On July 5th, 2016, The University of New Mexico (UNM) hosted the Southwest Regional Energy Innovation Forum, bringing together leading experts from academia, national laboratories and industry from the states of New Mexico, Arizona, Utah, Colorado and Idaho. This Forum was held in response to the Department of Energy’ (DOE) Mission Innovation initiative. We chose the theme of Materials Technologies for Clean Energy because of the significant contributions to advances in clean energy that have been made by innovators and researchers from throughout the Southwest Region. Panel members discussed the state of materials technology and the greatest challenges in hydrogen technology, solar conversion, electrical storage and nuclear energy.

Panelists highlighted the latest commercialized and emerging technologies in each of the four areas from the standpoint of materials-enabling breakthroughs, and presented potential revolutionary new approaches to clean energy production and utilization that will be enabled by advances in new materials technologies. In many cases the articulated needs, ideas and approaches overlapped between the different clean energy technologies explored, thus suggesting a fundamental synergy that is inherent in early stage innovation through materials research and integration. The need for critical experimental research, in conjunction with predictive modeling for materials properties, and emerging modes of collaboration between academia, the national laboratories, and industry were detailed and explored.
Years of gas, coal, and coal-bed methane mining and processing have rendered the “Four Corners” area a methane hot spot, providing an urgent impetus for rapid deployment of clean energy alternatives. It is both fortuitous and a tremendous advantage that the Region hosts a diversity of specialists in materials research and translation for clean energy applications. The Southwest Region is home to the National Renewable Energy Laboratory (NREL), Los Alamos National Laboratory (LANL), Sandia National Laboratories (SNL), and Idaho National Laboratory (INL), as well as to several top research universities, whose intellectual and technological capabilities have been leveraged into various multi-institutional, multi-sector collaborations.

**The July Energy Innovation Forum identified four important characteristics that make the Southwest Region uniquely poised to address the partnership goals of the Mission Innovation Initiative:**

1. There is a tremendous technological advantage in deliberately coupling fundamental research, development and integration of **new materials technologies** to the need for revolutionary advances in clean energy sources and processes. Thus a partnership devoted to energy materials development will form the foundation for expansion of the nation’s clean energy future.

2. The Southwest Region is a **national leader** in **materials research and development for energy applications** and is an established **hub** for **energy materials innovation** and **commercialization**.
3. Existing and well-established public/private partnerships within the Southwest Region can be leveraged in the development of materials solutions for clean energy and can be further enhanced as part of a regional partnership.

4. The Southwest Region is uniquely positioned intellectually and geographically to integrate and coordinate a multi-sector effort that can serve as a model for future, expanded programs in other Regions.

In conclusion, the Southwest Region will play an essential role in the development of materials to secure a clean energy future and will be central to the U.S. meeting its obligations under Mission Innovation.
The need for implementing better, low-carbon, clean energy technologies is becoming more urgent as average global temperatures increase, leading to rises in sea levels, persistent drought, encroachment of tropical diseases and severe weather events. The rapid deployment of innovations within the diverse spectrum of clean energy solutions and processes that can significantly reduce the emission of greenhouse gases is vital in mitigating the threats posed by climate change.

Last year President Obama announced at the United Nations Climate Summit in Paris the joint launching of Mission Innovation, a new twenty-one-member initiative that commits each partnering country to double their respective clean energy research and development (R&D) investment over five years. Mission Innovation seeks to accelerate the development of clean, carbon-reducing energy technologies throughout the energy sector in an effort to transform energy markets and create additional commercial opportunities in clean energy.

Through Mission Innovation, the U.S. has pledged to increase its energy R&D budget by 20% in 2017, with a concomitant $30 billion investment among the group of 21 members over five years. In a separate, complementary private sector-led effort, the Breakthrough Energy Coalition has pledged unprecedented levels of private capital investments to accelerate the development of clean energy solutions. The Breakthrough Energy Coalition is focused on early-stage, high risk innovations with the potential to reach scale-up mode quickly.
On July 5th, 2016, UNM hosted the Southwest Regional Energy Innovation Forum to explore how new materials technologies can enable clean energy devices and processes and bring transformative low carbon energy solutions to market. Experts from academia, industry and four national laboratories in New Mexico, Colorado, Arizona, Utah and Idaho came together to discuss materials for specific clean energy technologies of particular import to the Region, including fuel cells, solar conversion, battery storage and nuclear energy.

The Forum was a resounding success. Vigorous discussions identified many promising areas for future development. It also focused on overcoming the challenges to partnerships between academia, the national laboratories and industry and the overwhelming benefits to forming productive collaborations that will be necessary to address the grand challenge of developing viable solutions to combat climate change.

In attendance were the U.S. Secretary of Energy, Dr. Ernest Moniz; U.S. Senators from New Mexico, Tom Udall and Martin Heinrich; UNM President, Dr. Robert G. Frank; UNM Vice President for Research, Dr. Gabriel P. López; Director of the Los Alamos National Laboratory, Dr. Charles McMillan; and other distinguished participants representing academia (70), national laboratories (25), industry (23), the government sector (15) and NGOs (3), for a total of 136 participants.
“[There is] no doubt about the centrality of materials to so many of the energy technologies that we still need to invent and deploy.”

- Secretary Moniz

This impressive group of highly experienced policy leaders, researchers, innovators and entrepreneurs came together with a clear and common purpose, and the Forum clearly demonstrated the potential for a diverse group of constituencies to address important energy challenges, including:

- how advancements in materials technologies can help catalyze the development of revolutionary clean energy solutions;
- which technologies have near term potential in transforming the sector;
- what are the leading barriers to new materials development in each of the four areas;
- what steps do researchers, industry, and governmental officials need to take to help foster new technology developments;
- how to make clean energy technologies more affordable and whether affordability is the main obstacle to commercialization;
- what regulatory or other barriers prevent advancement;
- what manufacturing issues are limiting or could enable clean energy technologies; and
- what breakthroughs in manufacturing support getting the best materials into the market.
**Why the Southwest Region?**

In 2014, the “Four Corners” area of New Mexico, Arizona, Colorado and Utah was found to contain some of the highest levels of atmospheric methane in the country. The persistence of these high methane levels for more than a decade indicates the source is likely from established gas, coal, and coal-bed methane mining and processing. Because methane is 25 times more potent a greenhouse gas than carbon dioxide, the Region has the serious and time-sensitive task of finding energy alternatives. This urgency is compounded because the Southwest Region is also extremely vulnerable to prolonged droughts that are increasing in frequency with climate change.

While it is on the front lines of economic and security concerns related to climate change, the Southwest is also at the forefront of innovation in the area of materials technologies for clean energy. Excellence in materials research for energy applications has long been a hallmark of DOE research resources in the Southwest Region, including the National Renewable Energy Laboratory (NREL), the Los Alamos National Laboratory (LANL), the Sandia National Laboratories (SNL), and the Idaho National Laboratory (INL).

These national assets have a long history of close collaboration with the Region’s major research universities including UNM, Arizona State University, the University of Colorado, and the University of Utah, each of which have major federally funded research centers focused on materials research. All of these research institutions (i.e., academic and DOE) have also developed robust technology transfer, commercialization and industrial partnerships that link the requisite fundamental research expertise to R&D and commercial infrastructure necessary to dramatically accelerate public and private global clean energy innovation and quickly move new technologies out of the laboratory and into the commercial sphere.
Why Materials?

Recent growth and vibrancy of research institutions and the industrial sector in the greater Southwest Region, enhanced by increased collaborations with DOE laboratories, makes the Region superbly poised to undertake the challenges of developing clean energy solutions through new innovations in materials technologies. There are several reasons why the Southwest Forum was designed to focus on materials development for clean energy solutions. These include the facts that: 1) new materials technologies have been shown to be central to innovation in many, if not all, recently developed clean energy technologies; 2) the Southwest Region has been a leader in development of materials technologies for energy applications; and 3) new materials technologies can cut across and have impact on a number of new types of clean energy technologies, and thus can harness essential innovations from a large and diverse research and development community that will lead to faster integration of revolutionary energy technologies into large scale distributed networks.

Energy materials researchers and innovators in the Southwest Region routinely take advantage of the natural synergies provided by local DOE laboratories, universities and industry. A primary example is provided at UNM’s Center for Micro-Engineered Materials, which brings together academic and SNL-affiliated researchers (some with formal joint appointments) and which is co-housed within the UNM/SNL Advanced Materials Laboratory. Collectively, this unique resource is noted for its world class innovations in nanomaterial synthesis (including electrocatalytic and other materials for hydrogen fuel cell technology) and integration through 3D printing and advanced additive
manufacturing. These innovations have led to the formation of important strategic alliances with powerhouses in the energy (e.g., IRD Fuel Cells, LLC), energy materials (e.g., Ceramatec) and transportation (e.g., General Motors, Toyota/Daihatsu, Nissan/Renault) industries, as well as to promising, new commercial entities (e.g., Pajarito Powder, LLC). Similarly, the NSF-DOE Engineering Research Center (ERC) on Quantum Energy and Sustainable Solar Technologies (QESST), which is headquartered at Arizona State University—which includes the Center for High Technology Materials at UNM and the National Center for Photovoltaics at NREL as key partners—engages closely with a wide range of companies in the solar energy arena.

Each of the DOE national laboratories (INL, LANL, NREL, SNL) that participated in the Forum have extensive infrastructure and strategic assets devoted to fundamental and applied materials research for clean energy innovation. These include the DOE’s Office of Science Center for Integrated Nanotechnologies (SNL/LANL), the Los Alamos Neutron Science Center, NREL’s Materials Science Center, INL’s Materials and Fuels Complex, and the Joint Center for Energy Storage Research, which is headquartered at Argonne National Laboratory, but also includes research groups at SNL, NREL, University of Colorado and University of Utah. To augment these DOE resources in energy materials research, the Southwest Region enjoys funding from a rich pallet of NSF fundamental (Colorado School of Mines/NREL Renewable Energy Materials Research Science and Engineering Center (MRSEC), Utah MRSEC, and University of Colorado Soft Materials MRSEC) and applied research centers (QESST-ERC, Nanomanufacturing
To translate energy materials innovation into the marketplace, the Southwest Region is home to a burgeoning clean energy industry that includes many established companies, many start-up companies and several prominent incubation initiatives. Fourteen different companies from the clean energy industrial sector attended the conference along with several State and local organizations dedicated to fostering economic development in the energy sector (see Appendix 1). An important example is Innovate ABQ, Inc., a public-private partnership launched by the Board of Regents of UNM in late 2014. This unique concept will cohouse research and commercial labs with science and technology companies and business incubators in a single location in the heart of downtown Albuquerque. It will catalyze cross-pollination of ideas and technology, thus providing new high tech jobs and economic opportunity to Albuquerque and the Southwest Region. Given the proven track record of universities and national laboratories in this Region to generate advanced, commercially viable materials technologies for clean energy, energy materials will comprise a major portion of the technology commercialized through Innovate ABQ.

“By focusing on fundamental discovery, translation and commercialization of revolutionary advances in materials, the Southwest Region captures the most competitive and impactful ideas from a highly diverse spectrum of academic, federal and industrial researchers and innovators.”

- Dr. Gabriel López
Forum Organization and Content

The Energy Innovation Forum was opened with addresses by UNM Vice President for Research, Gabriel P. López, UNM President Robert G. Frank, U.S. Senators from New Mexico, Tom Udall and Martin Heinrich, and Secretary of Energy Ernest Moniz. Four panels, each representing one key clean energy technology, were convened as part of the one-day Forum. Each panel consisted of representatives from academia, industry and the four Regional DOE laboratories. Panelists presented a thirty-minute discussion regarding breakthroughs and future needs in their respective fields, followed by a question and answer period with members of the audience. Summaries of each of the four panels, with conclusions and points of nexus, follow.

Panel I: Enabling Materials For Hydrogen Technology and Infrastructure

Panel I consisted of Dr. Bryan Pivovar (Senior Scientist, Leader of Hydrogen and Fuel Cell Research, National Renewable Energy Laboratory; moderator); Mr. Thomas Stephenson (CEO & Chairman of Pajarito Powder, LLC); Dr. Plamen Atanassov (Distinguished Professor of Chemical and Biological Engineering and Chemistry & Chemical Biology, Director of the Center for Micro-Engineered Materials, University of New Mexico); and Dr. Rod Borup (Program Manager for Fuel Cell and Vehicle Technologies, Team Leader for Fuel Cells, Los Alamos National Laboratory).

Greenhouse gas emissions result primarily from the combustion of fossil fuels to provide energy to a multi-sector global economy. In order to lower greenhouse gas emissions, it will be necessary to either capture the emissions or to utilize zero-carbon energy sources. Energy needs in the U.S. are too high and too diverse for wind and solar alone to meet. In this regard, hydrogen has been identified as a zero-emission energy carrier with high potential for impact in the transportation sector and in energy storage applications.

Therefore, introducing hydrogen as an additional energy fuel will aid the U.S. in meeting its environmental and national security goals of reducing greenhouse gas emissions by 83% by 2050, with a concomitant reduction in energy imports. Hydrogen is an enabler of green processes and has the capacity to deeply decarbonize the energy system, including industrial processes and transportation, which are responsible for over 50%
of carbon dioxide emissions. Hydrogen can also help penetration of renewables by taking excess renewable capacity and turning it into a different chemical form.

The current centerpiece of hydrogen technology and the primary driver of the hydrogen fuel cell industry is the passenger car. The auto manufacturing industry recognizes the need for the electrification of vehicles, but reliance on a precious metal catalyst, platinum, as a central component of the fuel cell is cost prohibitive. In order to drive cost down and to commercialize fuel cell vehicles and other fuel cell applications on a large scale, better materials solutions that drastically reduce the platinum content and provide alternatives to precious metals are needed.

University of New Mexico pioneered a materials technology that enables robust synthesis of Platinum Group Metal-free (PGM-free) catalysts for fuel cells and electrolyzers. The success of this UNM technology platform was the demonstration of the first PGM-free fuel cell vehicle by Daihatsu Motor Company (Japan) in collaboration with UNM at the Tokyo Motor Shows of 2009, 2011 and 2013. The UNM Center for Micro-Engineered Materials is working closely with automotive technology leaders and specialty fuel cell developing companies across the world to advance state-of-the-art PGM-free catalysts. This UNM PGM-free catalysts technology was scaled-up and developed for various markets by Pajarito Powder, LLC, an Albuquerque startup. Pajarito Powder subsequently licensed technology from LANL, thus becoming a world leader in advanced non-platinum catalysts for fuel cells. Today Pajarito Powder reaches global markets and all automotive manufacturers with interest in fuel cell vehicles, electrical combined heat-and-power production and electrolytic hydrogen generation.

One subset of fuel cell technologies is polymer electrolyte membrane fuel cells which provide the attractive application of spanning three to four orders of magnitude of power generation capability, enough to power a reasonably-sized car, and operate at temperatures that automobile manufacturers are accustomed to. New technologies in medium temperature membranes (120° to 150° F) will eliminate the need for a catalyst to drive oxygen reduction, and thereby greatly reduce cost. Alkaline membrane fuel cell technology also allows for the elimination of a platinum catalyst, but the materials necessary for the rest of the fuel cell, especially the membrane itself, are not sufficiently developed and require additional materials research for further development. All these technology subsets have their representation in companies in the Southwest Region and in the research of scientists from Regional universities and national laboratories.

An important consideration in the broader introduction of hydrogen is the further development of the hydrogen infrastructure. In terms of hydrogen distribution, natural

**“Hydrogen... is an enabler of green processes, whether it is industrial processes or whether it is transportation.”**

- Dr. Bryan Pivovar
gas pipelines can move hydrogen at concentrations of about 10% without requiring substantial improvements to the existing infrastructure. But additional product development and the need to build hydrogen fueling stations, for example, raise questions regarding the valuation of system and infrastructure costs that may be incurred, and the policy implications and incentives necessary to determine what the value might be of more broadly introducing new energy resources.

Another factor contributing to valuation of hydrogen is the conceptual study of hydrogen generation introduction at scale. As technology allows for an increase in renewable energy generation, especially solar and wind, maintaining grid stability will become increasingly important. One solution is to take the excess renewable energy generated on the grid and produce value-added products such as hydrogen for other uses including biofuels, metal refining and synthesizing ammonia for fertilizer, which renders these industries low carbon dioxide generating, as well. The goal of the hydrogen at scale, therefore, is to enable increased production of clean and renewable energy for transportation and grid stabilization, while also generating more value-added products that are related to the industrial might of the country. Figure 1 illustrates the integration of hydrogen technology in the overall clean energy cycle.

At the moment, putting renewables on the grid is not decarbonizing the whole U.S. infrastructure. It is only decarbonizing the portion that is electrical with little impact on the fossil-fuel driven transportation infrastructure. The goal for many countries is to have their entire energy sector, including transportation, driven by renewable energy by 2050. For example, Germany is demonstrating up to 20% variable on the grid, and Denmark is generating 50% of their energy production from renewables. In the U.S., as more than

“Polymer electrolyte fuel cells... allow for practical application across 3-4 orders of magnitude of the power generation spectrum... from 1W or 5W to 1kW or 5kW.”

- Dr. Plamen Atanassov
20% of renewable energy is added to the grid, it is either going to have to be stored, used in the transportation sector or converted to value-added products, such as hydrogen. Hydrogen-fueled turbines could be a solution to this, creating hydrogen during load slumps for later use in energy ramps. Electrolyzer technology could be a solution that allows for greater value of hydrogen to be captured by storing it during periods of low usage and returning it to the grid during peak need.

Critical technology breakthroughs that are necessary today are advancements in battery materials to enable greater storage of electricity during non-peak periods; and in electrolyzer materials. Critical needs in the further development of electrolyzer technology to bring down costs are similar (and thus synergistic) to improvements needed for fuel-cells. But to date, investment in technologies to make renewable hydrogen as cheap as end-use hydrogen used in fuel cell vehicles has not been made. There is significant overlap and areas of commonality in which advanced materials can be used, including in fuel cells, electrolyzers and batteries.

Finally, the national trend of hydrogen usage could be enhanced by creating long-term demonstration projects that build into the future and demonstrate an economic path to viability of new technologies. For example, hydrogen-fueled cars have made strides in personal transportation, and these concepts can now be expanded to larger modes of transportation; e.g., the U.S. Postal Service could deliver mail utilizing a large fleet of hydrogen-fueled cars as a model of the technology. It is important for economic growth and job creation that the U.S. develop hydrogen-fueled technology to scale before other countries do. Currently the U.S. has an advantage, as the majority of materials technologies have been developed domestically, but other countries have shown willingness to invest heavily in fuel cell technology to ameliorate pollution problems, regardless of their immediate economic viability.

Panel II: Materials for Improving Efficiency and Lowering Manufacturing Costs for Photovoltaics

Panel II consisted of Dr. Kevin Malloy (Professor Emeritus of Physics and Astronomy, Special Assistant to the Vice President of Research for Science and Engineering, The University of New Mexico; moderator); Dr. Nancy Haegal (Center Director of the Materials Science Center, National Renewable Energy Laboratory); Dr. Christiana Honsberg (Professor, School of Computing, Electrical and Energy Engineering and Director, NSF and DOE Quantum Energy and Sustainable Solar Technologies Engineering Research Center, Arizona State University); and Dr. Pete Atherton (COO of mPower Technology, Inc., Former Senior Manager of Industry Partnerships, Sandia National Laboratories, Albuquerque, New Mexico).
Of all the low carbon, alternative energy sources under discussion in this Forum, solar is by far the most mature and entrenched. For example, California currently meets 10% of its energy needs from solar. Due to numerous advances in photovoltaic (PV) and other materials, the cost of solar energy is now competitive with fossil fuels, at $1/peak watt. Currently, the trillion dollar solar industry employs about 300,000 workers, making it a larger employer than the fossil fuel industry. All told, solar capacity should reach 1TW within the next 5 years. While photovoltaics and solar energy are relatively mature technologies, the materials comprising PV cells and enabling their integration into solar panels can be greatly improved. The maximum efficiency for a single junction silicon-based solar cell is 27.6%, far below the 34% efficiency limit imposed by thermodynamics for an ideal cell. Those currently on the market have a practical efficiency of about 20%. The National Renewable Energy Laboratory, based in Golden, CO, tracks the efficiency of emerging photovoltaic materials. Strongly correlated to efficiency, the maximum power output (open circuit voltage; $V_O$) is determined by the semiconductor band gap of the material. Silicon solar cells for example, have $V_O = 0.76$, whereas Gallium Arsenide (GaAs) and Cadmium Telluride (CdTe) can reach about 1V, with efficiencies of 28.8 and 22.1%, respectively. Perovskite solar cells are rivaling these, with $V_O = 0.83$ and an efficiency of 22.1%. Quantum dot PV cells offer tunable band gaps, enabling a $V_O = 1$; and while these cells have a theoretical efficiency limit of 62.2%, only 7% efficiency has been obtained.

While single-junction PV cells dominate the market, the exploration of multijunction PV cells promises leaps in both efficiency and $V_O$. The theoretical efficiency of multijunction cells approaches 90% (assuming an infinite number of layers); experimental systems developed at NREL have reached about half of that value (44%) for a 4-junction cell. The increased efficiency is due, in part, to the presence of multiple materials with different band gaps within the material, capturing more of the solar spectrum. These cells have power outputs similar to GaAs and CdTe; for III-V multijunction cells, the $V_O$ is about 1V.

In addition to optimizing efficiency and power output, integration of PV cells into solar arrays presents unique challenges imposed by geometry, flexibility and durability. For example, in current installations, cell and module breakage account for up to 10% of the cost of installation. Sandia National Laboratories has been a pioneer in developing high voltage, ultra-resilient, flexible solar cell arrays composed of interconnecting silicon PV dots.

“In Photovoltaics, we do have an entrenched materials science that has resulted in all those jobs to which the Secretary referred.”

- Dr. Kevin Malloy

Dr Abraham Ellis of Sandia National Labs discussing materials challenges to integrating photovoltaic/power conversion/power electronics into one package.
These Dragon Scales™ (Figure 2) will revolutionize solar power through higher efficiency, durability and flexibility, allowing them to extend solar power to convoluted surfaces. They have recently been commercialized by an Albuquerque start-up, mPower Technology, Inc.

Multiple synergies exist between PV and other types of clean energy. The most obvious of these is integration between solar electricity and solar thermal applications. These share a need for improved optical properties of PV cells. In addition, the high temperature tolerance of GaAs PV cells makes them ideal for integration of both technologies. Integrated circuit (IC) technology is also another point of synergy, because both ICs and PVs are currently dominated by silicon semiconductor technology. It is anticipated that such a synergy will provide increased utility in a number of areas, from consumer electronics to satellites. In addition, such integration may provide lightweight alternatives to current wiring technologies. Finally, such a synergy would enable co-manufacture of ICs and PV with minimal retooling of existing fabrication facilities, which would provide a new paradigm in solar power of consumer electronics. Another possible synergy is that between PV and semiconductor light emitting diodes.

It is clear that solar energy cannot be a standalone technology. Differences in light intensity throughout the day, although coinciding generally with peak usage, makes direct use of solar technology untenable for 24-hour output of electricity. With careful planning and coordination, however, solar energy can be integrated with battery or other storage technologies (see Panel III), or hydrogen technology (Panel I), to preserve energy produced at peak solar flux. Such systems are being realized in Indonesia with the incorporation of zinc-air batteries into pain-points within the solar grid, allowing for up to 24 hours of storage and distribution of energy to areas with less solar flux.

“We have heard about recent growth... There are more U.S. energy jobs in solar energy than in coal or oil.”
- Dr. Christiana Honsberg
Panel III: Materials Solutions for Electrical Energy Storage

This panel consisted of Dr. Babu Chalamala (Manager of the Energy Storage Technology & Systems Department, Sandia National Laboratories; moderator); Dr. Kevin Zavadil (Distinguished Member of Technical Staff, Sandia National Laboratories); Dr. Shelley Minteer (The Utah Science Technology and Research initiative Professor, Analytical, Biological & Materials Chemistry, University of Utah); and Dr. Cody Friesen (Fulton Engineering Professor of Innovation, Arizona State University, Founder and CEO, Zero Mass Water, Phoenix, Arizona).

Despite substantial progress in the last 10-20 years, large scale battery storage lags behind the rapid technological and cost improvements driving the deployment of solar and wind energy technologies. High current cost (> $100/kWh) coupled with low energy density and short cycle life limit the impact of batteries to accommodate the projected 1 TW renewable power to be integrated into the national base load. Innovations in materials used for electrodes and electrolytes are needed to create better batteries. Materials innovations have clearly played out over the last 25 years with lithium ion batteries (LIB) driving specific energy to 250 Wh/kg at a cost below $200/kWh. LIB technology is a good model to follow for innovation, but is rapidly approaching its limit in stored energy content, requiring the community to develop new concepts and materials for battery storage. Successful storage to meet the goals of an emerging renewable, low-carbon economy must extend cycle and calendar life, increase power performance (charging times), reduce cost ($100/kWh) and improve reliability and safety.

One clear path forward is the development of non-aqueous redox flow batteries using redox active organic compounds that can be produced at scale at low cost to replace the more traditional metal cation chemistries. Innovation in organic compound design to enhance capacity and extend lifetime of the redox active moieties is a key theme.

Figure 3. Renewable energy placed on the grid using scaled non-aqueous redox flow batteries could recharge the US fleet of electric vehicles powered by Li-S batteries. Courtesy of Dr. Kevin Zavadil.

Materials innovations are being made by exploring alternate battery chemistries and concepts. The Southwest Region is a participant in the DOE sponsored Joint Center for Energy Storage Research (JCESR), a private-public partnership funded to develop and demonstrate technologies beyond LIB for...
Both transportation and grid applications. Alternate chemistries for vehicle electrification include exploiting the electrochemical conversion reaction of elemental sulfur to a metal sulfide to form a Li-S battery. This is essentially a 16 electron process with a lightweight, low cost cathode material. Conversion redox chemistry benefits from much higher energy content because energy is stored in chemical bonds relative to the valence state change and electrostatics of ion based couples. Multivalent metal working ions such as magnesium are also explored as replacements to the lithium ion for insertion cathodes due to a doubling of charge, and consequently capacity. These chemistries implemented through the use of new, innovative materials promise to yield pack-level specific energies of 400 Wh/kg at $100/kWh. Materials innovation in grid storage is pursued by exploiting redox active molecules, oligomers and colloids in non-aqueous redox flow batteries to overcome the lifetime and cost limits imposed by state-of-the-art metal ion (e.g., vanadium) flow batteries.

Transportation storage solutions also require materials innovation. As an example, the energy density of the state-of-the-art Li-S system is currently limited by the need for excess Li metal, excess electrolyte and lost sulfur capacity from the cathode. New electrolyte and cathode designs are required to direct the redox pathway to reversibly interconvert the full capacity of sulfur to/from sulfide. Additionally, materials are needed to coat and protect the Li metal anode and eliminate parasitic loss of both lithium and electrolyte. Materials innovation is also required for creating viable magnesium (Mg) batteries. The current limitations are the lack of a suitable voltage insertion cathode and an electrolyte stable at both the anode and cathode potentials. Computational results indicate that the high charge density Mg(II) cation should have reasonable mobility in select higher voltage oxide cathodes, and effort is underway to synthesize and experimentally validate these predictions. New electrolytes are also under development and guided by computational insights that do not exhibit either salt or solvent breakdown at the cell voltage limits. Success in fielding the Li metal anode will accelerate the transition from today’s vehicles powered by Li ion batteries to tomorrow’s Li metal batteries.

Viable grid storage solutions also require new materials and concept innovations to produce storage that can be readily scaled in energy and power content, that lowers cost and that increases cycle life (> 10,000 cycles). One clear path forward is the development of non-aqueous redox flow batteries using redox active organic compounds that can be produced at scale at low cost to replace the more traditional metal cation chemistries. Innovation in organic compound design to enhance capacity and extend lifetime of the redox active moieties is a key theme. New concepts of redox active polymers and colloids appear as promising low cost replacements.

“Materials are going to play a fundamental role in how storage is going to evolve over the next 20 years.”

-Dr. Babu Chalamala
to simple organic compounds. Studies show that quantitative structure-activity relationship (QSAR) modeling is an effective tool for evaluating the lifetime of an active compound and therefore cycle life of a given flow chemistry. Lifetime and cost limits are also imposed by the ion conductive membrane used to separate the anode and cathode flow compartments in a flow cell. New strategies are being pursued using polymers of intrinsic microporosity to create highly transmissive ion conductors that prevent redox active molecule transport between the electrode compartments.

A good example of integrating battery storage within the context of low carbon technologies is the development of metal-air batteries by Fluidic Energy™, located in Scottsdale, Arizona. This company uses zinc-air batteries, large scale versions of those found in hearing aids, to supplement pain points in distributed electric grids that are normally covered by diesel engines. In Indonesia, for example, the microgrid covering the archipelago is fueled by solar energy. Due to varying cloud cover on different islands, and the diurnal pattern of solar irradiation, supplementary power used to be provided by diesel engines, which are both expensive and carbon dioxide-producing. The Fluidic Energy™ batteries replace these fossil fuel engines. They are charged during the day, and discharge at night or during cloudy weather. Over 250 MWh are currently being supplied in this form to remote villages in Indonesia, and are capable of providing up to 24 hours of energy storage.

The panel highlighted a number of additional, specific needs common among the emergent battery storage technologies discussed. An understanding of materials degradation during battery operation and its impact on performance and lifetime is needed. The capability to analyze systems beyond electrochemical parameters is also needed to better understand how the storage system evolves. Such an advance may also inform fuel cells and photovoltaic technologies. Lastly, “green” disposal methods and recycling of battery materials was also identified as a critical need for large scale storage.

Panel IV: Materials for Advanced Nuclear Energy Solutions

Participants in this panel were Dr. Chris Stanek (Nuclear Energy Advanced Modeling and Simulation (NEAMS) National Technical Director, Los Alamos National Laboratory; moderator) Dr. John Wagner (Chief Scientist for Materials and Fuels Complex (MFC) at Idaho National Laboratory), Dr. Tiangan Lian (Program Manager, Electric Power Research Institute), and Dr. Edward Blandford (Assistant Professor, Nuclear Engineering, University of New Mexico).

“Most pharmaceutical chemists would think about structure/activity relationships to predict structure/function relationships... Can we use those same principles...and apply them to the energy industry?”

-Dr. Shelley Minteer
“The biggest challenge we face is the lack of ability to predict how [nuclear] materials behave.”

- Dr. Tiangan Lian

Ninety-nine nuclear reactors operate within the United States, providing about 20% of the total power needs of the country and more than 60% of its zero-carbon baseline electricity. Thus, nuclear energy represents a key component in the quest for carbon-neutral energy production. Whether or not this will remain the case in the future is in serious doubt; the nuclear fleet is aging, with many power plants being 40 or more years old and needing operating lifetime extensions or replacement by 2030. In addition, competition from decreased prices of natural gas is forcing economically-driven shut down of up to 20 plants in the near future. It is predicted that the future of nuclear energy as an efficient, low-emission source of electricity will be in crisis within the next decade. Given that the time frame for validating new materials and reactor designs can take on the scale of decades, the rapid development of new materials, fuels and infrastructure design is paramount.

![Image of irradiated uranium oxide fuel](image-url)

Figure 4. 10 micro-meter sample of irradiated uranium oxide fuel being lifted out in a focused ion beam for microstructural characterization. Courtesy of Dr. John Wagner

Many of the key issues facing near-term nuclear energy R&D are driven by materials performance. Materials issues are readily encountered during efforts to optimize fuel in operating commercial reactors, accelerate the commercial deployment of small modular reactors or advanced reactors, and develop demonstrations/tests for special purpose reactors. Other critical materials challenges include the development of cladding and structural materials that can withstand the harsh environments (excess of 200 dpa) of next generation fission (and fusion) reactors, and the disposition of civilian nuclear waste. All of these issues would benefit from improved predictive models of materials performance.
A recurring technical theme related to many of these issues is the fundamental difficulty related to assessment of evolving materials behavior in conditions that make direct observation difficult, if not impossible. Myriad complex phenomena in irradiated materials, from damage accumulation in metals to chemical evolution in complex materials, are still beyond the reach of a true predictive capability. The ability to predict these effects begins with fundamental studies of the interaction of radiation with matter. This will lead to improved models that will provide better fundamental understanding, serve as the foundation for the design of new materials with enhanced performance and perhaps shift the life-cycle/licensing for nuclear systems, structures and components to allow for shorter time scales for component replacement.

As noted, fuel stability and composition represent a major materials challenge. The radiative process may itself change the materials property of the fuel, and the high temperatures inherent in the nuclear process may cause an accident. Recent advances in this area include embedding uranium dioxide into silicon carbide and/or zircon matrices to allow fuels to resist the effects of high temperatures within the reactors, thus rendering them accident safe. Additive manufacturing has amazing, yet unproven, potential for nuclear fuels and materials, e.g., the potential to expand design space by fabricating components with characteristics that are not currently possible, improve quality and predictability of nuclear-grade components, and reduce cost. For example, for nuclear fuel it may be possible to optimize fuel performance through varying enrichment, burnable neutron absorbers, and/or thermal, conducting material within the fuel pellet in ways that are not currently possible. Because uranium dioxide pellets are traditionally homogeneous, this could provide a dramatic improvement in fuel performance. Finally, nano-engineered materials that provide better mechanical properties remain largely unproven for nuclear, but the limited work that has been performed on them has been extremely promising and is worth pursuing.

Helping to meet these and other challenges, the DOE has a variety of experimental facilities across several national laboratories. One example includes the Materials and Fuels Complex (MFC) at Idaho National Laboratory, which has as its mission developing advanced fuels and materials, including nuclear waste. Several components comprise the MFC, including facilities for characterizing irradiated materials, examining hot fuels, and those for experimental fuels and integration in reactor design. LANL and SNL also have key experimental facilities that are capable of investigating advanced materials, including the Los Alamos Neutron Science Center (LANSE) at LANL and the Ion Beam Laboratory (IBL) at SNL.

While the materials questions associated with generating electricity are unique, integrating them into a distributed energy infrastructure will rely on successful integration with other low-carbon strategies.
Regarding the ability of reactor components to withstand the corrosion due to the use of water as both a coolant and a neutron moderator in light water reactors, some of these issues have been addressed by reference to development of aerospace materials. For example, Alloy 600, whose failure had been cited in over 70 reactors, has been replaced with the higher chromium containing Alloy 690 in steam generator tubes, reactor upper and lower head penetrations, increasing the reliability of these parts. Also, Alloy 52/152 (weld materials for Alloy 690) is being proposed to replace Alloy 82/152 (associated weld materials for Alloy 600) for welding dissimilar metals in the primary system piping. Alternative coolants, such as molten sodium or salts, gases (such as helium and carbon dioxide) and hydrocarbons have been explored, with limited success, indicating the need for further development in this area.

Leading the way in reactor component design is the Electric Power Research Institute (EPRI), a nonprofit organization funded by energy utilities. EPRI serves as a conduit to transfer knowledge from research to application - or, in other words, to convert technology from a scientific base to an engineering base. The goal of EPRI is to work with members and partners to provide society with safe, reliable, affordable and environmentally responsible energy. Materials research is an important part of EPRI’s research portfolio.

For example, a major component of its research is in materials degradation, with a goal of understanding materials aging mechanisms in nuclear reactors and developing technologies to mitigate and monitor degradation. Such efforts include understanding corrosion processes resulting from stress corrosion and irradiation-induced corrosion, the unique issues facing steam generation (i.e. water chemistry, inspection limitations, material performance issues and the presence of foreign objects) and materials for welding and repair.

In 2013, the DOE introduced the Nuclear Energy University Program (NEUP) and Nuclear Science User Facilities (NSUF), administered through Idaho National Laboratory, of which EPRI is a partner. This program has produced a large number of university-led research programs in partnership with national labs and industry developing advanced materials modeling and simulation in addition to critical experimental nuclear materials investigations. One example of such a program includes developing alternate means for irradiating materials to high doses using non-traditional methods such as ion beam sources. The facility sponsored under this NEUP funding will collect materials from around the world, as well as archival samples, to experimentally validate physics-based models of the effects of extreme radiation. It should be able to test such parameters as path-dependence of materials within a nuclear reactor, information that is not currently available. Facilities of this sort will enable designing experiments.
Overall, the panel emphasized the need for integration and coordination of experimental and computational modeling efforts throughout the materials development and demonstration process to enable materials breakthroughs through advanced understanding, enable the ability to develop and demonstrate predictive computational modeling capabilities, and reduce nuclear materials RD&D timelines and costs.

LANL, Sandia and INL, therefore, have long experience with actinide-bearing materials, study of radiation effects in both fuel and structural materials, advanced modeling and simulation science, and challenging measurements of evolving materials properties in harsh environments. To address outstanding materials issues requires proactive integration of materials synthesis, advanced characterization, and multiscale mod-sim. Within each of these are specific capability improvements. However, being strategic requires the integration of these three activities, where the ultimate products are a validated engineering scale performance/safety model and design principles for the next generation of nuclear energy materials.

While the materials questions associated with generating electricity using nuclear fission are unique, integrating them into a distributed energy infrastructure will rely on successful integration with other low-carbon strategies. There are current efforts through NEUP support looking at plants capable of providing both baseload and peak power for integration into such a grid. Such integration will complicate the power history of the materials in the reactor, something that is very important to understand. The need for storage of power generated, either in a battery or by using the energy of hydrogen for use in other modalities, will require far more complex predictive models for operations of facilities in addition to the materials.
The Southwest Regional Energy Forum brought together experts from academia, the national laboratories and industry to share ideas regarding the state of energy materials as related to meeting the challenges articulated in Mission Innovation. A common interest in materials for energy applications brought the group together, but in the process, a number of synergies became apparent.

The Synergy of Urgency and Opportunity. The Southwest Region is being drastically affected by climate change and is also the site of the largest atmospheric methane hotspots in the nation. Thus, the development of clean, low carbon, renewable energy is essential to the future well-being of this unique environment. At the same time, the region is host to a robust, cooperative intellectual and technological hub for the development of unique materials to address these issues. Existing collaborations between regional academic institutions, four DOE national laboratories and innovative energy companies makes the Southwest Region a natural leader in the pursuit of solutions to regional, national and global problems related to carbon dioxide emissions.

The Synergy of Diverse Materials Research, Development Approaches and Solutions. It is clear from the panelists that understanding and developing materials cuts across all energy applications. Within these programs, common materials needs can be easily identified. Materials research in flow cells will inform energy storage and electrolysis; the semiconductor technology for creating and integrating photovoltaics may apply to storage and fuel cells; integrating nuclear energy with solar into distributed networks will create new materials challenges in reactors. A common theme throughout the panels was the need for computational power to model materials properties that will meet both the individual needs of each technology, as well as the combined needs of integrated systems. The strength of materials research in the Southwest Region and the established interrelationships between academic and national laboratories are already in place.
Partners in the Southwest Region will tackle the need for clean energy by leveraging and strengthening existing ties, as well as serving as a nexus for development of future collaborations and dissemination of new ideas and technologies to the region, the country and the world.

**The Synergy of Innovation and Industry.** The Southwest Region has an established track record of turning ideas into marketable products, several of which, including hydrogen fuel cells, photovoltaic cells and low cost batteries, were discussed during the panel discussions. UNM and SNL, in particular, have a long record of collaboration in commercialization and have the infrastructure and programmatic supports in place to foster further innovation. UNM is a leading partner in Innovate ABQ, which, along with local government, is seeking to invigorate the local economy through technology transfer, particularly within the energy sector. Such ventures across the region form the nexus of collaboration between DOE national laboratories, academia and industry.

**In summary, the Southwest Regional Energy Innovation Forum on Materials Technology for Clean Energy was an excellent venue for bringing key regional partners together to discuss new opportunities for collaboration and mechanisms for revolutionary advances toward clean energy.** The Forum also reaffirmed the commitment of partnering institutions to collaborate closely on materials innovations that support clean energy solutions. Strategies for how the region can contribute to breakthrough innovations in materials technologies that will lead to an abundance of clean energy are being developed in the wake of the Forum and will continue to take shape as the partnership develops.
This report was made possible through technical contributions and support from the following people:

**The Panelists, Mr. Michael J. Workman** (PhD Candidate and NSF Graduate Research Fellow, The University of New Mexico), **Mr. Noel Dawson** (PhD Candidate, The University of New Mexico), **Ms. Hannah Height** (Graduate Student, The University of New Mexico), **Mr. Joel Hughes** (PhD Candidate, The University of New Mexico), **Dr. Linnea Ista** (Research Assistant Professor, Center for Biomedical Engineering, The University of New Mexico), **Dr. Carman Melendrez** (Research Scholar, Faculty Research Development Office, The University of New Mexico), **Ms. Vanessa Tan** (Training and Communications Specialist, Office of the Vice President for Research, The University of New Mexico) and **Dr. Gabriel P. López** (Vice President for Research, The University of New Mexico). We are grateful for financial support from the Office of the Vice President for Research at The University of New Mexico.
Appendix 1: Participating Organizations and Institutions by Sector

**ACADEMIC INSTITUTIONS**
- Arizona State University
- Colorado State University
- New Mexico Institute of Mining and Technology
- New Mexico State University
- Northern Arizona University
- Prairie View A&M University
- University of Arizona
- University of Colorado - Boulder
- The University of New Mexico
- University of Northern Colorado
- University of Texas at El Paso
- University of Utah
- Utah State University

**INDUSTRY**
- Affordable Solar
- Electric Power Research Institute (EPRI)
- Energy Related Devices, Inc.
- EverGuard Solar
- mPower Technology, Inc.
- Osecola Energy
- Pajarito Powder, LLC
- Public Service Company of New Mexico
- Shimizu Corporation
- STC.UNM
- Suncore Photovoltaics, Inc.
- Van Scyoc Associates
- Zero Mass Water
- Zia Suns Green Construction Co. LLC

**NATIONAL LABORATORIES**
- Idaho National Laboratory (INL)
- Los Alamos National Laboratory (LANL)
- National Renewable Energy Laboratory (NREL)
- Sandia National Laboratories (SNL)

**GOVERNMENT**
- New Mexico Public Regulation Commission
- New Mexico State Representative Idalia Lechuga
- Office of U.S. Congressman Ben R. Lujan
- Office of U.S. Congressman Steve Pearce
- Office of U.S. Representative Michelle Lujan Grisham
- Office of U.S. Senator Martin Heinrich
- Office of U.S. Senator Tom Udall
- U.S. Department of Energy

**NON GOVERNMENTAL ORGANIZATIONS**
- Los Alamos Study Group
- North American Electric Reliability Corporation (NERC)
- Prizm Foundation
Southwest Regional Energy Innovation Forum
MATERIALS TECHNOLOGY FOR CLEAN ENERGY
July 5, 2016 | The University of New Mexico | Albuquerque, New Mexico

10:30 AM - 6:00 PM
Student Union Building Ballroom BC
Welcome
Thank you for joining us in the Southwest Regional Energy Forum! We hope to use this time to connect & discuss clean energy solutions relevant to our region & help inform the Department of Energy as they steer their policy direction in the coming years.

SCHEDULE

BALLROOM LOBBY
10:30 AM
Registration & Refreshments

BALLROOM C
11:30 AM
Master of Ceremonies Introductory Remarks by Gabriel P. López, Vice President for Research, The University of New Mexico & 2016 STC.UNM Innovation Fellow

Welcome & Opening Remarks by Robert G. Frank, President, The University of New Mexico

Congressional Remarks by the Honorable Tom Udall, US Senate & the Honorable Martin Heinrich, US Senate

Forum Address by the Honorable Ernest Moniz, Secretary, US Department of Energy

BALLROOM B
12:30 PM
Buffet Lunch Line

BALLROOM C
12:40 PM
Luncheon Discussion with Panel I - Enabling Materials for Hydrogen Technology & Infrastructure moderated by Bryan Pivovar, Program Manager, National Renewable Energy Laboratory
Panel II - Materials for Improving Efficiency & Lowering Manufacturing Costs for Photovoltaics moderated by Kevin Malloy, Professor Emeritus of Physics & Astronomy, Special Assistant to the VPR for Science & Engineering, The University of New Mexico

Panelists include: Nancy Haegel, Center Director of the Materials Science Center, National Renewable Energy Laboratory | Christiana Honsberg, Director, Quantum Energy & Sustainable Solar Technologies Engineering Research Center, Arizona State University | Pete Atherton, COO of mPower Technology, Former Senior Manager of Industry Partnerships, Sandia National Laboratories, Albuquerque, New Mexico

2:42 PM  Break

2:52 PM  Panel III - Materials Solutions for Electrical Energy Storage moderated by Babu Chalamala, Manager of the Energy Storage Technology & Systems Department, Sandia National Laboratories

Panelists include: Kevin Zavadil, Distinguished Member of Technical Staff, Sandia National Laboratories | Shelley Minteer, USTAR Professor, University of Utah | Cody Friesen, CEO, Zero Mass Water, Phoenix, Arizona

3:53 PM  Panel IV - Materials for Advanced Nuclear Energy Systems moderated by Chris Stanek, NEAMS National Technical Director, Los Alamos National Laboratory

Panelists include: John Wagner, Chief Scientist, Idaho National Laboratory | Edward Blanford, Assistant Professor, Nuclear Engineering, The University of New Mexico | Tiangan Lian, Program Manager, Electric Power Research Institute, Palo Alto, California
Please visit the UNM Research Events website at http://reseachevents.unm.edu to provide your feedback & comments in the “Interactive Discussion” section so that we can keep this conversation going!