has seen CO₂ emissions decrease over the past 10 years due to concerted efforts to reduce emissions as well as shifts in the U.S. industrial mix.

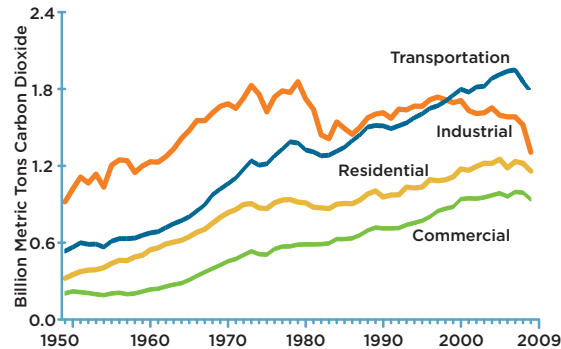
While absolute energy consumption has steadily risen in the past decades, energy intensity (energy consumed per constant dollar of GDP) has gradually declined, from

**Figure 4. Energy Consumption in the Industrial Sector, 2006
Primary Energy Consumption
(32.5 quadrillion Btu)**



Source: Manufacturing Energy Consumption Survey (MECS 2006)

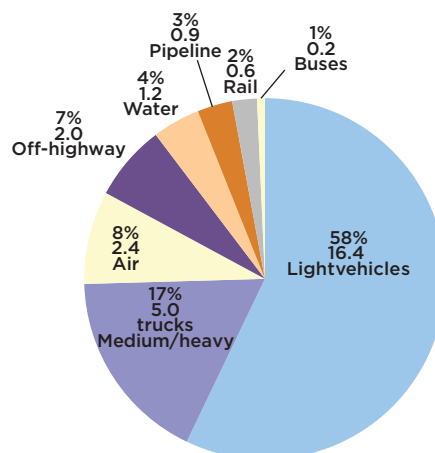
Figure 3. Total Energy-Related Carbon Dioxide Emissions by Sector (1949-2009)



about 14,800 Btu/dollar GDP in 1975 to about 7,400 Btu/dollar GDP in 2009 (EIA, 2009). This important trend demonstrates the United States' ability to address energy and carbon emission concerns while maintaining economic growth. While some of this decline in energy intensity is attributable to a shift toward a more service-based U.S. economy, much of the decline is attributable to technological innovations that allow U.S. vehicles, buildings, and manufacturing plants to do more while using less energy.

Figures 4 and 5 provide a closer look at the industrial and transportation sectors, respectively. The U.S. chemicals, petroleum refining, and forest products industries together constitute 55% of total industrial

**Figure 5. Energy Consumption in the Transportation Sector, 2008
Primary Energy Consumption
(28.8 quadrillion Btu)**



Source: Transportation Energy Data Book, 29th Edition. Table 2.6

energy consumption. The steel and food-and-beverage industries follow, with each accounting for 6% of total energy consumption.

In the transportation sector, 75% of energy consumption occurs on the nation's roads, with the majority being consumed by light-duty vehicles. Nearly all of the energy consumed in transportation is derived from petroleum, while the industrial sector relies on a mix of energy sources that includes large amounts of natural gas and electricity in addition to petroleum. To partially address the transportation sector, the Energy Independence and Security Act of 2007 (EISA-2007) increases corporate average fuel economy (CAFE) standards for light vehicles to 35 mpg by 2020.

Many opportunities exist for reducing the energy and carbon intensity of the United States while maintaining economic growth. Yet, the urgency to address both sides of the intensity equation—the numerator (energy use, carbon emissions) and denominator (GDP)—is great and growing, demanding innovation and leadership. To this end, President Obama signed an Executive Order on Federal Sustainability, committing the Federal Government to lead by example by reducing greenhouse gas emissions by 28% by 2020, increasing energy efficiency, and reducing fleet petroleum consumption.

THE POTENTIAL IMPACT OF MATERIALS SCIENCE AND ENGINEERING

Pursuing and realizing the opportunities for significant improvements in energy efficiency, greenhouse gas reduction, and economic development will require transformations in products and the industrial processes used to make them. Underlying these product and process innovations are materials and materials processing developments that enable performance breakthroughs and radical cost reduction.

Previous studies, noted in Appendix A, have focused on materials needs for specific areas of energy generation or use, or on broad technology development or policy needs. Many technology roadmaps address materials along with materials processing and manufacturing innovation needs that, if filled, would address only a specific energy area or meet one particular industry's needs. The U.S. Climate Change Technology Program Strategic Plan names broad research and innovation needs to enable the provision of low-carbon energy, but it does not generally describe the fundamental research needed if the identified technological hurdles are to be surmounted, or the transition path of such

research to product and/or manufacturing process implementation. In addition to these technology-specific roadmaps, many different groups have elaborated policy recommendations for addressing climate change and energy security, and others have created assessments and projections for the expected future. Beyond the previous technical and policy roadmaps and projections, other studies have focused on the basic science needs for materials in meeting energy and carbon reduction challenges, such as the “Basic Research Needs Workshop Series” conducted between 2003 and 2010 by the U.S. DOE's Office of Science program in Basic Energy Sciences. In the UK, the government published a strategic plan outlining the national energy sector's materials R&D needs over 5, 10, and 20 year timeframes.

The need to better connect basic research and application of this research is well-recognized. A recent report from the Department of Energy's Basic Energy Sciences Advisory Committee entitled “Science for Energy Technology: Strengthening the Link between Basic Research and Industry” is a specific example. It notes that “to accelerate the innovation and development of critically needed energy solutions, effective communication is essential between, on one side, fundamental research developed in the DOE Office of Basic Energy Sciences and, on the other side, the applied community, in the DOE technology offices and in industry.”

The current work further focuses on the connection between research and application by addressing the potential impacts of materials science and engineering, and identifying key breakthrough areas, across energy generation and use sectors. It also specifically addresses the “applied research to commercial readiness” space often referred to as the “valley of death”. Opportunities for economic development from growth in the clean energy industry area as well as enhancement for a broader base of industry sectors are also considered.

OVERVIEW AND PROCESS OF THE CURRENT STUDY

The Minerals, Metals, and Materials Society (TMS), with support from the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy, Industrial Technologies Program sought to address these issues and opportunities through this study, titled *Linking Transformational Materials and Processing for an Energy Efficient and Low-Carbon Economy: Creating the Vision and Accelerating Realization*.

The purpose of this study was to uncover opportunities for transformational impact by:

- Identifying areas where MSE has the greatest leverage
- Taking a holistic materials and manufacturing process perspective and identifying common elements across multiple application areas
- Seeking ways to compress the time from discovery to commercial readiness
- Informing the focus for the nation's MSE R&D portfolio

Phase I of the study entailed convening the Energy Materials Blue Ribbon Panel, consisting of 21 materials community thought leaders representing industry, academia, federally funded R&D laboratories, and government, to:

- Assess opportunities for transformational MSE contributions to energy sources, energy carriers and transmission, and energy use
- Identify high-impact, cross-cutting materials and processing technologies
- Evaluate the status of the U.S. science and technology infrastructure in these opportunity areas

Vision of the Energy Materials Blue Ribbon Panel

Materials science and engineering (MSE) breakthroughs will enable the United States to greatly reduce the energy and carbon intensity of its economy. Near-term improvements in the materials employed in today's massive energy infrastructure will deliver significant payoffs that will serve a critical role in the ability of the United States to meet its national energy needs. Meanwhile, transformational innovations in MSE hold promise to revolutionize the way the nation produces, transports, and consumes energy in the long term. By pursuing a balanced approach to material and manufacturing science R&D, the United States can deliver near-term improvements while also laying the foundation for radical advances in the longer term.

This Panel identified a vital role for MSE as reflected in its Vision statement in the accompanying text box.

The Panel identified several areas where MSE breakthroughs could be the key enabler for high impact energy efficiency and carbon reduction solutions. Shown in Figure 6 are these priority energy application areas in both the near-term and long-term timeframes.

The Panel next identified the materials and processing-driven elements that could make the highest impact across energy source and use. These elements were

Figure 6. Energy Application Areas with Greatest Promise for Transformational Near-Term and Long-Term Impact Through MSE Technologies

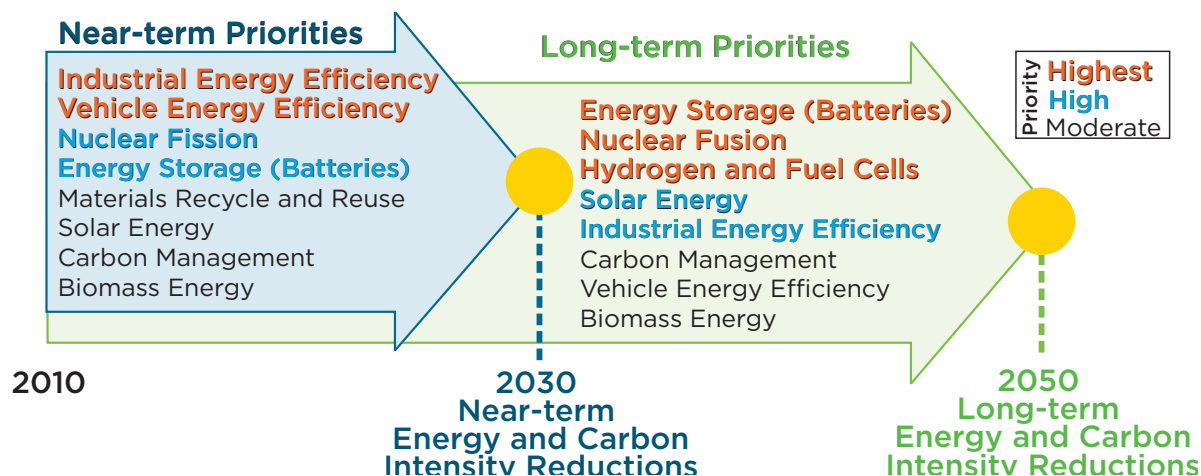
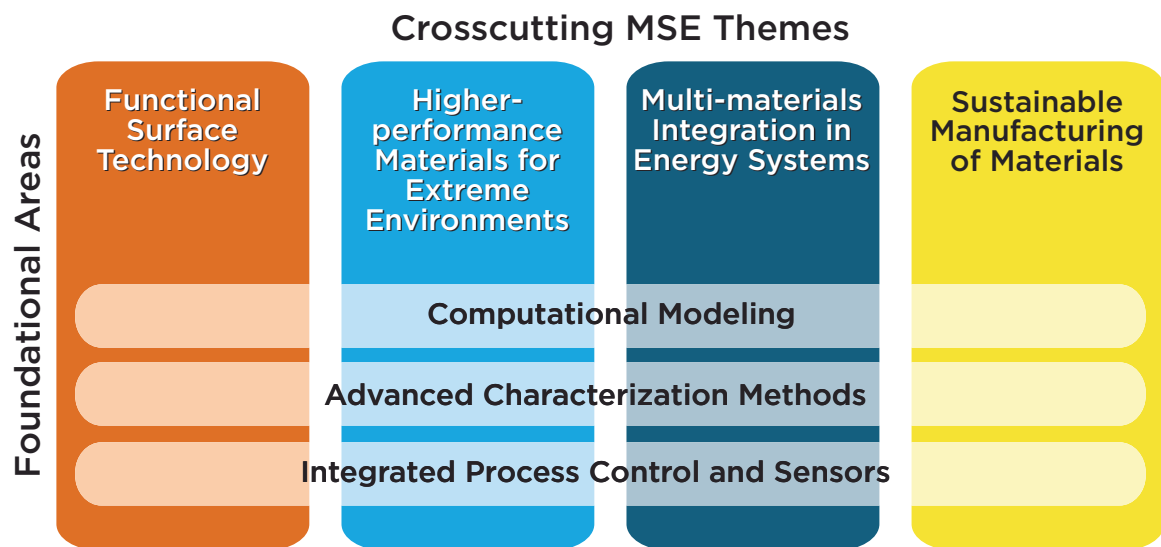


Figure 7. MSE Themes and Foundational Areas



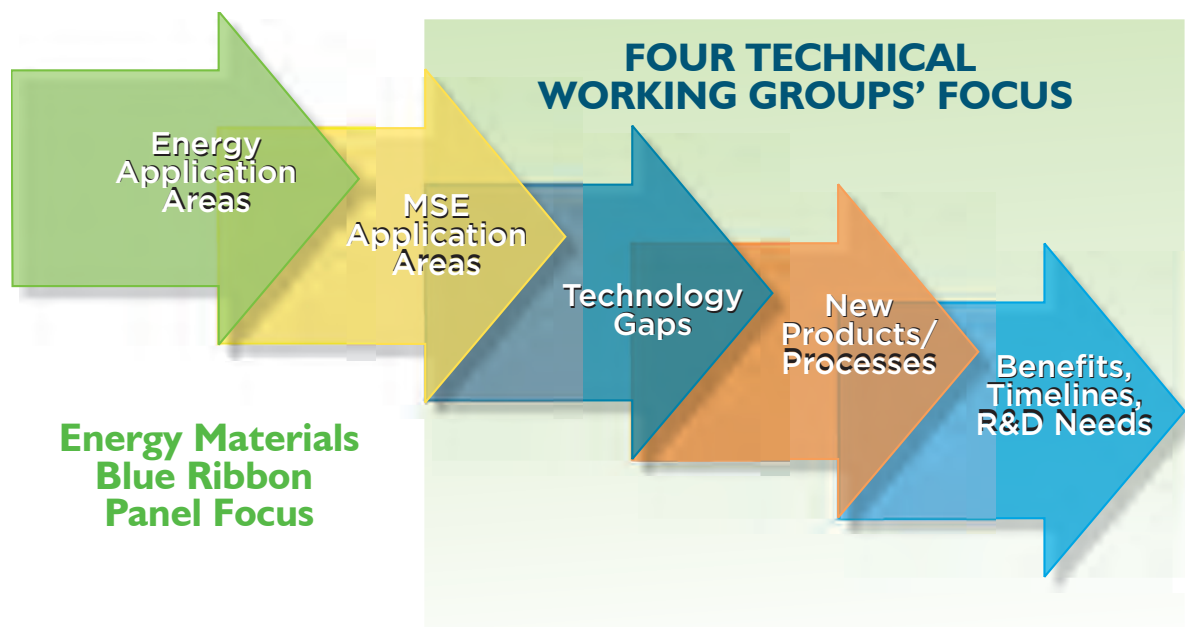
classified into the four crosscutting MSE themes, which were in turn supported by three foundational areas, illustrated in Figure 7.

With this background, four Technical Working Groups were engaged and organized according to each of the four crosscutting MSE themes in Figure 7 in Phase II of the study. These groups were again comprised of members from industrial, academic, federally funded R&D laboratories, and government organizations (a

listing of the Technical Working Group members is presented in Appendix C). The Technical Working Groups met for a facilitated workshop on September 16-17, 2010 in Pittsburgh, PA. This report represents the output and recommendations of this Phase II study.

The logic flow of the Technical Working Group's efforts as a continuation of the focus of the Energy Materials Blue Ribbon Panel is illustrated in Figure 8.

Figure 8. Logic Flow of Blue Ribbon Panel and Technical Working Groups' Outputs



Specifically, the Technical Working Group efforts were focused on achieving the following outcomes:

- Consensus around **key application areas** where materials technology advances will make significant energy and carbon reduction impacts
- A prioritized set of **limitations and gaps in materials technologies** that, if overcome, could enable breakthrough processes and products
- A **prioritized set of new products and manufacturing processes** that hold potential to deliver significant energy and/or carbon reductions and can be realized through MSE breakthroughs
- **Semi-quantification of the energy and carbon reduction benefits** projected from the new products and processes identified
- A **preliminary time line** for when new technologies could achieve commercialization

- **Preliminary lists of R&D** needed to achieve MSE breakthroughs to enable new products and processes that deliver energy and carbon savings

In addition, each Technical Working Group was asked to consider ways in which the three Foundational Areas illustrated in Figure 7 factored into their specific MSE area.

In the following chapters, the output from each of the four Technical Working Groups is summarized in succession. (Note that the summaries presented are visually keyed to the MSE Themes and Foundational Areas illustrated in Figure 7 for easy reference.) In each of these four chapters, summaries of key product and process opportunities are provided using the framework of the desired outcomes listed above.

II. MSE THEME 1: FUNCTIONAL SURFACE TECHNOLOGY

Advances in functional surfaces will play a fundamental role in achieving energy and carbon benefits in many sectors of the U.S. economy. Enhanced functional surface technologies enable surfaces to interact with process conditions to improve efficiency, speed reaction times, produce and store energy more efficiently, and withstand demanding operating conditions longer. Functional surface innovations can improve renewable energy technologies, storage and distribution, transportation and industrial efficiency, and carbon management applications throughout the U.S. energy sector. Specific examples of envisioned advances include:

- Improving conversion efficiencies in industrial processes and hydrogen fuel cells using highly reactive catalysts
- Enabling vehicle lightweighting through the use of cost-effective, high-strength lightweight materials that can withstand demanding operating conditions
- Radically extending component life through innovative surface restoration
- Enabling large-scale and prolific carbon management through selective separation advances enabled by functional surfaces (e.g., membranes)

- Improving the efficiency of solar photovoltaics by creating surfaces that absorb light more effectively and increase conversion efficiency

PRODUCT AND PROCESS INNOVATIONS

Innovations in products that utilize functional surfaces and processes that enable their deployment at scale are needed to realize the promising benefits of functional surface technology. The following table outlines products and processes that, if developed and commercialized successfully, can deliver significant energy and carbon savings. The highest-priority items—those that were identified as holding the greatest potential for delivering energy and/or carbon reductions—are identified by bold underlined font and are further explained later in this chapter. The innovations are associated with key application areas of the energy sector to demonstrate the primary sector where the innovation will deliver energy and carbon savings. However, several of the innovations could have broad impact in multiple areas of the energy sector if successfully realized.

Table 1. Potential Product and Process Innovations – Functional Surface Technology

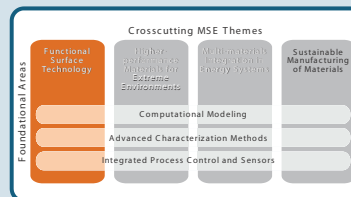
ENERGY APPLICATION AREA	MSE PRODUCT/PROCESS INNOVATION
Industrial Energy Efficiency	<p>Improved catalysts for industrial processes</p> <ul style="list-style-type: none"> • <u>Catalysts with high selectivity and conversion efficiency</u> • Catalysts that perform like today's advanced catalysts but use common metals <p>High thermal conductivity materials and improved thermal barrier conditions</p> <ul style="list-style-type: none"> • Non-fouling surfaces for heat exchange in industrial processes • Thermal barrier coatings (TBCs) with low thermal conductivity, higher strain tolerance, better adhesion, and better environmental resistance <p>Materials for energy efficient high-temperature performance and aggressive environment resistance</p> <ul style="list-style-type: none"> • Thermal barrier coating (TBC) that adds 100°C operating temperature to turbines with ~1% reduction in specific fuel composition • Environmental barrier coating that adds 200°C to operating temperature of ceramics for combustion at high pressure ratios
Vehicle Energy Efficiency	<p>Reduction of friction and wear</p> <ul style="list-style-type: none"> • <u>Smart coating/lubricant systems for lightweight alloys</u> • Surface prep techniques for strong coating adhesion on Al, Mg, Ti, and composites for internal combustion engines and drive trains; tough coatings for Al, Mg, and Ti with tailored interfaces • Alloyed and composite coatings that apply multiple elements in a single process <p>Novel, robust, lightweight materials with adequate properties for vehicle applications</p> <ul style="list-style-type: none"> • <u>Coatings to inhibit galvanic corrosion</u>
Hydrogen and Fuel Cells	<p>Efficient photo-catalytic materials for hydrogen production</p> <ul style="list-style-type: none"> • Low-cost materials that absorb light more effectively and use more than the UV range <p>Better solid state H₂ storage materials</p> <ul style="list-style-type: none"> • Materials with better energetics and faster kinetics • High gravimetric and volumetric H₂ storage materials
Solar Energy	<p>New materials that utilize a broader spectrum of light</p> <ul style="list-style-type: none"> • <u>New solar photovoltaic materials that utilize a broader spectrum of light</u>
Materials Recycle and Reuse	<p>Life extension of components to reduce replacement</p> <ul style="list-style-type: none"> • <u>New surface treatment process to rebuild or enhance surfaces</u> • Coatings with visual indicator of condition – e.g., fatigue sensor, and cost-effective way to strip and replace coatings
Carbon Management	<p>New CO₂ capture materials</p> <ul style="list-style-type: none"> • <u>High flux membrane for selective separation of atmospheric gases</u> • Surface with selective absorption of CO₂ versus N₂ (or vice versa); also able to readily release it
Lighting	<p>Commercial lighting with reduced CO₂ emissions</p> <ul style="list-style-type: none"> • LED lighting that offers a broader spectrum of light and lower cost

The following pages showcase the highest-priority product and process innovations as identified by the Function Surface Technology Technical Working Group. These summaries provide more details regarding the benefits of the innovation, the timing in which those benefits might be realized, the gaps

and limitations that must be addressed to achieve the benefits, and R&D needed to do so. While quantitative estimates of the benefits are estimated, the actual benefits will depend on market uptake of the new products and processes that result from a concerted R&D effort.

Catalysts with High Selectivity and Conversion Efficiency

The production of ammonia, ethylene, and almost all industrially important chemicals involves catalysis. Catalysts with high selectivity and conversion efficiency improve industrial process energy efficiency by optimizing chemistry and structure to result in more efficient surface catalysis reactions and enable more cost-effective manufacturing.



How will it save energy and carbon?

- A more active catalyst can allow operation at lower temperatures. For example, ammonia (NH_3) synthesis currently runs at $\sim 500^\circ\text{C}$. Improved catalysts could result in a 100°C lower reaction temperature and therefore achieve significant energy savings
- Improved catalysts may also allow direct synthesis pathways and replace the indirect methods that exist today. For example, 60%–70% of the cost of methane (CH_4) to methanol (CH_3OH) production is due to syngas production. Removing this step through the use of a direct methanol synthesis pathway enabled by new catalysts can reduce both energy and carbon dioxide emissions

Potential savings

- 3%–5% reduction in energy use in ammonia production

Time until commercialization

- Ammonia production: 5–20 years
- Methanol production: 5–10 years – likely a shorter timeframe than advances in ammonia production

Gaps and Limitations to Overcome

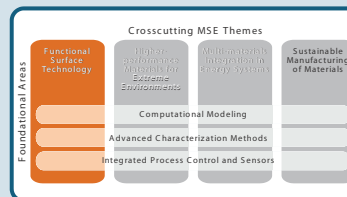
- Nanoparticles currently melt and sinter at low temperatures relative to bulk materials. The sintering of catalytic particles results in reduced efficiency and life of catalysts relying on nanoparticles for improved activity and efficiency.
- Many advanced catalysts have inadequate mechanical stability, resistance to contamination, or both. This limits their efficiency, lifetime, and range of application.
- Some advanced catalysts rely on noble metals, creating cost and resource availability concerns.
- Certain catalysts have insufficient low-temperature reactivity (e.g., catalysts for ammonia synthesis).
- Materials scientists lack adequate understanding and capabilities for predicting the reactive properties of new catalysts, and therefore require a trial-and-error approach to identifying new catalysts.
- Microscopic analysis capabilities are inadequate, preventing material scientists from fully characterizing catalyst surfaces and defects and distinguishing the relative reactivity of various geometric regions of the catalyst structure (e.g., crystal surfaces versus terraces).

R&D Needs for Market Readiness

- Research to improve the stability of catalysts
- Research to increase catalyst reactivity at lower temperatures
- Computational and atomistic modeling to identify new catalysts materials in a predictive manner
- Development of characterization methods such as atomic-scale, in-situ, high-speed microscopic techniques
- Development of low-cost, efficient manufacturing methods for nanocatalysts

Smart Coating/Lubricant Systems for Lightweight Alloys

Lightweight alloyed materials in vehicles are subject to degradation by friction and wear. Smart coating/lubricant systems offer thermal stability and wear resistance in order to broaden the opportunities for use of lightweight alloys that are typically inadequate for such high-wear environments as vehicle applications. These coatings offer good coating-substrate adhesion, do not degrade the substrate during deposition, and are strain-tolerant allowing for the retention of critical dimensions of moving sealing surfaces.



How will it save energy and carbon?

- Smart, wear-resistant and thermally stable coatings/lubricants allow the use of lightweight alloys, such as aluminum (Al) and magnesium (Mg) in vehicles which result in mass reduction and increased fuel economy
- Improved dimensional tolerance of engine components reduces carbon emissions

Potential savings

- 10% reduction in mass results in 6% increased fuel economy
- 5-15% of energy in a car is lost due to friction

Time until commercialization

- Coatings: 1–5 years
- Lubricants: 5–10 years—slightly longer timeframe than coatings

Gaps and Limitations to Overcome

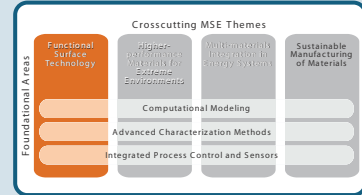
- Many lightweight materials have inherently poor corrosion and wear resistance. Materials scientists have few wear-resistant and thermally-stable coatings and surface treatments for Al and Mg-based alloys, limiting their life and adequacy for vehicle applications.
- Both the cost and the deposition process limit the choice of wear-resistant compounds for vehicle energy efficiency. The ability to adhere many coatings to the substrate is limited, especially for composite substrates or when the bulk thermal coefficients of expansion of the coating and substrate are mismatched. Many current coating deposition processes degrade the substrate, raising fatigue and strength challenges.
- Inadequate ASTM tests, terminology and vocabulary, and property database information exist for coatings.
- Interactions among surface material, surface shape, and lubricants are poorly understood, and lubricant additives that function with coatings are lacking.
- Due to the lack of in-situ characterization and sensors that can function in industrial environments, residual stress and how it relates to coatings is poorly understood.
- In saltwater environments or when damaged, coatings often create local galvanic corrosion coupled with aluminum and magnesium.

R&D Needs for Market Readiness

- Improvements in choice of wear resistant compounds that can be deposited, the deposition process (address degradation of substrate, fatigue, and strength), and the overall cost-effectiveness
- Increased understanding of residual stress and how it relates to coatings, and development of coatings with better strain tolerance
- Research to better understand what happens to the boundary layer between coating and substrate base
- Research to better understand how surface material, surface shape, and lubricants interact
- Development of boundary lubricants
- Development of additive packages for lubricants compatible with coatings, to increase the lubricants' effectiveness and durability and help self-heal damage done

Coatings to Inhibit Galvanic Corrosion

Lightweight automotive materials can experience severe galvanic corrosion, posing a major challenge to the use of alloys for lightweighting. Coatings and coating deposition processes that inhibit galvanic corrosion of materials such as aluminum (Al) and magnesium (Mg) allow the more widespread use of these materials in automotive and other applications by improving the surface properties of lightweight materials to increase their adequacy for high-wear environments over the long term.



How will it save energy and carbon?

- As pure magnesium is about one-third lighter than aluminum and two-thirds lighter than conventional steel, more widespread use of magnesium in vehicles would lead to significant weight savings
- As lighter weight translates into greater fuel efficiency, magnesium alloys are very attractive to the automobile industry
- Significant overall mass savings would result if 100 lb of Mg were placed in a car

Potential savings

- 2% lighter cars would result from increasing current use of Mg (10lb) to 100lb
- About 48 million gallons of gasoline per year could be saved

Time until commercialization

- 3–5 years for better coatings addressing more problems at once

Gaps and Limitations to Overcome

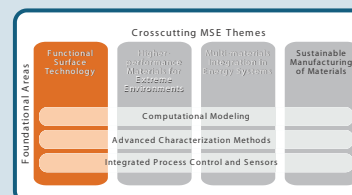
- Current corrosion mitigation strategies and materials are inadequate to meet the needs posed by multi-materials vehicles and by the use of enhanced performance materials.
- Insufficient fundamental research has been conducted to date on mechanisms for galvanic corrosion, new coatings and new surface treatments to address it, and accelerated test procedures.

R&D Needs for Market Readiness

- Research to design better coatings to deal with multiple problems at once
- Techniques to optimize energy system design
- Development of better coatings to isolate dissimilar metals (such as those at joints and other contact areas)
- More and better test procedures, including accelerated testing
- Fundamental understanding of how corrosion occurs, especially thermodynamic, mechanical, and chemical processes/mechanisms

New Solar Photovoltaic Materials that Utilize a Broader Spectrum of Light

In order to achieve high conversion efficiency in producing electricity from solar energy, solar cells must absorb photons from a broad portion of the solar spectrum. Each photovoltaic material responds and absorbs a narrow range of solar energies (low-energy infrared to high-energy ultraviolet), corresponding to its characteristic band gap. Photons with energy lower than the band gap escape unabsorbed; photons with higher energy are absorbed, but most of their energy is wasted as heat. New materials could allow for tuning the band gaps to enable solar cells to absorb and utilize a broader and more controllable spectrum of light in order to increase the amount of energy collected.



How will it save energy and carbon?

- Solar photovoltaic technologies provide low carbon energy
- Increased conversion efficiency should lead to better economics and market uptake of solar technologies

Potential Savings

- Potentially large carbon emissions reductions, if conversion efficiency can be increased substantially

Time until commercialization

- Depends on the extent the absorbed spectrum is broadened
- 10% broadening may be possible in 1-5 years
- Doubling the absorbed spectrum may take much longer
- If new discovery is needed, then >20 years

Gaps and Limitations to Overcome

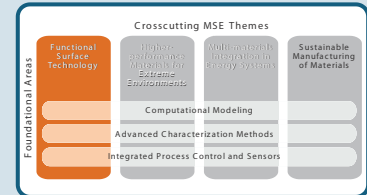
- Materials scientists are currently unable to control the band gap of photovoltaic materials to optimize capture of the solar spectrum and thereby increase the efficiency of light's conversion into electrical current. In particular, inadequate concepts are available for tuning the band-gaps of oxide semiconductors.
- Although most widely available and robust materials have a wide band gap, the narrower the band gap, the more solar energy is captured. Most light escapes because low energy photons do not have enough energy to excite electron-hole pairs across the energy gap, and high energy photons excite pairs with energy above the gap resulting in heat energy loss rather than useable electrical energy. Materials scientists have not yet been able to optimize power input, which increases as bandwidth increases.
- Even where current devices capture a good deal of light, too much of the energy is currently dissipated. Better knowledge of, and ability to manipulate, the interface between the dye molecule and surface is needed to minimize energy loss.
- Current oxide semiconductor devices have limited ability to absorb light from the visible range.

R&D Needs for Market Readiness

- Identifying new, low-cost materials with tunable band gap; better interface and control for energy conversion
- Developing new processing techniques for such materials
- Address the issue of power loss due to loss of low-energy and excessively high-energy photons
- Establishing enhanced photonics modeling capabilities
- Improving computational modeling tools

New Surface Treatment Processes to Rebuild or Enhance Surfaces

Achievements in materials recycling and reuse hinge on restoration and refurbishing processes that extend the life of components while addressing issues such as surface fatigue, strain accommodation, and damage tolerance. New surface treatment processes to rebuild surfaces are needed for high-strain applications and other component repair and refurbishment applications including engines and aircraft. Opportunities exist for restoration processes allowing diffusional bonding between old and new surfaces.



How will it save energy and carbon?

- Reduced need for replacement materials and increased use of refurbishment/repair in a variety of applications saves energy
- Surface rebuilding processes are applicable to ferrous-based as well as aluminum-based components

Potential savings

- Salvaging old parts saves 85% of energy needed to make the original part

Time until commercialization

- 1–5 years

Gaps and Limitations to Overcome

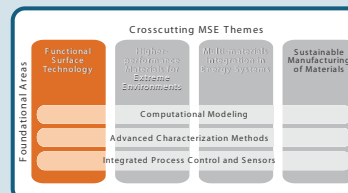
- Current surface restoration processes are incapable of performing in high-strain applications, and also lack adequate damage tolerance and fatigue life (e.g., for crankshafts).
- Most materials now in use lack “materials autonomy”—i.e., the ability to respond actively at the first onset of weakness to avoid corrosion or other forms of breakdown.
- Although residual compression techniques hold promise for extending the fatigue life of materials to be reused, materials scientists currently lack any gauge or process for sensing residual compression in an inexpensive, reliable way.
- Inadequate repair/remanufacturing processes exist for many advanced high-performance materials.

R&D Needs for Market Readiness

- Process development that yields new interfaces between base material and rebuilt surface
- Accelerated test procedures to gather long-term performance data in shorter time frames

High Flux Membranes for Selective Separation of Atmospheric Gases

Carbon management requires materials for CO₂ separation, capture, or both. Improved selectivity of separation decreases the energy cost associated with carbon capture and therefore improves the economics. High flux membranes address the intrinsic challenges of efficiently separating CO₂ from N₂, such as their similar molecular sizes (0.33nm vs. 0.36nm, respectively) and CO₂ molecules' tendency to move through membranes relatively slowly.



How will it save energy and carbon?

- Reduction in the energy penalty associated with carbon capture
- For example, the heat and power requirements for operating the separation equipment, currently impose a 40%–50% (and up to 80%) energy penalty
- Reducing the energy penalty will decrease the energy consumption and costs associated with carbon capture, helping move the technology closer to widespread use
- Direct carbon avoidance

Potential savings

- 12% minimum energy penalty is the theoretical limit
- 20% energy penalty may be a realistic target

Time until commercialization

- 1–5 years—many related research projects are now underway

Gaps and Limitations to Overcome

- Given that carbon capture now requires 25–80% of the energy produced, existing separation concepts and paradigms are insufficient to support broad implementation.
- Due to the similar molecular diameters of N₂ and CO₂ (0.33nm vs. 0.36nm, respectively), separating CO₂ from flue gas is intrinsically challenging and inefficient.
- Current technical approaches to separation draw a parasitic energy load for releasing the CO₂.
- CO₂ molecules currently move too slowly through membranes.
- Today's separation membranes for carbon capture are inadequately selective, and use materials with low contaminant resistance.

R&D Needs for Market Readiness

- Conduct research to better understand what happens to the boundary level, and achieve both faster kinetics and better selectivity
- Create an organic framework using composite materials such as polymer membranes with metals
- Improve computational methods

III. MSE THEME 2: HIGHER-PERFORMANCE MATERIALS FOR EXTREME ENVIRONMENTS

For many energy systems, the path to realizing greater energy efficiency requires operation in harsher environments characterized by varying thermal, chemical, mechanical, and radiation stresses. Materials are frequently the limiting factor for pushing energy systems to these extremes. In these environments, materials must maintain the chemical and physical properties necessary to enable the energy systems to operate efficiently without reducing component and system life. Although surface aspects of materials play a significant role in determining material performance in extreme environments, improvements in bulk material properties are also needed to maximize the efficiency of energy systems operating with extreme environments.

To develop technologies that can improve industrial and vehicle energy efficiency; advance nuclear fission, fusion, and solar technologies; and enable the affordable use of hydrogen fuel cells, it is necessary to develop breakthrough materials that can maintain their structural integrity under these extreme conditions. Examples of the breakthroughs needed are provided below.

- Increasing the efficiency of industrial combustion and conversion systems requires corrosion- and chemical-resistant materials capable of withstanding higher temperatures and aggressive chemicals such as sulfur, hydrogen, chlorine, and water.
- Nuclear fission and fusion requires radiation-tolerant materials and new fuel systems to

improve energy efficiency. These materials must be cost-effective and may require new materials manufacturing techniques.

- The cost-effective development of new materials for tomorrow's energy systems requires improved methods of predicting material properties and performance with limited operating data and design experience.
- New models are needed for researchers to better understand and predict environmental degradation modes on material lifetimes.
- Methods to rapidly detect damage to energy system materials in service will enable systems to maintain their maximum operation efficiencies.

PRODUCT AND PROCESS INNOVATIONS

Materials innovations are essential to the development of new product and processes needed to realize the advantages of operating in more extreme environments. The following table outlines identified products and processes that, when commercialized successfully, can deliver significant energy and carbon savings. The highest-priority items—those that hold the greatest potential for delivering energy and/or carbon reductions—are identified by bold underlined text.

Table 2. Potential Product and Process Innovations – Higher-Performance Materials for Extreme Environments

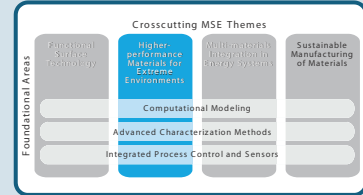
ENERGY APPLICATION AREA	MSE PRODUCT/PROCESS INNOVATION
Industrial Energy Efficiency	<p>Materials for energy efficient high-temperature performance and aggressive environment resistance</p> <ul style="list-style-type: none"> • <u>High-temperature, phase-stable alloys</u> • High-temperature (>600°C) alloys for engine applications • High-temperature (> 650°C) alloys that are highly resistant to aggressive (e.g., sulfur, chlorine, water) environments <p>Materials for managing thermal energy loss</p> <ul style="list-style-type: none"> • <u>Thermoelectric materials with high conversion efficiency</u> • Thin-walled recuperators for service in exhaust gas with high water contents at $\geq 700^{\circ}\text{C}$ for 40,000 hours • More user-friendly modeling software or computer programs for process engineers and academics to optimize thermoelectric devices • Energy-harvesting materials
Vehicle Energy Efficiency	<p>Materials and processing for lighter and fuel-efficient vehicles</p> <ul style="list-style-type: none"> • <u>Light, high-strength ductile materials</u> • Co-extrusion of complex multi-layered materials • Layered metals/alloys produced via solidification processing • A corrosion resistant, damage tolerant, formable magnesium alloy <p>Surface engineering for advanced vehicles</p> <ul style="list-style-type: none"> • Processing for making strong and/or lightweight materials/alloys surface stable • Surface engineering/coatings for improved formability and corrosion resistance
Nuclear Fission	<p>Radiation-resistant structural materials</p> <ul style="list-style-type: none"> • <u>Irradiation-resistant structural alloys for nuclear applications</u> <p>Advanced nuclear fuels</p> <ul style="list-style-type: none"> • Proliferation-resistant nuclear fuels to enable worldwide deployment of safe, secure nuclear energy • Fuel with energy density and thermal conductivity of metallic fuel that can be burned to 400 gigawatt day per ton (40% burnup)
Hydrogen and Fuel Cells	<ul style="list-style-type: none"> • <u>High pressure hydrogen-resistant materials</u> • A robust, efficient photocatalyst that splits water into hydrogen and oxygen at room temperature under concentrated sunlight
Materials Recycle and Reuse	<ul style="list-style-type: none"> • Portable remediation strategies for materials degraded in service
Advanced Characterization Methods	<ul style="list-style-type: none"> • <u>Collaborative, comprehensive materials database</u> • A non-destructive evaluation method to determine current conditions of components and remaining life
Computational Modeling	<ul style="list-style-type: none"> • <u>Predictive materials performance code</u>

The following summaries provide more information about the top product and process innovations in higher-performance materials for extreme environments. These summaries identify how the innovations will

save energy, the potential savings that could be realized through successful commercialization, their expected time to market, key challenges, and the R&D needed to move the technology from current status to market readiness.

High-Temperature, Phase-Stable Alloys

Increasing the efficiency of industrial combustion and conversion systems requires corrosion- and chemical-resistant materials capable of withstanding temperatures greater than 650°C and aggressive chemicals such as sulfur, hydrogen, chlorine, and water. High-strength, phase-stable alloys are needed for extended service at temperatures greater than 650°C. These alloys will be manufactured by advanced techniques, such as combining strong, corrosion-resistant steel with advanced surface engineering processes.



How will it save energy and carbon?

- Enables the power generation steam cycle to operate at temperatures greater than 650°C, thereby increasing the energy efficiency of electricity production
- Enables oxy-fuel combustion, i.e., fuel combustion in pure oxygen
- Improves waste heat recovery

Potential savings

- 5% added efficiency in steam cycle from operation at 650°C
- 10% added efficiency from operation at 750°C
- Oxy-fuel combustion produces pure carbon dioxide, facilitating carbon capture

Time until commercialization

- 5–20 years for a 5% energy conversion efficiency gain due to materials able to perform at 650°C
- Greater than 20 years for a 10% efficiency gain due to materials able to perform at 750°C

Gaps and Limitations to Overcome

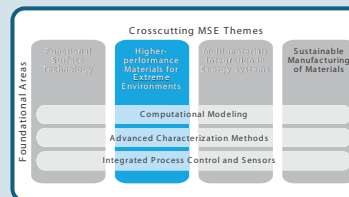
- For many energy systems, the path to realizing greater energy efficiency requires operation in harsher environments characterized by varying thermal, chemical, mechanical, and radiation stresses. Materials are frequently the limiting factor for pushing energy systems to these extremes. Insufficient structural/functional materials exist that are resistant to high-temperature, high-steam content environments, and for turbine applications demanding strength, corrosion-resistance, and high-temperature performance.
- Few materials exist that have low coefficients of thermal expansion (CTE) and can tolerate high-temperature conditions. Existing low-CTE materials are too expensive, and the melting points of traditional structural alloys are too low.
- Inadequate manufacturing know-how and capabilities to produce advanced high temperature alloys of the sizes needed for high efficiency energy conversion and utilization applications.
- Insufficient performance data exists for radiation tolerant materials for high-burnup nuclear applications, and existing materials are inadequate for these applications.
- Current methods for predicting material properties with limited operating data and experience are inadequate to support the cost-effective development of new materials for extreme environment energy systems. New models are needed for researchers to better understand and predict environmental degradation modes on material lifetimes.
- Existing methods are unable to rapidly detect damages to energy system materials in service and thereby enable systems to maintain their maximum operation efficiencies.

R&D Needs for Market Readiness

- Developing new alloys that offer higher-temperature performance
- Creating testing procedures, both accelerated aging testing and long-term testing
- Establishing models that can predict material aging and performance
- Developing improved thermomechanical processing
- Creating new codes and standards that incorporate newly developed alloys
- Improving corrosion and thermal stability of microstructure
- Creating models to better predict environmental degradation modes on material lifetimes

Thermoelectric Materials with High Conversion Efficiency

Thermoelectric (TE) materials are used to convert waste heat into useful electricity. The higher a TE material's ZT value (thermoelectric figure of merit), the greater its thermodynamic efficiency. TE materials, especially P-types, with high ZT values and improved thermal cycling properties offer an efficient alternative to mechanical generation and refrigeration. They also allow the harvesting of waste heat, thereby increasing energy and fuel efficiency of diverse processes.



How will it save energy and carbon?

- TE generation from waste heat recovery improves vehicle fuel efficiency. TE conversion of waste heat to electric energy in a current BMW car has been shown to provide 1-2% increased fuel economy
- New higher-efficiency TE materials will improve waste heat capture and conversion to additional electricity in industry and power generation. As such, TE devices to harvest waste heat will become increasingly prevalent and represent a large opportunity for energy savings
- Thermoelectric cooling results in more efficient cooling in air conditioning units and computers

Potential savings

- Several % increase in vehicle fuel economy is possible
- Waste heat capture represents a huge opportunity—even a 1% improvement would have large implications for energy savings

Time until commercialization

- Additional improved TE materials: 5-10 years (some advanced materials are currently available)
- Must either achieve ZT of 3 or lower cost and/or toxicity of TE materials to enable large-scale commercial success

Gaps and Limitations to Overcome

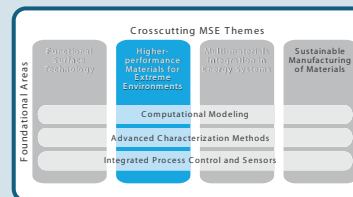
- Too few materials exist with sufficient thermal and electrical conductivity for high-heat, high-load thermoelectrics with figures of merit (ZT) in excess of 1.5-2. The best bulk N-type materials now available have a ZT of 1.6. Few P-type device materials are available, and synthesis of P-type materials with the desired properties is challenging.
- Limitations on the process of doping with P-type semiconductor materials hinder the construction of thermoelectrics with high conversion efficiencies.
- Current cost and toxicity of thermoelectrics are incompatible with large-scale use. Affordable materials and structures lack high-ZT performance, and therefore produce low energy yields or require high volumes.
- For advanced thermal management in vehicles, thermoelectric conversion efficiency is currently inadequate at automotive exhaust temperatures.
- Thermoelectric energy conversion at lower temperatures cannot withstand chemical environments, and current thermoelectric devices have inadequate mechanical properties to withstand thermal cycling.
- Predictive capability for materials design and property prediction is inadequate to narrow the list of potential thermoelectric materials.
- Design engineers who may not be modeling experts find current computer modeling tools challenging to use.

R&D Needs for Market Readiness

- Development of P-type materials compatible with N-type materials
- Research to improve mechanical stability of TE materials – how to support, consolidate, and/or make more robust; whether thermoelectrics made of matrix composites have potential
- Achievement of high ZT values (>3) and reduced costs and toxicity
- High throughput methods for TE materials discovery
- Computational modeling for new materials – computer program that can characterize intrinsic TE properties under a range of conditions
- Thermoelectric system-level or device-level modeling – use for optimization of design, characterization of performance, and understanding of design (e.g., size) and behavior of such characteristics as TE junctions

Lightweight, High-Strength Ductile Materials

Lightweight, damage-tolerant, and corrosion-resistant materials serve roles in transportation body and structural applications. These high-strength materials include composites, aluminum, magnesium, titanium, and high-strength steel alloys, hybrid materials, and polymer-based materials. Today, the use of such materials is limited by a variety of factors, including their relatively high cost, corrosion issues, forming and assembly challenges, and end-of-life materials management challenges.



How will it save energy and carbon?

- Performance at lighter weights increases mileage per gallon of fuel, reducing fuel use

Potential savings

- 1.5 mpg increase (~7%) per 250 lb reduction in automobile weight
- Fuel mileage gains for other types of vehicles, including aircraft

Time until commercialization

- 5–20 years

Gaps and Limitations to Overcome

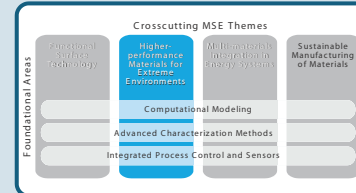
- Today's lightweight materials have poor corrosion and wear resistance. In particular, the surface properties of affordable lightweight alloys are often inadequate for high-wear environments.
- Few integration strategies exist for dissimilar materials systems, such as for automotive body structure. Interfacial properties of composites including dissimilar materials are unknown.
- No low-cost synthesis, processing, and manufacturing technologies exist for Ti, Mg, and composites that can meet targeted costs, weight reductions, and properties.
- Lightweight materials (e.g., composites) often contain a non-uniform distribution of phases.
- Inability to detect damage to low-cost, lightweight materials in-situ, and performing off-site analyses requires more energy

R&D Needs for Market Readiness

- Developing new materials (alloys, composites, polymers) with the desired properties and costs
- Improving corrosion resistance of these materials methods
- Developing new thermomechanical processing methods
- Establishing advanced joining process suited to these materials
- Enhancing the formability of lightweight materials
- Developing inexpensive material repair methods

Irradiation-Resistant Structural Alloys for Nuclear Applications

Nuclear applications require structural alloys that retain their strength, ductility, and dimensional stability when exposed to radiation levels up to 100 displacements per atom (dpa). These alloys must not only resist irradiation, but also offer superior mechanical strength and resistance to swelling, similar to oxide dispersion strengthened steels.



How will it save energy and carbon?

- Higher irradiation-resistance will enable better use (i.e., high burnup) of uranium in nuclear fission
- Increased fuel efficiency will increase the overall efficiency of nuclear electricity production with ultra-supercritical or supercritical water or other coolants
- New nuclear power plants will replace aging, inefficient fossil energy plants

Potential savings

- Doubling of plant service life (to greater than 60 years)
- 10x more energy derived from uranium fuel
- Additional 5%–10% improvement in overall nuclear electricity production efficiency
- Direct carbon avoidance

Time until commercialization

- 5–20 years to increase energy derived from fuel by a factor of 2
- Greater than 20 years to increase energy derived from fuel by a factor of 10
- Greater than 20 years to realize full electricity generation efficiency gains

Gaps and Limitations to Overcome

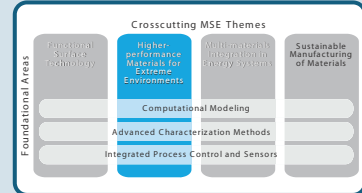
- Today's clad materials have inadequate toughness and corrosion-resistance. No existing clad can withstand the doses of radiation associated with high fuel burnup levels.
- Nuclear fission requires materials that resist neutron embrittlement, or are recoverable. Materials scientists' limited ability to deal with fission gases, fission product "attack," and swelling hinders the development of high burnup reactors.
- Existing nuclear materials have an excessively broad and unpredictable spread in properties.
- Different tailored and functionally-graded materials are inadequately compatible with each other under fusion reactor conditions due to a lack of processes to improve compatibility.

R&D Needs for Market Readiness

- Alloy development
- Novel surface treatments
- Testing procedures
- Thermomechanical processing
- Accelerated aging testing and prediction
- Long-term testing
- Radiation testing
- Nuclear testing within the U.S.
- Codes and standards, ASME standards, etc.

High-Pressure Hydrogen-Resistant Materials

Structural materials resistant to high-pressure hydrogen enable advancements in hydrogen storage and handling applications, such as hydrogen containers and compressors that could enable the more rapid commercial deployment of hydrogen fuel cell vehicles.



How will it save energy and carbon?

- High-pressure hydrogen-resistant materials will enable widespread use of hydrogen for automobiles by providing affordable hydrogen storage and compressor components

Potential savings

- Enables the commercialization of a hydrogen fuel cell car
- Avoids the use of carbon-based fuels

Time until commercialization

- 1–20 years

Gaps and Limitations to Overcome

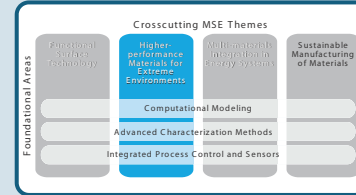
- Current predictive capability for new materials properties is inadequate to drive advancement in the solid-state storage of hydrogen.
- Automotive applications will require low-cost H_2 storage materials for ambient conditions and complex thermal loads. Given that no “clear winner” has emerged for room temperature operation, an unmet need exists for new alloys and compositions with greater hydrogen diffusion rates for the charge-discharge cycle, as well as faster kinetics for the take-up and release of hydrogen.
- Although the goal has been set at 6%, insufficient weight percent of hydrogen has been stored in the system for vehicle applications.
- Some solid-state H_2 storage materials suffer from ongoing surface poisoning issues.
- Inadequate methods exist to reduce hydrogen embrittlement.
- Fuel cell manufacturing is too expensive.
- Fuel cell reliability is poor due to start-stop fatigue in joints.

R&D Needs for Market Readiness

- Establishing new joining techniques
- Improving resistance to hydrogen embrittlement
- Improving formability of hydrogen storage materials
- Developing new alloy, potentially focusing on nonferrous metals
- Enhancing thermomechanical processing techniques
- Establishing hydrogen permeation barriers for storage materials

Collaborative, Comprehensive Materials Database

A collaborative, comprehensive materials database including images and material property and characterization data (e.g., conductivity, structure, microstructure data, diffusion, corrosion resistance, and viscosity) that is user-friendly, searchable, and relational stands to provide cross-cutting support for materials scientists working in highly diverse technical areas.



How will it save energy and carbon?

- Accelerates the development of advanced materials and reduces the development and product cost of materials science and engineering products that are designed to increase energy efficiency and/or accelerate the development of energy technologies that avoid the use of carbon-intensive fuels.

Potential savings

- Reduces the development time and cost of MSE products

Time until commercialization

- 1–20 years

Gaps and Limitations to Overcome

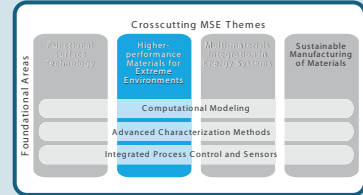
- No collaborative, comprehensive materials database exists.

R&D Needs for Market Readiness

- Code development
- Human/computer or user-friendliness interaction testing
- International collaboration
- Resolve Intellectual Property issues
- Data standardization
- Identify and resolve security issues
- Integration with existing digital materials infrastructure
- Exploitation of advanced techniques in knowledge generation (e.g. neural networks) and management

Predictive Materials Performance Code

Predictive calculations enable the design of novel materials across many application areas. A user-friendly materials code is able to predict quantitatively the chemistry, mechanical, and physical performance properties under various conditions of temperature, pressure, and strain as a function of time.



How will it save energy and carbon?

- Predictive calculations enable the design of novel materials across many application areas. A user-friendly materials code is able to predict quantitatively the chemistry, mechanical, and physical performance properties under various conditions of temperature, pressure, and strain as a function of time.

Potential savings

- Reduces the development and product cost of MSE products

Time until commercialization

- 5–20+ years

Gaps and Limitations to Overcome

- Materials scientists do not have access to adequate predictive capability for applications including modeling the range of potential thermoelectric materials and modeling solid state and high-capacity storage of hydrogen.
- Current materials testing procedures and capabilities, such as those that would provide improved materials lifetime predictions, are either unrealistic or insufficiently accelerated and coupled to models. A lack of good predictive life models particularly hinders advancements in higher-burnup nuclear reactors, particularly at extremes.

R&D Needs for Market Readiness

- Integrated disciplinary experiments and modeling
- Computer code development
- Developing the predictive model, incorporating multi-scale, time, and spatial elements over time
- Validation and verification by experiments
- Integrated computational materials engineering (ICME)
- 3D models, code, experimentation
- Multi-scale, time, and spatial

IV. MSE THEME 3: MULTI-MATERIALS INTEGRATION IN ENERGY SYSTEMS

Every energy system requires different materials working together to deliver desired functionality. Integrating new materials, including those with intrinsic heterogeneity like composites and smart materials, creates design and manufacturing challenges, especially as systems become more complex and service environments become more demanding. However, this approach also holds promise to yield significant energy and carbon emissions reductions in many parts of the U.S. energy sector. Specific examples are provided below.

- Broad use of low-cost carbon fibers and composites in vehicle manufacturing can reduce body weight by up to 50 percent and correspondingly reduce vehicle fuel consumption by 20 to 30 percent.
- Advances in low-cost, abuse tolerant, and long life cycle cathode materials for batteries can lead to transformational improvements in cost and efficiency of battery technologies.
- Low-cost fuel cells utilizing cheaper alternatives to platinum can promote a wider adoption of fuel cells for vehicular use. Together with improved vehicular efficiency and increased use of biofuels or synthetic fuels, this technology can lead to over 90 percent reduction in petroleum use by light-duty vehicles by 2050.
- Improved computational modeling capabilities in multi-materials science can allow researchers to simultaneously model material capabilities, engineering product performance and associated manufacturing processes, compressing overall development time for new materials and processes by up to 50 percent. In the best case, a 20-year development cycle can be reduced to less than 5 years by using new modeling capabilities.

Designing materials that can work reliably and deliver the desired functionality when integrated into a single system requires many innovations, including:

- New joining processes for disparate materials (e.g., by using lasers, plasma or chemical reaction to join materials)
- Creating low-cost composite materials with wide applicability
- Effective thermal management of materials and processes to improve the efficiency and reliability of energy systems
- Design and manufacturing of smart materials such as shape memory alloys and materials with embedded sensors for monitoring and verification
- Sensors to enable self-healing materials that can repair damage incurred during normal use
- Improving the ability to accurately predict the performance and reliability of disparate material systems to allow designers of energy systems to take full advantage of all material capabilities in order to maximize the efficiency and performance of the entire system

PRODUCT AND PROCESS INNOVATIONS

Substantial product and process innovations are required to fully realize the benefits of multi-materials integration. The following table outlines products and processes that, when commercialized successfully, can deliver significant energy and carbon savings. The highest-priority items—those that hold the greatest potential for delivering energy and/or carbon reductions—are identified by bold underlined text.

Table 3. Potential Product and Process Innovations – Multi-Materials Integration in Energy Systems

ENERGY APPLICATION AREA	MSE PRODUCT/PROCESS INNOVATION
Industrial Energy Efficiency	<p>Materials and processes to increase the efficiency of industrial heat exchangers used for converting heat into useful energy</p> <ul style="list-style-type: none"> • Thermally conductive polymers and polymer matrix composites • Next generation heat exchanger construction with dedicated heat recovery systems • New processing techniques for high-temperature, thin gauge materials for use in solar-thermal energy systems • New process for laser-based sintering of metals to fabricate complex parts • Ceramic matrix composites that can resist oxidation and corrosion under high-temperature conditions • Robust bearings and seals for operation under high-temperature conditions • New materials that change temperature when exposed to magnetic fields for use in environmentally-friendly refrigeration systems
Vehicle Energy Efficiency	<p>Materials for lighter and fuel-efficient vehicles</p> <ul style="list-style-type: none"> • <u>Low-cost carbon fibers and composites manufacturing processes</u> • Strong, lightweight, and layered (“sandwich-based”) materials having the density of magnesium and the strength of low-carbon steel • A new acoustic or ultrasonic process to increase material hardness and homogeneity of microstructures (e.g., electromagnetic acoustic transducer process) • New thermo-magnetic process to produce high-temperature alloys and other structural materials with enhanced strength and durability <p>Advanced processes and equipment for joining dissimilar materials</p> <ul style="list-style-type: none"> • Joining process for assembling multi-material structures • Solid-state joining process that retains original material strength (e.g. by using friction-stir welding techniques) • Highly adhesive coatings with improved functional grading and ceramic interaction to prevent materials interaction and corrosion • Next generation joining equipment manufacturing and quality assurance strategies
Energy Storage (Batteries)	<p>Materials to improve battery efficiency, usability, and storage life</p> <ul style="list-style-type: none"> • <u>High energy density, low cost battery cathodes</u> • Co-extrudable battery electrodes and separators (i.e., layers painted separately and stamped, extrusion of multiple layers simultaneously) • Core shell materials for use in battery cathodes (i.e., high energy cores surrounded by a safe long-life shell) • Batteries with long storage times for vehicle and electric-grid storage applications • Solid membranes with improved conductivity at normal working conditions for use in advanced Na-S batteries • High-volume manufacturing process for graphene used as anode material in Lithium-ion batteries
Nuclear Fission and Nuclear Fusion	<ul style="list-style-type: none"> • Ceramic matrix composite materials having oxidation- and corrosion-resisting properties for use in high temperature conditions
Hydrogen and Fuel Cells	<p>Low-cost, robust, multi-purpose fuel cells for use in automotive and electric grid applications</p> <ul style="list-style-type: none"> • <u>Low-cost fuel cell catalyst</u> • Improved and economically-priced interconnect seals for solid oxide fuel cells • Materials to absorb and store hydrogen gas at room temperature

Table 3. Potential Product and Process Innovations – Multi-Materials Integration in Energy Systems *continued*

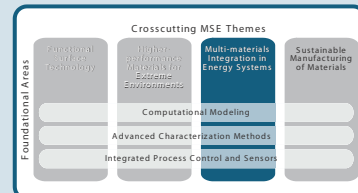
ENERGY APPLICATION AREA	MSE PRODUCT/PROCESS INNOVATION
Solar Energy	<ul style="list-style-type: none"> • Advanced membranes and durable, high temperature catalysts to produce liquid hydrocarbon fuels from the capture and solar-assisted transformation of carbon dioxide to syngas • Manufacturing processes to integrate electronic circuitry directly onto solar cells to reduce cost and improve reliability and efficiency • New materials with thermal conductivity better than that of copper and having low coefficient of thermal expansion for use in concentrating photovoltaic applications • New ceramic-based composite materials that can withstand high-temperature conditions • Salts with lower corrosivity and low melting temperatures (for storage of solar energy)
Integrated Process Control and Sensors	<ul style="list-style-type: none"> • Direct write processes for smart structural materials with built-in sensors to measure strain, temperature or other phenomenon and transmit data using wireless connectivity for use in photovoltaic and other energy systems
Computational Modeling	<ul style="list-style-type: none"> • Integrated computational materials engineering modeling package

The following summaries provide additional information about the top-priority product and process innovations in multi-materials integration. These summaries identify how the innovations will save energy, the potential

savings that could be realized through successful commercialization, their expected time to market, and the key R&D needs to move the technology from where it is today to market readiness.

Low-Cost Carbon Fibers and Composites Manufacturing Processes

Carbon fibers and composite materials consume less energy during their manufacture than the metals they replace. Their use also enables parts to be consolidated, creating lower-density and corrosion resistant materials and allowing for repairing of materials during their use. To be broadly used in energy systems, manufacturing costs must be lowered.



How will it save energy and carbon?

- Use of low-density composites can improve fuel consumption in vehicles and aircraft through weight reduction.
- Composite manufacturing processes can enable parts consolidation.
- Corrosion-resistant properties of composite materials can extend product lifetimes.
- Incorporation of structural carbon fibers in wind turbine blades leads to lighter blades, allowing longer blades to be supported by existing structure and resulting in better energy capture.

Potential savings

- A 10 percent reduction in vehicle weight leads to 4 to 6 percent savings in fuel consumption

Time until commercialization

- 5 years (composite materials manufacturing)
- 10 years (carbon fiber manufacturing)

Gaps and Limitations to Overcome

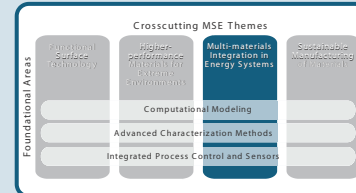
- Processes to produce complex geometries from lightweight materials are expensive and energy-intensive. No low-cost synthesis, net-shape processing, or manufacturing technologies exist that can meet targeted costs and properties for titanium, magnesium, and other composites.
- Prediction of final microstructure after processing into complex geometries is not currently possible.
- Processes to create composites are costly and time-intensive. Manufacturing of layered/hybrid systems for damage tolerance and corrosion resistance is only possible at high costs. In particular, the carbonization step is too energy-intensive.
- Fiber-substrate adhesion limits the strength of composites.
- Application of coating to composites is not straightforward.
- Availability of raw materials hinders the creation of materials for automotive lightweighting.

R&D Needs for Market Readiness

- High-volume, low-cost out of autoclave composite processes
- High volume, low-cost manufacturing processes to produce class A surface quality automotive body parts
- Metal matrix composites
- Low-cost, low-temperature carbonization process
- Design guidelines and predictive performance tools for composites and hybrid-composites

Joining Process for Assembling Multi-Material Structures

Joining of dissimilar materials enables the use of lighter-weight or greater strength materials with conventional metals. New joining processes stand to improve the corrosion-resistance properties, strength, and performance of the joined connections.



How will it save energy and carbon?

- Enables the use of multi-materials in automobiles, contributing to vehicle weight reduction by up to 50%
- Leads to increased system efficiencies due to improved heat exchanger design
- Enables joining of metals with ceramics, withstanding thermo-chemical fatigue over tens of years for solid oxide fuel cells

Potential savings

- 10 percent reduction in vehicle weight leads to 4 to 6 percent savings in fuel consumption

Time until commercialization

- 1-5 years

Gaps and Limitations to Overcome

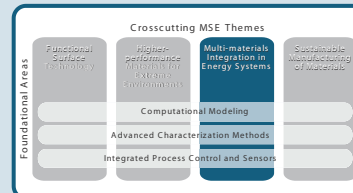
- Effectively joining metallurgically incompatible materials (e.g., joining light-weight aluminum to steel or magnesium to steel) is persistently difficult, hindering the development of lightweight vehicles. Strength, performance, and reparability at the interface of the joined materials are typically less than desired.
- Today's solid oxide fuel cells lack quality joining and seals, for example, to join ceramics with metals. Such seals will need to be able to operate at higher temperatures, and also provide improved ionic conductivity at lower temperatures.
- Thermal cycling stresses currently cause degradation of the joints on a heat exchanger. Current technology is generally inadequate for creating interconnects for differential temperature regime elements, e.g., high temperature to low temperature with different materials for the hot and cold ends.
- A novel, low-cost multi-alloy composite fabrication process is not yet available to provide to stiff and lightweight materials.

R&D Needs for Market Readiness

- Joining of steel to dissimilar materials (e.g., polymers)
- Solid-state joining processes
- Rapid thermal cycle processing
- Next-generation adhesive technology
- Solid free-form fabrication of metal alloys
- Heat compatibility issues

High Energy Density, Low-Cost Battery Cathodes

The cathode, along with the electrolyte and anode, is a key part of battery technology. High energy density, low-cost, abuse tolerant, and long cycle-life cathodes in particular have key MSE challenges that if overcome, would enable transformational battery technologies.



How will it save energy and carbon?

- Enables vehicle fleet electrification through the development of advanced batteries for electrical energy storage (EES)
- Enables integration of renewable energy electricity generation technologies through increased EES capabilities

Potential savings

- 10% energy savings from the integration of renewables into the grid
- Up to 100% carbon savings from vehicle fleet electrification

Time until commercialization

- 1-5 years for existing materials
- 5-20 years for new material discovery

Gaps and Limitations to Overcome

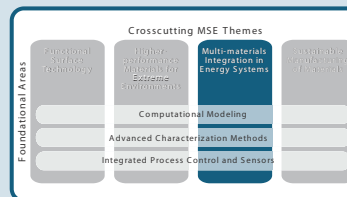
- Materials scientists have an inadequate understanding of solid electrolyte interfaces, high ionic-conductivity electrolytes at room temperature, and low environmental impact materials to enable improved performance and lower-cost battery materials, including new robust and compatible electrodes and electrolytes.
- Available battery materials with even moderate performance are expensive and not amenable to easy or large-scale processing. In particular, low-cost materials for large-scale energy storage and processing are not available.
- Both the positive and negative electrodes on automotive lithium-ion batteries are currently too expensive and heavy.

R&D Needs for Market Readiness

- Electrode fabrication processes compatible with new materials
- Low-cost precursors, preferably aqueous processing
- Stable electrolytes, e.g., at higher voltages
- Environmentally safe or recoverable materials
- Higher energy density materials, e.g., high energy core with a safe, long-life shell
- Materials development to identify high energy density, low-cost materials that intercalate lithium (lithium batteries)
- Compatibility to electrolyte

Low-Cost Fuel Cell Catalyst

The development of a low-cost polymer electrolyte fuel cell catalyst with cost equivalent of less than 10 grams of platinum per vehicle enables the commercial production and use of fuel cells at economic prices for a variety of vehicle-based and stationary applications.



How will it save energy and carbon?

- Enables wider adoption of alternative vehicle propulsion technologies which can save both energy and carbon
- Use of renewable sources for hydrogen in fuel cell may lead to even larger carbon and energy savings

Potential savings

- Petroleum use can be reduced by up to 90 percent and carbon emissions can be reduced from 10 to 100 percent, depending on the source of hydrogen

Time until commercialization

- 5 to 20 years

Gaps and Limitations to Overcome

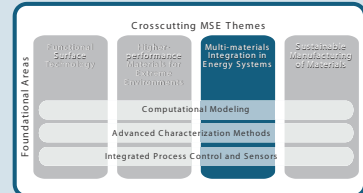
- Today's automotive fuel cells demand too much platinum for the fuel cell catalyst. A lower-cost fuel cell catalyst is needed to advance fuel cell technology for automotive and stationary applications.
- Next-generation hydrogen and fuel cell technologies will require more efficient oxygen reduction catalysts, nanostructured catalysts for hydrogen generation and carbon dioxide reduction, and efficient photocatalytic materials for hydrogen production.
- Room temperature hydrogen storage now relies on compressed hydrogen because no room-temperature absorbents exist.

R&D Needs for Market Readiness

- New materials for fuel cells (e.g., an affordable core with a platinum shell or a platinum-free material)
- Improved understanding of fuel cell chemistry (through morphological evaluations)
- Understanding of the oxygen reduction reaction in fuel cells
- Durability studies for fuel cells
- Improved understanding of surface kinetics
- Studies for long-term use of fuel cells

Integrated Computational Materials Engineering Modeling Package

An integrated computation materials engineering modeling package integrates materials information with engineering product performance analysis and manufacturing process simulations, enabling researchers to model materials-related processes and components (e.g., oxidation, joining, welding, brazing, electrodes, and electrolytes), help design functionally graded materials, and model accelerated degradation of materials during their use.



How will it save energy and carbon?

- Enables accelerated research and development of new materials and processes
- Allows for improved optimization of new materials and processes
- Shortens time to market for new materials and processes, accelerating energy and carbon savings

Potential savings

- 30 to 50 percent reduction in new material and process development time
- Reduction of a 10 to 20-year development cycle into 2 to 3 years, in the best cases

Time until commercialization

- Midterm (5 to 20 years) to develop detailed and reliable models
- Timeframe may vary depending on the type of modeling application
- Preliminary packages currently in use at Ford and GE

Gaps and Limitations to Overcome

- It is not yet possible to predict materials properties such as phase constitution, chemistry, reactivity, etc. Uncertainties in existing predictions have rarely been quantified.
- Predictions of materials lifetimes are often impossible in extreme environments with limited operating data or experience. Materials scientists have an inadequate understanding of multiple, synergistic environmental degradation modes (e.g., simultaneous pressure and cycling effects) on material lifetime.
- Multiple modeling tools are inadequately integrated with experimental tools for model verification, integrated across disciplines and scales, or quantitatively validated.
- Little progress has been made on process modeling or on science-based fuel performance codes with predictive capabilities.
- Computational modeling has not yet been able to provide a good understanding of the relationships among materials' history, microstructure, and properties. Relatedly, materials scientists' ability to control microstructures is underdeveloped.
- Non-destructive evaluation and remnant life modeling are not yet available based on the degradation mechanism.
- Many key materials do not have available life-cycle modeling.
- 2D modeling and characterization methodologies miss 3D effects.
- Specimen size may bias the answer for current test technologies.
- Multi-scale modeling and fundamental microstructure modeling are still immature. Effective multi-materials integration will require such modeling at all length and time scales, including of transient behavior.
- Computational methods are lacking for multi-phase and heterogeneous materials (e.g., solidification modeling of heterogeneous and multi-structure composites).
- In situ, real-time characterization, such as by using neutrons, is not yet available to materials scientists.
- Accelerating aging diagnostics and high-throughput testing are unavailable for storage batteries.
- Quantitative methods for neutron characterization are unavailable. Only poor visualization techniques exist for structure and composition of materials at the atomic level.

R&D Needs for Market Readiness

- Development of new models for oxidation, joining, electrodes, electrolytes and functionally gradient materials
- Improved predictive modeling capability for [damage] rate and materials lifetime
- Improved modeling of computational fluid dynamics
- Better understanding of failure mechanisms, chemical reactions, solid mechanics, and electrochemistry
- Modeling needs for the aerospace industry

V. MSE THEME 4: SUSTAINABLE MANUFACTURING OF MATERIALS

Manufacturing materials such as steel, aluminum, and cement is fundamentally energy-intensive. Other, lower-volume materials can be even more energy-intensive to produce due to the specialized processing techniques, low abundance in the earth (increasing mining and extraction energy requirements), or complex chemistries and compositions of the final material. Further, the waste of material resources, both during a product's manufacture and at the end of its life, can be substantial. Minimizing the loss of both energy and materials is at the core of sustainable manufacturing. Yet today's approaches for doing so often require unacceptably high costs. Breakthrough innovations are needed to achieve improvements to realize true sustainability in materials manufacturing. Such innovations hold great promise to generate energy- and carbon-intensity reductions. Examples are provided below.

- Net-shape processing cannot only reduce material waste in industry, but it can also produce metal components and composites with better material properties for enhanced vehicle energy efficiency.

- Energy storage technologies can be advanced via the use of earth abundant materials capable of high energy densities.
- Solar energy technologies can benefit from additive manufacturing techniques in the manufacturing of solar panel components.
- The efficiency of materials recycling and reuse can be increased through selective, high-throughput separation methods.

PRODUCT AND PROCESS INNOVATIONS

Material science and engineering innovations are needed to realize the new products and processes that can yield sustainable manufacturing. The following table outlines these products and processes that, when commercialized successfully, can deliver significant energy and carbon savings. The highest-priority items—those that hold the greatest potential for delivering energy and/or carbon reductions—are identified by bold underlined text.

Table 4. Potential Product and Process Innovations – Sustainable Manufacturing of Materials

ENERGY APPLICATION AREA	MSE PRODUCT/PROCESS INNOVATION
Industrial Energy Efficiency	<p>Enhanced Industrial Energy Efficiency</p> <ul style="list-style-type: none"> • Materials and processes for waste heat recovery • New, non-destructive methods for damage detection and damage monitoring on real structures • Novel electrolysis (e.g., low-temperature) for production of aluminum • Solar heating for process heat • Low-cost, small-scale combined heat and power (CHP) units that withstand harsh environments (for low-volume and low-temperature applications) • Lower cost regenerative systems for smaller applications (e.g., smaller burners, furnaces) • Refractory materials with longer life • Material substitutes for energy critical materials used in industrial processes (e.g., rare earth elements, precious metals) • More advanced surface processes for wear and impact resistance (e.g., laser shock, etc.) • Refractory materials with better insulating properties and non-wetting properties • New generation of low-cost and lower material-intensive catalysts

Table 4. Potential Product and Process Innovations – Sustainable Manufacturing of Materials *continued*

ENERGY APPLICATION AREA	MSE PRODUCT/PROCESS INNOVATION
Vehicle Energy Efficiency	<p>Near-Net-Shape Materials and Products</p> <ul style="list-style-type: none"> • <u>Net shape processing of structural metals</u> • <u>Additive manufacturing of components and systems</u> <p>Low-Cost, Lightweight Materials for Transportation</p> <ul style="list-style-type: none"> • <u>Low-cost processing and energy reduction technology for metals</u> • Joining in solid state of metallic materials (friction stir processes) of typically unweldable or dissimilar materials • Advanced conversion of low-cost carbon fiber to reduce energy consumption by 50% • In-situ production of metal composites (molten metal - Ti, Al, Mg; metal matrix nano-composites with uniform distribution through casting and/or powder metallurgy) • Develop continuous manufacturing processes (i.e., eliminate steps) for lightweight metals • New methods to repair damaged materials (cold spray, friction stir processing) • Methods for thermal barrier coatings with higher temperature ranges • Methods to build layered materials and smart materials with embedded sensors and self-repair capabilities • New design methods (integrated) for low safety factors
Energy Storage	<p>Materials for Low-Cost Vehicle Batteries</p> <ul style="list-style-type: none"> • Processing of materials beyond lithium for batteries • Processing of materials for low-temperature sodium beta batteries • Low-cost ceramic nano-fiber filters and membranes produced by non-woven paper/fabric techniques for high and low temperature applications <p>Energy Storage Materials with High Energy Density (Earth Abundant)</p> <ul style="list-style-type: none"> • Printing of battery and capacitor parts for energy storage (utility scale) • High-stability, high-surface-area platinum structures • Production of low-cost, no-fluorine, low-humidity proton exchange membranes • Production of low-cost ionic liquids for energy storage
Materials Recycle and Reuse	<p>Energy Efficient Recycling of Materials</p> <ul style="list-style-type: none"> • <u>Separation of materials for recycling</u> • Recycling processes for rare earth and refractory metals • Sorting systems to remove contamination and sort mixed materials into high grade/pure materials for recycling • More efficient transportation of molten metals • Systems to measure and quantify materials in feed scraps (total composition of scrap stream) • ‘Smart’ analytical lab in the recycling plant • Recycling of high and low level nuclear materials
Solar Energy	<p>Low-Cost, Low Energy Manufacturing of Solar Panels</p> <ul style="list-style-type: none"> • Additive (low-cost, low waste) manufacturing of components and systems (e.g., thermo-electrics; solar panels; novel inks and printing technologies) • Self-assembling nano-structures for solar absorption • Non-vacuum deposition of photovoltaic (PV) materials on low-cost substrates • High-volume, lower-purity silicone substrates for solar panels by electrochemical deposition

Table 4. Potential Product and Process Innovations – Sustainable Manufacturing of Materials *continued*

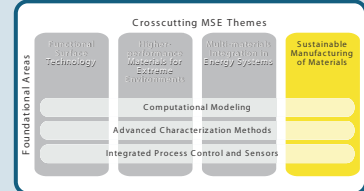
ENERGY APPLICATION AREA	MSE PRODUCT/PROCESS INNOVATION
Computational Modeling	<ul style="list-style-type: none"> • Modeling integrated across all length scales (atomistic to processing), including economics, energy, and life-cycle analysis • Computational design of novel 3D material architectures at the micro-scale • Property prediction modeling tools for metals and composites (dynamic and non-linear)
Advanced Characterization Methods	<ul style="list-style-type: none"> • Integrated multi-sensor vision/spectrographic technology systems employing x-ray fluorescence (XRF), x-ray transmission (XRT), laser-induced breakdown spectroscopy (LIBS), optic, and neutron irradiation for rapid characterization
Integrated Process Control and Sensors	<ul style="list-style-type: none"> • <u>Real-time sensor technology for gases and molten metals</u>
Building Materials	<ul style="list-style-type: none"> • Cement that cures/heals faster and at lower temperatures and therefore releases less CO₂ in the chemical reaction process

The following summaries provide greater information about the highest rated product and process innovations in sustainable manufacturing of materials. These summaries identify how the innovations will save energy,

the potential savings that could be realized through successful commercialization, their expected time to market, and the key R&D needs to move the technology from where it is today to market readiness.

Net-Shape Processing of Structural Metals

Net-shape processing of metals such as Al, Ti, and Mg include thixocasting, rheo-casting, and powder metallurgy – all at lower cost and with better material properties. Other processes include net-shape forging, castings, and laser processing.



How will it save energy and carbon?

- Reduces scrap, thereby reducing embedded energy within processes such as melting, casting, rolling, etc.
- Eliminates or reduces the number of processing steps, such as melting and re-melting steps
- Achieves downstream savings in lightweight transportation manufacturing

Potential savings

- 35% energy savings through scrap reduction
- 5% energy savings in processing steps
- 10% weight reduction results in 6% fuel savings in transportation

Time until commercialization

- 5 to 20 years

Gaps and Limitations to Overcome

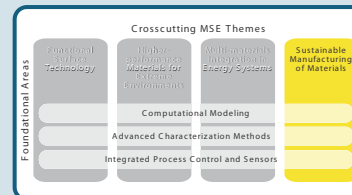
- Creation of automotive lightweighting composites is currently too costly and requires lengthy process times to produce targeted properties.
- Magnesium formability is highly challenging.
- After today's processing techniques are applied to lightweight materials, prediction of final microstructure is not possible.
- Today's casting is done with high extra material to reduce surface defects and eliminate warping.
- Due to shortcomings in computational design, materials scientists are unable to "tailor" microstructures to needed specifications.

R&D Needs for Market Readiness

- Computational modeling of casting, injection, and other processing steps
- Optimization of heat treating processes
- Casting process research
- Powder metallurgy research
- Welding and joining research

Additive Manufacturing of Components and Systems

Additive (consolidating two or more parts into a single design), low-cost, low-waste manufacturing of components and systems, such as thermoelectrics and solar panels.



How will it save energy and carbon?

- Reduces scrap and lessens use of energy-intensive materials, which also lowers carbon footprint
- Facilitates technology for waste heat recovery and other processes

Potential savings

- 50% embedded energy savings in the manufacturing of flexible photovoltaic cells/other electronics, and bulk near-net shape components such as metals, ceramics, and thermo-electrics

Time until commercialization

- Between 1 to 20 years

Gaps and Limitations to Overcome

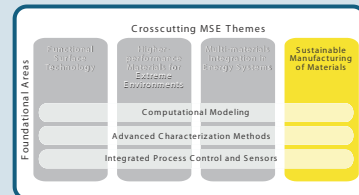
- Today's solar and thermoelectric materials are processed in batches rather than in a continuous manner. Low-cost processing of photovoltaics does not currently exist.
- Materials for high-temperature receiver technology for solar thermal applications currently meet temperature limitations at about 1,000°C, while continuous operating temperatures are expected to remain between 500°C and 1,000°C.

R&D Needs for Market Readiness

- Developing capabilities for multi-material flexibility, providing multiple materials capable of performing at comparable levels
- Advancing self-assembly of materials (i.e., formation of molecules into specific structures), with particular emphasis on materials that offer specific properties, such as increased corrosion resistance
- Developing capabilities for large-volume synthesis of precursor materials

Low-Cost Processing and Energy Reduction Technology for Metals

New, low-cost, energy-efficient, primary reduction and processing technology for titanium, aluminum, and magnesium.



How will it save energy and carbon?

- Because of its higher energy efficiency than conventional processes, this technology saves energy in the reduction of titanium, aluminum, and magnesium.

Potential savings

- Between 5% to 20% energy efficiency improvements in the reduction of titanium, aluminum, and magnesium

Time until commercialization

- Greater than 20 years

Gaps and Limitations to Overcome

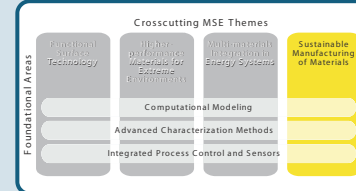
- Multi-sensor, integrated spectrum devices and software for solid, liquid, and gas process control, such as metal ion sensors for molten metal processing, are not available

R&D Needs for Market Readiness

- Develop improved electrodes for processing technologies
- Develop novel, low-temperature electrolytes
- Advance carbothermic reductions (high-temperature chemical reactions that use carbon as the reducing agent) of aluminum

Separation of Materials for Recycling

Selective separation of materials allows for increased recycling rates and reduced solid waste streams.



How will it save energy and carbon?

- Facilitates recycling of energy-intensive materials, saving embedded energy (energy used to make, market, and recycle the product)

Potential savings

- Improves recycling rates by 5% to 10%, which results in embedded energy savings

Time until commercialization

- Between 1 and 5 years

Gaps and Limitations to Overcome

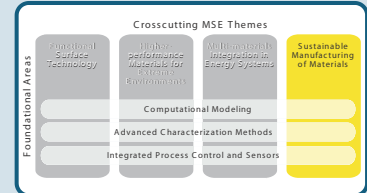
- Recycling processes for carbon fiber composites that preserve properties are not currently available at affordable costs.
- Inadequate systems exist for quantifying materials in scrap streams.
- Current processes are incapable of sorting dirty, low-grade materials into high-grade, pure materials. Systems to remove physical contaminants are poor, and current elemental removal systems (selective separations) are inefficient.
- Rapid screening processes and efficient systems for sorting have not yet been developed.
- The inability to reuse lower-grade scrap in vehicles poses a challenge.
- Reliance on inefficient combustion heating in thermal processes for recycling is a problem. There is a need for low-temperature recycling processes.

R&D Needs for Market Readiness

- Develop better technologies for screening and sorting of materials.
- Develop high-throughput, multi-sensor approaches to identify mixed materials (e.g., metal alloys, plastics).
- Develop low-temperature recycling processes.

Real-Time Sensor Technology for Gases and Molten Metals

Advanced characterization and sensors are needed for damage detection in the processing and service of high-performance materials. Multi-sensor, integrated spectrum devices and software would serve to enable solid and liquid process control and material identification (e.g., metal ion sensors for molten metal processing). Real-time sensor technologies facilitate improved control in the various steps involved in the processing of gases and metals, such as melting, heat treating, and combustion, across the manufacturing sector.



How will it save energy and carbon?

- Provides real-time control optimization, minimizing energy lost during processing steps

Potential savings

- 15% process efficiency gains in the production of plastics, metals, and other materials

Time until commercialization

- Between 1 to 20 years; applying sensors to Al and Ti processes are shorter term, while processes for cast alloys and Ni-based materials are mid-to-longer term

Gaps and Limitations to Overcome

- Cost-effective material integration for embedded sensor technology is yet to be developed.
- Multi-sensor, integrated spectrum devices and software would serve to enable solid and liquid process control and material identification (e.g., metal ion sensors for molten metal processing).
- Validated model-based closed loop controls often do not exist.

R&D Needs for Market Readiness

- Developing sensors or remote-sensing technologies for high temperature environments
- Developing model-based, closed-loop controls to optimize processes in real time

VI. NEXT STEPS

The previously published Vision Report of the Energy Materials Blue Ribbon Panel combined with this Opportunity Analysis for Materials Science and Engineering have culminated in identification of a set of important areas for product and process innovation. These innovations offer both performance breakthroughs and radical cost reduction opportunities which, if realized, could significantly impact the United States' progress toward enhanced sustainability and economic growth.

In the near term, the MSE community in government, the federally funded research laboratories, academia, and industry can begin to immediately pursue breakthrough innovations in the opportunity areas identified in this document by structuring projects and programs to focus on these key areas. Further,

a significant investment in Integrated Computational Materials Engineering (ICME) will ensure that this foundational tool set will offer the enabling power needed to accelerate progress.

As a next step, it is necessary to focus on each of the high-priority areas identified in this report in greater depth to establish specific performance goals needed to realize maximum impact but also to identify the R&D pathways needed to accomplish those goals in an accelerated timeframe that reflects the urgency of the issues. This detailed analysis should be a key element of Phase III of this work, resulting in clearly defined and compelling impacts for each innovation area coupled with R&D roadmaps for realizing this impact. TMS and the MSE community stand ready to assist in moving this process ahead.

APPENDIX A: REFERENCES

Bourell et. al., eds. 2009. "Roadmap for Additive Manufacturing: Identifying the Future of Freeform Processing." <http://wohlersassociates.com/roadmap2009.pdf> (accessed 23 December 2009).

Committee for the National Academies Summit on America's Energy Future. 2009. "America's Energy Future: Technology and Transformation." (accessed 7 September 2010).

Materials UK Energy Review 2007. "Energy materials—a strategic research agenda." 2007. http://www.matuk.co.uk/docs/1_StrategicResearchAgenda%20FINAL.pdf (accessed 3 December 2009).

McKinsey Global Energy and Materials. 2009. "Unlocking Energy Efficiency in the U.S. Economy." (accessed 7 September 2010).

The Minerals, Metals, and Materials Society. Linking Transformational Materials and Processing for an Energy Efficient and Low-Carbon Economy: Creating the Vision and Accelerating Realization. Vision Report of the Energy Materials Blue Ribbon Panel in support of the U.S. Department of Energy, Energy Efficiency & Renewable Energy, Industrial Technologies Program. 2010.

U.S. Department of Energy, Basic Energy Sciences Advisory Committee. Science for Energy Technology: Strengthening the Link between Basic Research and Industry. Washington, DC: Argonne National Laboratory, 2010.

U.S. Department of Energy, Energy Information Administration, 2010. "Annual Energy Outlook 2010: With Projections to 2035." accessed 7 September 2010).

U.S. Department of Energy, Energy Information Administration. "Table 1.7 Primary Energy Consumption per Real Dollar of Gross Domestic Product." Monthly Energy Review. November 2010. http://www.eia.doe.gov/emeu/mer/pdf/pages/sec1_16.pdf.

U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE), Office of Industrial Technologies (OIT). 2000. "Mining Industry of the Future Mineral Processing Technology Roadmap." <http://www1.eere.energy.gov/industry/mining/pdfs/mptr roadmap.pdf> (accessed 22 December 2009).

U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE), Office of Industrial Technologies (OIT). "Roadmap for Process Heating Technology: Priority Research and Development Goals and Near-Term Non-Research Goals to Improve Industrial Process Heating." http://www1.eere.energy.gov/industry/bestpractices/pdfs/process_heating_0401.pdf (accessed 28 January 2010).

U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE), Office of Industrial Technologies (OIT). 2000. "Vision 2020 Chemical Industry of the Future: Technology Roadmap for Materials." http://www1.eere.energy.gov/industry/chemicals/pdfs/materials_tech_roadmap.pdf (accessed 4 February 2010).

U.S. Department of Energy (DOE), Office of Science (OS), Office of Basic Energy Sciences (BES). "The 'Basic Research Needs' Workshop Series." http://www.science.doe.gov/bes/reports/files/BRN_workshops.pdf (accessed 12 December 2010).

U.S. Department of Energy (DOE), U.S. Climate Change Technology Program. "Strategic Plan." <http://www.climatechange.gov/stratplan/final/CCTP-StratPlan-Sep-2006.pdf> (accessed 4 February 2010).

U.S. Photovoltaic Industry Roadmap Steering Committee. 2003. Solar-Electric Power: The U.S. Photovoltaic Industry Roadmap. <http://www.nrel.gov/docs/gen/fy03/30150.pdf> (accessed 22 December 2009).

World Resources Institute. "A Roadmap for a Secure, Low-Carbon Energy Economy." <http://www.wri.org/publication/roadmap-for-a-secure-low-carbon-energy-economy> (accessed 4 February 2010).

APPENDIX B: ACRONYMS

ANL	Argonne National Laboratory	MSE	materials science and engineering
ASTM	standards development organization originally known as the American Society for Testing and Materials	NAS	National Academy of Sciences
CCS	carbon capture and sequestration	n-type	negative type (semiconductor)
CHP	combined heat and power	ODS	oxide dispersion strengthened
CMC	ceramic matrix composite	P	pressure
CPV	common pressure vessel	PAFC	phosphoric acid fuel cell
CTE	coefficient of thermal expansion	PCHX	heat exchanger made from thermally conductive polymer matrix composites
DMFC	direct methanol fuel cell	PEMFC	proton exchange membrane fuel cell
dpa	displacements per atom	PMC	polymer matrix composite
EIM	energy-intensive manufacturing	p-type	positive type (semiconductor)
EMAT	electromagnetic acoustic transducer	PV	photovoltaic(s)
EV	electric vehicle	PVD	physical vapor deposition
FSW	friction-stir welding	RFID	radio-frequency identification
GMCE	giant magnetocaloric effect	RTP	room temperature and pressure
HEV	hybrid electric vehicles	SEI	solid electrolyte interphase
HX	heat exchanger	SOFC	solid oxide fuel cell
ICME	Integrated Computational Materials Engineering	T	temperature
IP	intellectual property	TBC	thermal barrier coating
JOM	The member journal of TMS	TCE	thermal coefficient of expansion
k	thermal conductivity	TE	thermoelectric
LED	light-emitting diode	USABC	United States Advanced Battery Consortium
LIBS	laser-induced breakdown spectroscopy	XRF	X-ray fluorescence
MCFC	Molten carbonate fuel cell	XRT	X-ray transmission
MMV	Multi-materials vehicle	ZT	thermoelectric figure of merit

APPENDIX C: LIST OF PARTICIPANTS

Functional Surface Technology Technical Working Group

Arvind Agarwal	Florida International University
Raghavan Ayer	Exxon Mobil
Clark Cooper	National Science Foundation
Mike Dugger	Sandia National Laboratories
Jonah Erlebacher	Johns Hopkins University
Steven George	University of Colorado at Boulder
Jan Herbst	GM R&D
Yancy Riddle	UCT Coatings
Dan Sordelet	Caterpillar
Götz Vesper	University of Pittsburgh
Zhenyu Zheng	ORNL
Brajendra Mishra	Colorado School of Mines (Group Chair)

Higher-Performance Materials Technical Working Group

Bill Brindley	Rolls Royce Corp
Ivan Cornejo	Corning Incorporated
Thomas Felter	Sandia National Laboratories
Warren Garrison	Carnegie Mellon University
Brian Gleeson	University of Pittsburgh
Wayne King	Lawrence Livermore National Lab
John Lewandowski	Case Western Reserve University
Xingbo Liu	West Virginia University
Peter Tortorelli	Oak Ridge National Lab
Bill Tredway	United Technologies Research Center
Patrice Turchi	Lawrence Livermore National Lab
Brian Wirth	ORNL/University of Tennessee
Chris Wolverton	Northwestern University
Steve Zinkle	Oak Ridge National Laboratory
George Spanos	TMS (Group Chair)

Multi-Materials Integration Technical Working Group

Glenn Daehn	Ohio State University
David Dietrich	Boeing
Jerry Gould	Edison Welding Institute
Darrell Herling	Pacific Northwest National Lab
Robert Hyers	University of Massachusetts
Bruce Kelley	Sandia National Laboratories
Gerry Ludtka	Oak Ridge National Lab
Jaime Marian	Lawrence Livermore National Laboratory
Angelo Mascarenhas	National Renewable Energy Laboratory
Mark Mathias	General Motors Research
Michael Wixom	AI23Systems
Carl Zweben	Consultant, Zweben Composites and Advanced Thermal Materials
Warren Hunt	TMS (Group Chair)

Sustainable Manufacturing of Materials Technical Working Group

John Barnes	Lockheed Martin Aeronautics
Cindy Belt	Superior Industries
Craig Blue	Oak Ridge National Laboratory
James Evans	UC-Berkeley
Jackie Isaacs	Northeastern University
Randy Kirchain	Massachusetts Institute of Technology
Anantha Krishnan	Lawrence Livermore National Laboratory
Diana Lados	Worcester Polytechnic Institute
Ramana Reddy	University of Alabama
Mark Smith	Pacific Northwest National Laboratory
Susan Smyth	GM Research
David Spencer	wTe, Inc.
Ellen Stechel	Sandia National Laboratories
Brian Thomas	University of Illinois; Urbana-Champaign
Ray Peterson	Aleris International (Group Chair)

