## INNOVATION IN SOLAR FUELS, ELECTRICITY STORAGE, AND ADVANCED MATERIALS

## **HEARING**

BEFORE THE

# SUBCOMMITTEE ON ENERGY COMMITTEE ON SCIENCE, SPACE, AND TECHNOLOGY HOUSE OF REPRESENTATIVES

ONE HUNDRED FOURTEENTH CONGRESS

SECOND SESSION

June 15, 2016

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WASHINGTON: 2017

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#### INNOVATION IN SOLAR FUELS, ELECTRICITY STORAGE, AND ADVANCED MATERIALS

#### WEDNESDAY, JUNE 15, 2016

House of Representatives, Subcommittee on Energy, Committee on Science, Space, and Technology, Washington, D.C.

The Subcommittee met, pursuant to call, at 10:07 a.m., in Room 2318 of the Rayburn House Office Building, Hon. Randy Weber [Chairman of the Subcommittee] presiding.

EDDIE BERNICE JOHNSON, Texas RANKING MEMBER

## Congress of the United States

#### House of Representatives

COMMITTEE ON SCIENCE, SPACE, AND TECHNOLOGY

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Subcommittee on Energy

#### Innovation in Solar Fuels, Electricity Storage, and Advanced Materials

Wednesday, June 15, 2016 10:00 a.m. – 12:00 p.m. 2318 Rayburn House Office Building

#### Witness

Dr. Nate Lewis, Professor, California Institute of Technology
Dr. Daniel Scherson, Professor, Case Western Reserve University
Dr. Collin Broholm, Professor, Johns Hopkins University
Dr. Daniel Hallinan Jr., Assistant Professor, Florida A&M University – Florida State University College of Engineering

#### U.S. HOUSE OF REPRESENTATIVES COMMITTEE ON SCIENCE, SPACE, AND TECHNOLOGY

#### **HEARING CHARTER**

Wednesday, June 15, 2016

TO: Members, Subcommittee on Energy

FROM: Majority Staff, Committee on Science, Space, and Technology

SUBJECT: Subcommittee hearing: "Innovation in Solar Fuels, Electricity Storage, and

Advanced Materials"

The Subcommittee on Energy will hold a hearing titled *Innovation in Solar Fuels*, *Electricity Storage, and Advanced Materials* on Wednesday, June 15, 2016, at 10:00 a.m. in Room 2318 of the Rayburn House Office Building.

#### **Hearing Purpose:**

The purpose of this hearing is to examine the status of basic research on energy in the United States, including research related to solar fuels, electricity storage, and advanced materials. The Department of Energy's Basic Energy Sciences (BES) program within the Office of Science funds basic research which, among other things, provides the foundations for new energy technologies. For FY 2016, BES is funded at \$1.85 billion and the FY 2017 budget request is \$1.94 billion.

#### Witness List

- Dr. Nate Lewis, Professor, California Institute of Technology
- Dr. Daniel Scherson, Professor, Case Western Reserve University
- Dr. Collin Broholm, Professor, Johns Hopkins University
- Dr. Daniel Hallinan Jr., Assistant Professor, Florida A&M University Florida State University College of Engineering

#### **Staff Contact**

For questions related to the hearing, please contact Aaron Weston of the Majority Staff at 202-225-6371.

Chairman Weber. The Subcommittee on Energy will come to order. Without objection, the Chair is authorized to declare recesses of the Subcommittee at any time.

Welcome to today's hearing entitled "Innovation in Solar Fuels, Electricity Storage, and Advanced Materials." I recognize myself for

an opening statement.

Good morning. Today, we will hear from a panel of experts on the status of America's basic research portfolio, which provides the foundation for development of solar fuels, electricity storage, and quantum computing systems. Hearings like today help remind us of the Science Committee's core focus: the basic research that pro-

vides the foundation of technology through breakthroughs.

We're going to discuss the science behind potentially groundbreaking technology today. But before America ever sees the deployment of a commercial solar fuel system or we move to quantum computing, a lot of discovery science must be accomplished. For the solar fuel process, also known as artificial photosynthesis, new materials and catalysts will need to be developed through research. If this research yields the right materials, scientists could create a system that could consolidate solar power and energy storage into one cohesive process. This would potentially remove the intermittency of solar energy and make it a reliable power source for chemical fuels production. That is a game-changer.

In the field of electricity storage research, there is a lot of excitement—or as I like to say there's electricity in the air—about more efficient batteries that could operate for longer durations under decreased charge times. But not enough people are asking just how could we design a battery system that moves more electrons at the atomic level, a key aspect to—excuse me—drastically increasing the efficiency or power of a battery. This transformational approach, known as multivalent ion intercalation, will use foundational study of electrochemistry to build a better battery

from the ground up.

And then finally, there is quantum computing, which relies on a thorough understanding of quantum mechanics, a challenging concept that is a longer discussion for a different hearing. For today, I hope we can discuss how a quantum computing system could change the way computers operate. In order to achieve this kind of revolutionary improvement in computing, we're going to need foundational knowledge in the materials needed to build those systems also known as quantum materials.

I look forward to hearing from Dr. Broholm—have I got that right, Doctor-

Dr. Broholm. Yes.

Chairman Weber. —in his research—your research in that field. Today, we hear a lot of enthusiasm for solar power, batteries, and high-performance computing technology, yet few innovators are talking about how these technologies could be transformed at the fundamental level. In Congress, we have to take the long-term view and be patient, making smart investments in research that can lead to the next big discovery.

When it comes to providing strong support for basic research, this Science Committee won't get any major accolades or headlines today. But someday, someday, when the next disruptive technology changes our economy for the better, I firmly believe that discovery

science will play that central role.

DOE must prioritize basic research over grants for technology that is ready for commercial deployment. When the government steps in to push today's technology in the energy market, it's actually competing against private investors and it uses limited resources to do so. But when the government supports basic research and development, everyone has the opportunity to access the fundamental knowledge that can lead to the development of future energy technologies.

I want to thank our accomplished panel of witnesses for testi-

fying today, and I look forward to a productive discussion about the DOE basic energy research portfolio.

[The prepared statement of Chairman Weber follows:]



For Immediate Release June 15, 2016 Media Contacts: Alicia Criscuolo, Thea McDonald (202) 225-6371

#### Statement of Energy Subcommittee Chairman Randy Weber (R-Texas) Innovation in Solar Fuels, Electricity Storage, and Advanced Materials

**Chairman Weber**: Good morning and welcome to today's Energy Subcommittee hearing. Today, we will hear from a panel of experts on the status of America's basic research portfolio, which provides the foundation for development of solar fuels, electricity storage, and quantum computing systems.

Hearings like today's help remind us of the Science Committee's core focus – the basic research that provides the foundation for technology breakthroughs. We're going to discuss the science behind potentially ground breaking technology today. But before America ever sees the deployment of a commercial solar fuel system or we move to quantum computing, a lot of discovery science has to be accomplished.

For the solar fuel process, also known as artificial photosynthesis, new materials and catalysts will need to be developed through research. If this research yields the right materials, scientists could create a system that could consolidate solar power and energy storage into a cohesive process. This would potentially remove the intermittency of solar energy and make it a reliable power source for chemical fuels production. *That* is a game changer.

In the field of electricity storage research, there is a lot of excitement about more efficient batteries that could operate for longer durations under decreased charge times. But not enough people are asking how we could design a battery system that moves more electrons at the atomic level – a key aspect to drastically increasing the efficiency or power in a battery. This transformational approach, known as multivalent ion intercalation, will use foundational study of electrochemistry to build a better battery from the ground up.

Finally, there is quantum computing, which relies on a thorough understanding of quantum mechanics... a challenging concept that is a longer discussion for a different hearing! For today, I hope we can discuss how a quantum computing system could change the way computers operate. In order to achieve this kind of revolutionary improvement in computing, we're going to need foundational knowledge in the materials needed to build these systems, known as quantum materials. I look forward to hearing from Dr. Broholm about his research in that field.

Today, we hear a lot of enthusiasm for solar power, batteries, and high performance computing technology. Yet few innovators are talking about how these technologies could be transformed at the fundamental level. In Congress, we have to take the long-term view and be patient, making smart investments in research that can lead to the next big discovery.

When it comes to providing strong support for basic research, the Science Committee won't get any major accolades or headlines today. But someday, when the next disruptive technology changes our economy for the better, I firmly believe that discovery science will play a central role.

DOE must prioritize basic research over grants for technology that is ready for commercial deployment. When the government steps in to push today's technology in the energy market, it competes against private investors and uses limited resources to do so. But when the government supports basic research and development, everyone has the opportunity to access the fundamental knowledge that can lead to the development of future energy technologies.

I want to thank our accomplished panel of witnesses for testifying today, and I look forward to a productive discussion about the DOE basic energy research portfolio.

Chairman Weber. I now recognize the Ranking Member.

Mr. GRAYSON. Sorry, would the Committee Chair like to precede me? Would the Committee Chair like to precede me?

Chairman SMITH. I'd be happy to. I thank the gentleman. And

let me thank the Chairman as well.

Today, we will examine American innovation in solar fuels, electricity storage, and advanced materials. The Department of Energy's Office of Science is the nation's lead federal agency for basic research in the physical sciences. This type of fundamental research allows scientists to make groundbreaking discoveries about everything from our universe to the smallest particle. It has led to transformative breakthroughs in energy science that will allow the private sector to develop innovative energy technologies.

Today's hearing will provide a status update on the Department's basic research in solar chemistry, energy storage, and advanced materials. Electricity storage is one of the next frontiers in energy research and development. Innovation in batteries could help bring affordable renewable energy to the market without costly subsidies

or mandates.

By investing in the basic scientific research that will underpin and lead to new advanced battery technology, we can enable utilities and others to store and deliver power produced elsewhere. This will allow us to take advantage of energy from the diverse natural resources available across the country.

Another high-reward application of energy basic research is solar fuels, also known as artificial photosynthesis. Through the study of chemistry and materials science, researchers are developing systems that can use energy from sunlight to yield a range of chemical fuels.

Our last topic for today's hearing is advanced materials research. By examining substances at the atomic level, researchers can develop materials with the exact qualities necessary for an application, like thickness, strength, or heat resistance. These new materials could provide the capability for quantum computing systems that will fundamentally change the way we move and process data.

Basic scientific research like the work funded by DÔE's Office of Science requires a long-term commitment. While this groundbreaking science can eventually support the development of new advanced energy technologies by the private sector, Congress must ensure limited federal dollars are spent wisely and efficiently. Federal research and development can build the foundation for the next major scientific breakthrough.

As we shape the future of the Department of Energy, our priority must be basic energy science and research that only the federal government has the resources and mission to pursue. This will enable the private sector, driven by the profit motive, to develop and move groundbreaking technology to the market across the energy spectrum, create jobs, and grow our economy.

Thank you, Mr. Chairman. I want to thank the Ranking Member

for letting me precede him as well.

[The prepared statement of Chairman Smith follows:]



For Immediate Release June 15, 2016 Media Contacts: Alicia Criscuolo, Thea McDonald (202) 225-6371

#### Statement of Chairman Lamar Smith (R-Texas)

Innovation in Solar Fuels, Electricity Storage, and Advanced Materials

**Chairman Smith:** Thank you, Mr. Chairman. Today we will examine American innovation in solar fuels, electricity storage and advanced materials.

The Department of Energy's Office of Science is the nation's lead federal agency for basic research in the physical sciences. This type of fundamental research allows scientists to make groundbreaking discoveries about everything from our universe to the smallest particle. It has led to transformative breakthroughs in energy science that will allow the private sector to develop innovative energy technologies.

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This will enable the private sector, driven by the profit motive, to develop and move groundbreaking technology to the market across the energy spectrum, create jobs, and grow our economy.

###

Chairman Weber. I thank the gentleman.

Now, the Ranking Member is recognized for a five minute opening statement.

Mr. GRAYSON. Thank you, Chairman Weber. Thank you, Chairman Smith, for holding this hearing, and thank you to the wit-

nesses for providing your testimony today.

The Basic Energy Sciences program in the Department of Energy's Office of Science supports fundamental research in materials science, physics, chemistry, and engineering with an emphasis on energy applications. BES is the largest program in the Office of Science, and it's home to several state-of-the-art facilities that provide world-class capabilities to the scientific community. BES is home to five of the world's Advanced Light Sources, to unique neutron scattering facilities, and five nanoscale research centers.

All these BES facilities are considered user facilities meaning that they provide broad access not only to scientific government inquiry but also to university researchers and private industry. That

being said, please do not try neutron scattering at home.

Each year, over 14,000 scientists use these facilities, and the demand for access to facilities can exceed the time available. In many cases, the high demand for these facilities requires weightless and extensive efforts to fit as many interested users into the schedule

as possible.

The vast array of research and diverse collection of scientists that take advantage of these facilities make them fertile ground for scientific collaboration and also innovation cutting across scientific specialties. The knowledge gained through research supported by BES underpins the applied energy research supported by other DOE programs and by the private sector. Innovation and materials science, chemical analysis, geological imagery, and electrochemistry can have far-reaching impacts on renewable energy, energy efficiency, battery storage, and nuclear power to name just a few subjects.

I look forward to hearing from our witnesses as to how they put benefited from federal support that we provided to build these user facilities, as well as other resources provided by BES. I'd particularly like to welcome Dr. Hallinan from Florida A&M and Florida State University's College of Engineering to today's hearing. His research has the potential to achieve considerable gains in battery storage, which would help the renewable energy sector play an even larger role in our economy in the coming years.

Solving renewable energy's day-versus-night challenge could allow for a faster transition to a low-carbon energy future for the United States and the world. Also, it would be good if you can make the sun shine at night, but that's probably outside the scope

of your research.

Dr. Hallinan, as we will hear, has relied upon the Advanced Light Source and the Advanced Photon Source facilities to advance his work by testing new solid polymers that can be used as battery electrolytes. His work is an excellent example of what we can accomplish if we fund the vital research and facilities of the Office of Science amply.

Last week, the Basic Energy Science Advisory Committee released a new report on the prioritization of upgrades to the major BES facilities. One of the witnesses here today may have been directly involved in developing this report. I hope we can consider revisiting this topic in the near future with a closer look at the facility upgrades that are currently under consideration. These proposed upgrades represent major government investments and thus major opportunities. Prioritizing and funding the research that's being highlighted today should certainly be a bipartisan issue and one in which we should make considerable progress on by working together.

together.
With that, I yield the balance of my time. Thank you, Mr. Chair-

[The prepared statement of Mr. Grayson follows:]

#### **OPENING STATEMENT**

# Ranking Member Alan Grayson (D-FL) of the Subcommittee on Energy

House Committee on Science, Space, and Technology
Subcommittee on Energy
"Innovation in Solar Fuels, Electricity Storage, and Advanced Materials"
June 15, 2016

Thank you Chairman Weber for holding this hearing, and thank you to the witnesses for providing your testimonies today.

The Basic Energy Sciences program (BES) in the Department of Energy's Office of Science supports fundamental research in materials sciences, physics, chemistry, and engineering with an emphasis on energy applications. BES is the largest program in the Office of Science and is home to several state-of-the-art facilities that provide world-class capabilities to the scientific community. BES is home to five of the world's most advanced light sources, two unique neutron scattering facilities, and five nanoscale research centers.

All of these BES facilities are considered "user facilities," meaning they provide broad access, not only to government scientists, but also to university researchers and private industry. Each year, over 14,000 scientists use these facilities, and the demand for access to the facilities can exceed the time available. In many cases the high demand for these facilities requires wait lists and extensive efforts to fit as many interested users into the schedule as possible. The vast array of research and diverse collection of scientists that take advantage of these facilities makes them fertile ground for scientific collaboration and crosscutting innovations.

The knowledge gained through research supported by BES underpins the applied energy research supported by other DOE programs and by the private sector. Innovations in materials science, chemical analysis, geological imaging, or electrochemistry can have far-reaching impacts on renewable energy, energy efficiency, battery storage, and nuclear power – just to name a few.

I look forward to hearing how our witnesses have benefited from the federal support that we've provided to build these user facilities as well as other resources provided by BES. I'd particularly like to welcome Dr. Hallinan from Florida A&M and Florida State University's College of Engineering to today's hearing. Dr. Hallinan's research has the potential to achieve considerable gains in battery storage which could help the renewable energy sector play an even larger role in our economy in the coming years. Solving renewable energy's intermittency challenge in the near term could allow for a faster transition to a low-carbon energy future for the United States and the world.

Dr. Hallinan, as we will hear, has relied on the Advanced Light Source and the Advanced Photon Source facilities to advance his work by testing new solid polymers that can be used as battery electrolytes. His work is an excellent example of what we can accomplish if we robustly fund the vital research and facilities in the Office of Science.

Last week, the Basic Energy Sciences Advisory Committee released a new report on the prioritization of upgrades to the major BES facilities. While my understanding is that none of the witnesses here today were directly involved in developing this report, I hope we can consider revisiting this topic in the near future, with a closer look at the facility upgrades that are currently under consideration. These proposed upgrades represent major government investments, and I believe this issue warrants a closer examination from Congress.

Prioritizing and funding the research that is being highlighted today should certainly be a bipartisan issue and one I believe we can make considerable progress on.

With that, I yield back the balance of my time. Thank you, Mr. Chairman.

Chairman Weber. And I thank the gentleman. Again, I thank you for letting the Ranking—I mean, for our full Committee Chair

go first.

Let me introduce our witnesses today. Our first witness today is Dr. Nathan Lewis, Professor at the California Institute of Technology. Dr. Lewis is an inorganic materials chemist who is a globally recognized authority in artificial photosynthesis. Perhaps he's the one that needs to make the space in the night. Dr. Lewis received his Ph.D. in chemistry from MIT.

Our second witness today is Dr. Daniel Scherson, Professor at Case Western Reserve University. Dr. Scherson received his Ph.D.

in chemistry from the University of California Davis.

Our next witness today is Dr. Collin Broholm. Am I saying that correctly, Doctor?

Dr. Broholm. Yes.

Chairman Weber. Yes. A Professor at Johns Hopkins University, Dr. Broholm received his Ph.D. from the University of Copenhagen. And I will now yield to the Ranking Member to introduce our final witness.

Mr. Grayson. Thank you. Dr. Daniel Hallinan is unaccountably only Assistant Professor—I don't get that at all; you should be a full professor—in the College of Engineering at Florida A&M and Florida State University. As an independent investigator, he researches the use of solid polymers as electrolyte membranes in batteries, which have the potential to offer a safer, longer-lasting battery.

During his career, he has utilized both the Advanced Photon Source at Argonne National Lab and the Advanced Light Source at Lawrence Berkeley National Lab. His current research allows him to visit the Advanced Photon Source with his students regularly to explore the fundamental makeup of the materials that they're testing and from time to time actually insert the students into the photon source and light them up. No, no, that's not what he does. Never mind that.

Dr. Hallinan has degrees in chemical engineering and philosophy from Lafayette College and a Ph.D. in chemical engineering from Drexel University. His passion for science and innovative research has certainly been an inspiration to his students, and his work is a perfect example of our conversation today about supporting basic energy sciences and why it is so important. Thank you for testifying.

Chairman Weber. Thank you, Mr. Grayson.

I now recognize Dr. Lewis for five minutes to present his testimony. Dr. Lewis?

# TESTIMONY OF DR. NATE LEWIS, PROFESSOR, CALIFORNIA INSTITUTE OF TECHNOLOGY

Dr. Lewis. Chairman Smith, Chairman Weber, Ranking Member Grayson, Members of the Subcommittee, thank you very much for the opportunity to discuss this very exciting and timely research area of artificial photosynthesis, which is the direct production of fuels from sunlight.

Artificial photosynthesis has the potential indeed to be a gamechanging energy technology, cost-effectively producing fuels that are compatible with our existing infrastructure, and providing us

with both energy and environmental security.

Artificial photosynthesis is inspired by plants except that it can be over 10 times more efficient than natural photosynthesis, avoiding the need to trade food for fuel and producing a fuel unlike lignocellulose that we can directly used to power our vehicles, to potentially make ammonia for fertilizer to feed people around the world, and for other uses that they may develop.

Solar fuels production would also solve massive grid-scale energy storage so when the sun doesn't shine at night, we can still provide power to whenever people need it and carbon-neutral transportation fuels, which are both critical gaps at present that research

is needed to obtain a full carbon-neutral energy system.

Artificial photosynthesis does not look like a leaf, nor does it look like a solar panel. Instead, imagine a high-performance fabric that could be rolled out like artificial turf, supply that with sunlight, water, and perhaps other feedstocks from the air like nitrogen or carbon dioxide, and produce a fuel that gets wicked out into drainage pipes and collected for use. It's that simple in principle.

Many approaches to solar fuels are being pursued. Some are taking biological molecules like the green pigment chlorophylls and using them coupled to manmade catalysts. Others use all inorganic materials like semiconductors at the nanoscale and couple them to catalysts like ones used in fuel cells. Still others use metal com-

plexes as dyes and couple them to molecular catalysts.

Laboratories like mine at Caltech have already demonstrated functional solar fuels systems through advances in nanoscience that have enabled us to fabricate nanofibers of semiconductors that can absorb light and couple them to catalysts all in a piece of plastic. So we know this is possible, but we need to continue to innovate and perform fundamental research to make it practical.

A full system of solar fuels needs five components, two materials to absorb sunlight, one to capture the blue part of the rainbow, the other to capture the red part of the rainbow to make it very efficient. We need two catalysts, one to oxidize water from the air to provide electrons to make the reduced catalyst make the fuel that we want to harvest. We also need a membrane to separate those products to ensure that the system is safe and doesn't explode.

We actually have all of those pieces. What we don't have is all of those pieces all working together seamlessly in one system where they all are stable and mutually compatible. Research opportunities include the use of high-performance computation to design new catalysts, to design new semiconductors, and to do modeling and simulation to help us understand how to make the system

work as a whole, not just the pieces.

Many approaches are useful, and many fuels could be produced. We might produce a liquid fuel directly. We might produce a gaseous fuel and then convert it to a liquid fuel. We might think about a solar refinery the way we have an oil refinery where in comes our solar crude and then we convert it to various fuels as the output using the stained chemical processes that we use today.

In closing, I also would like to make two points. One is that many other countries now have burgeoning efforts in solar fuels. There are large efforts starting in Korea, Japan, China, Sweden, Germany, and the EU. We should beneficially leverage those efforts. We're well-positioned to do that given our historical leadership in solar fuels in the United States.

The second point is that solar fuels is an intellectual challenge that stimulates our young scientists, our graduate students, our postdocs involving nanoscience, material science, and fundamental research and energy broadly to give us better options for energy technologies than the ones that we have now. Thank you.

[The prepared statement of Dr. Lewis follows:]

#### **Congressional Testimony**

# Committee on Science, Space, and Technology Subcommittee on Energy U.S. House of Representatives

June 15, 2016

Dr. Nathan S. Lewis, California Institute of Technology

Mr. Chairman and Members of the Subcommittee:

Thank you for the opportunity to discuss the exciting and timely research opportunities in artificial photosynthesis—the direct production of fuels from sunlight.

Artificial photosynthesis has the potential to be a game-changing energy technology, cost-effectively producing fuels that are compatible with our existing infrastructure, and providing both energy and environmental security to our nation.

Artificial photosynthesis is inspired by plants, except that it can be over 10 times more efficient than natural photosynthesis, avoiding the need to trade food for fuel, while producing a fuel that we can directly use in our existing infrastructure, such as gasoline, diesel, methanol, or producing hydrogen that can be converted with nitrogen in the air into ammonia for use as agricultural fertilizer, as well as for other uses as they may develop.

Solar fuels production would allow for massive grid-scale energy storage, and for carbon-neutral transportation fuels, both of which are critical gaps at present towards reaching a full carbon-neutral energy system.

Artificial photosynthesis does not look like a leaf, nor does it look like a solar panel. Instead imagine a high performance fabric that can be rolled out like artificial turf, supplied with sunlight, water, and perhaps other feedstocks in the air such as nitrogen and/or carbon dioxide, and produces a fuel that is wicked out into drainage pipes and collected for use.

Many approaches to solar fuels generators are being pursued. Some are taking biological molecules like chlorophylls, and using them in artificial systems coupled to man-made catalysts for fuel production. Others are using all inorganic materials such as semiconductors like those used in solar panels and coupling them to catalysts like those used in fuel cells. Still others are using metal complexes as dyes to absorb the light and coupling the energy to molecular catalysts to produce the desired fuels.

Laboratories like mine at Caltech have already demonstrated functional solar fuels systems, through advances in nanoscience that have enabled the fabrication of nanofibers

of semiconductors that can absorb sunlight and coupled them to catalysts that can seamlessly produce fuel in one integrated assembly. We thus know that this is possible, but we need to continue to innovate and perform fundamental research on such systems to make it practical.

A full solar fuels system needs five components; two materials to absorb sunlight, one to capture the blue part of the spectrum and the other to capture the red part of the spectrum, two catalysts, one to make oxygen from water and the other make the fuel; and a membrane to ensure safe and efficient operation. We have all of these pieces, but do not yet have them all working together in a system that is simultaneously cost-effective, safe, efficient and stable.

Research opportunities include the use of high performance computation to design new fuel-producing catalysts that are both stable and inexpensive; development of new semiconducting materials using nanoscience and materials science to absorb the sunlight at the needed wavelengths; and use of modeling and simulation methods to design a system that will be safe, scalable, and efficient. Although challenging, we are making great progress, and more will be enabled by leveraging the expertise of interdisciplinary teams of scientists and engineers to focus on this use-inspired research area.

Many scientific approaches to solar fuels production are promising and should be pursued in parallel at this early stage of the field. Similarly, many types of solar fuels can be produced, including gases and liquids, hydrogen, methanol, methane, and gasoline. Since fuels can readily be interconverted, all options should be pursued in parallel to determine which are the most technically feasible and promising for implementation. The key is producing a fuel from the sun, and it is not nearly as important which fuel that is, because we can always convert one fuel into another as needed for end-use.

Within the past few years, other countries, including Korea, Japan, China, Sweden, Germany, and the European Union as a whole, have each launched burgeoning research programs in solar fuels. We can beneficially leverage these international efforts, but need to stay in the lead domestically on the research front. We are well-positioned to do this, given our historical leadership in the solar fuels area.

Solar fuels research offers an intellectual challenge to our young scientists such as graduate students and post-doctoral fellows, because it simultaneously involves frontier research challenges in nanoscience, materials science, applied physics, chemistry, and chemical engineering. It is a wonderful focal point for use-inspired, cross-disciplinary research, because the prize is so great. Moreover, the need for fundamental research is compelling, and challenges our scientists and engineers to apply their talents to discovering and designing the new molecules, materials, and systems that will make solar fuels and artificial photosynthesis a reality, and ultimately an option at scale for sustainable fuel production globally. Humans were inspired by biology to fly, but we don't build airplanes out of feathers, and airplanes fly faster and farther than any bird. Similarly, we are poised to beat nature at its own game: through artificial photosynthesis, we can harness the biggest energy source known to mankind, the Sun, and convert its

energy efficiently into a storable, dense form, namely into chemical fuels. Through research we can develop technology that can provide better energy options than those that we have now available, insuring a safe and secure energy future domestically and internationally.

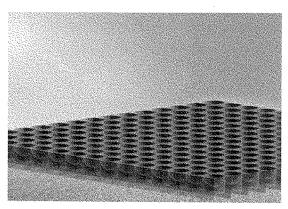


# How Does The Lewis Group Approach Making Fuels from Sunlight?

In order to radically reduce the costs of making fuels from sunlight, we focus on developing single-step devices from Earth-abundant elements, using techniques which minimize the total costs of materials without compromising on efficiency or safety. Since capital costs – for example labor, wiring, and equipment – need to be reduced significantly for solar fuels to be cost-competitive with fossil fuels, we focus on an architecture compatible with flexible materials, and envision a system that can be installed simply, like unrolling bubble wrap or artificial turf.

#### What Might a Solar Fuels Device Look Like?

We are designing systems that can make fuels from sunlight efficiently and safely. We use modeling and simulation tools to evaluate device designs so that we understand the theoretical limits to the design, and so



Bubble-wrap design for a solar fuels device, consisting of plastic cells that concentrate sunlight, with each cell containing a small active component (semiconductors, catalysts, and membranes) and water.

that we understand which parameters have the greatest impact on performance. Much of this modeling is done in collaboration with the team of Chengxiang Xiang, a Lewis Group alumnus and a Principal Investigator with the Joint Center for Artificial Photosynthesis.

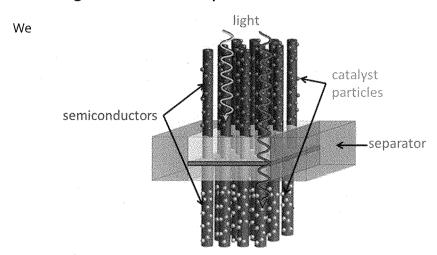
The bubble-wrap design sketched on this page consists of an array of plastic cells, each of which contains a small active component and water. This design uses simple, inexpensive plastic lenses to concentrate sunlight, and therefore allows a ten-fold reduction in the materials used for the active components relative to the materials requirements for devices without concentrating lenses. Since most of the design is plastic, the materials costs would be low, and the structure would be flexible, allowing it to be rolled out like bubble wrap or artificial turf, radically reducing installation costs relative to current solar fuels technologies. Other designs, for example an array of long cells based on trough-shaped plastic lenses, would achieve comparable efficiency while reducing materials and installation costs.

The optimal designs (on cost and efficiency metrics) vary depending on whether the device makes hydrogen from sunlight and water or carbon-based fuels from carbon dioxide, water, and sunlight. Devices designed to produce hydrogen fuel typically contain either acidic or alkaline water, while those designed to produce carbon-based fuels typically contain water buffered with carbonate salts. Some designs allow cells to fed either by humidified air, or by humidified deoxygenated air.

The active components of a solar fuels device are light absorbers and catalysts. For safety and efficiency purposes, solar fuels devices also need separators to prevent mixing of the chemical products of the reaction (fuels and oxygen).

Read more about devices in the Lewis Group Research pages.

#### What Might the Active Components Look Like?



envision active components consisting of wire-shaped semiconductors that are decorated with catalyst particles and embedded within a separator.

#### Semiconductors

The function of the semiconductors is to absorb sunlight and convert the energy in the absorbed sunlight into the potential energy of separated positive and negative charges.

Since sunlight is multispectral – it contains a wide range of energies (higher energies for violet and blue, lower energies for red) – we envision two complementary semiconductors, one on top which absorbs only higher energy light, and the other on the bottom to absorb any light which passes through the top (lower energies).

We can use silicon as the bottom absorber, but we are looking for a semiconductor for the top absorber that will not corrode and that can be made inexpensively from Earth-abundant elements.

Read more about semiconductors in the Lewis Group Research pages.

#### Catalysts

The active component needs two catalysts: one for the chemical reaction that yields fuels, and the other for the chemical reaction that yields oxygen gas. The reaction that forms oxygen gas is a necessary partner to the fuel-forming reaction, providing the electronic charges needed for the fuel-forming reaction, and closing a combustion-based fuel cycle.

Without catalysts, these reactions would proceed very slowly (if at all). Although the reactions are thermodynamically favored under the operating conditions in a solar fuels device, the reactions first need an uphill push – for example, electronic charges and molecules need to get close enough to react. Catalysts increase the reaction rates by decreasing the height of the hill.

Catalysts used in devices which make fuels from sunlight need long-term stability, preferably decades of stability under operating conditions. The catalysts need to attach firmly to the semiconductors, and can't dissolve, corrode, or undergo any other chemical reactions that would reduce their effectiveness. Stable catalysts are often based on expensive and rare elements – platinum, iridium, ruthenium and rhodium are a few examples. We are looking for catalysts based on Earth-abundant elements, such as nickel, iron, cobalt, or zinc. Ideally the catalysts would be transparent to sunlight, so that they don't block light from reaching the semiconductors; however, we have developed strategies for catalyst placement and loading that would considerably reduce the amount of light blocked by an opaque catalyst.

Several catalysts based on Earth-abundant elements and capable of making hydrogen fuel from water have been discovered as a result of solar fuels research. This set of catalysts – transition metal phosphides and nickel-molybdenum – offers options for stability and efficiency for either acidic or alkaline water. We also have catalysts – nickel-iron oxide

and cobalt oxide – that offer stability and efficiency for making oxygen from alkaline water.

We are looking for catalysts that can make carbon-based fuels from carbon dioxide and water. We are also looking for catalysts that can make oxygen from acidic water. We collaborate with Professor Ray Schaak at the Pennsylvania State University for many of our catalyst-discovery efforts.

Read more about catalysts in the Lewis Group Research pages.

#### **Separators**

Separators are critical components in a solar fuels device. For safety reasons, separators must prevent the fuels and oxygen formed by solar fuels devices from mixing in the cell or in the output streams. In order for the devices to function, separators must also allow ionic current to pass.

Without a separator ionic current would pass, but the products (fuels and oxygen) would not readily be separated. If fuels and oxygen are not separated everywhere and all the time: 1) The products from desired chemical reactions – fuels and oxygen – will recombine yielding the starting materials while releasing, possibly explosively, the energy of sunlight that was stored as chemical bonds; and, 2) Reverse chemical reactions will occur that convert fuels back to water (and carbon dioxide for carbon-based fuels) and that convert oxygen back to water, wasting the energy from sunlight that had been stored in the chemical bonds of the fuel.

# Where Can I Get More Information on Solar Fuels Research?

- Check out Who is Making Fuels from Sunlight?
- · Check out the Lewis Group Research pages.

- Read "Research Opportunities to Advance Solar Energy Utilization" published in *Science* (volume 351, 2016) and written by Prof. Nate Lewis.
- Read "Will Solar-Driven Water-Splitting Devices See the Light of Day" published in Chemistry of Materials (volume 26, 2014, pages 407–414) and written by Lewis Group alumnus James McKone, Prof. Harry Gray, and Prof. Nate Lewis.

by Kimberly Papadantonakis, June 2016.



More energy from the Sun hits the Earth in one hour than humans use in an entire year

#### Why Make Fuels from Sunlight?

Solar is by far the most abundant source of renewable energy available on Earth.

However, the sun is an intermittent and variable resource at any given location on the Earth's surface. Therefore, a reliable energy system in which solar plays a significant role will require a way to store the energy captured from sunlight so that it will be available upon demand, at any time of day or year.

The chemical bonds found in fuels are the most dense way to store energy outside of an atomic nucleus. For example, the energy density of gasoline is 60 times that of the best battery. In other words, 60 tons of batteries would be needed to store the energy contained in 1 ton of gasoline.



Making fuels from sunlight would store solar energy so it can be used on demand at any time of the day (or night).

Fuels made from sunlight would:

- Provide the massive grid-scale energy storage that is needed to compensate for the intermittency of solar power;
- 2. Provide an abundant source of the liquid fuels that are needed to power heavy-duty trucks, ships, and aircraft. Together these vehicles currently use ~40% of transportation fuels globally, and demand and will grow further as global commerce expands especially in developing nations. Unlike automobiles, these vehicles cannot run on batteries alone.



Airplanes, ships, and heavy-duty trucks cannot run on batteries alone and require energy-dense fuels.

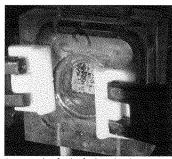
#### What is Solar Fuels Technology?

Solar fuels technologies are developmental systems that use robust, cheap, and highly efficient components to produce fuels that can readily be used in our existing energy

infrastructure. Solar fuels technologies use sunlight, water, carbon dioxide, and nitrogen from the air to produce fuels. Solar fuels are sustainable and produce no net emissions of carbon dioxide.

Solar fuels technologies are analogous to natural photosynthesis – plants make fuels (biomass) from sunlight. However, the fastest growing crops store <1% of the sunlight they receive as biomass. In order to be compatible with our energy infrastructure, the primary biomass made by plants – lignocelluose – must be converted into ethanol, biodiesel, or gasoline. This conversion requires energy and labor. Converting crops to fuels raises significant land-use concerns, specifically with regard to trading food for fuel.

We could make a fuel – hydrogen gas – from sunlight simply by pumping electricity from solar panels into water. This process is called water electrolysis, and making solar fuels this way would use two proven technologies: solar panels and



An example of solar fuels technology. Oxygen gas bubbles form at the center of the front of this water-containing cell when it is illuminated, and bubbles of hydrogen fuel form and are collected at the back of the cell.<sup>1</sup>

electrolyzers. Although mature, both of these technologies remain expensive, and the hydrogen that would be produced this way would be prohibitively costly when compared to hydrogen as it is currently produced at large scale from natural gas. Furthermore, commercial electrolyzers typically use precious metal catalysts (e.g., platinum and iridium), which imposes a barrier to scaling this technology globally.

#### What Fuels Can Be Made From Sunlight?

The Lewis Group leads the development of solar fuels technologies that produce hydrogen gas directly from sunlight and water. Carbon-containing fuels such as natural gas (methane) or liquid fuels such as methanol or ethanol might be produced from sunlight, water, and carbon dioxide. Ammonia for use as fertilizer in agriculture can be made indirectly from solar hydrogen or directly as a solar fuel from sunlight, water, and nitrogen in the air. Fuels can be readily interconverted using well-known processes implemented in petrochemical refineries.

Solar fuels would provide the same quality and quantity of energy services that end-users are used to, without a massive change in infrastructure, and hence would produce "drop-in" fuels that could serve critical sectors of the energy economy both in the developed and developing world. The feedstocks for solar fuels are abundant: sunlight, water, carbon dioxide, and nitrogen from the air. Solar fuels are sustainable and produce no net carbon dioxide emissions.

Are Solar Fuels Technologies Ready for Commercialization?

Solar fuels technologies are developmental systems that are not yet ready for commercialization. Although a number of prototypes have been demonstrated, they can't now compete with existing energy technologies, and can't yet provide the long-term (20 years) stability that would be needed.

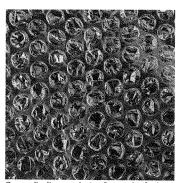
#### What are the Key Hurdles?

The key hurdles to making fuels from sunlight commercially are:

- Cost competitiveness Using current technologies, hydrogen made from sunlight would cost about ten times more than hydrogen made from fossil fuels. The high cost of solar fuels is primarily driven by costs such as labor, wiring, equipment, and materials for mounting solar panels.
- Materials discovery and system design Because fuels made from sunlight using current technologies would cost so much more than fossil fuels, radically new materials and system designs, that can be installed simply and at low costs, are needed.

#### What are Scientists Doing to Overcome the Hurdles?

Several approaches are being pursued to construct a demonstration solar fuels system. In one approach, the molecular components of natural photosynthesis, such as chlorophylls, are synthesized and modified chemically to attempt to construct a complete, functional photosynthetic system in the absence of a living organism such as a plant or photosynthetic bacteria or algae. In another approach, inorganic molecules, such as transition metal complexes, are used instead of chlorophylls as the light absorbers, and these complees are either coupled chemically to biological catalysts or are coupled to inorganic catalysts, such as metallic colloids or particles to generate solar fuels. In yet another approach, metal dyes are bonded to titania films to absorb light, and the dyes are also chemically are coupled to transition metal catalysts to produce solar fuels. Inorganic



One radically new design for a solar fuels technology looks like bubble wrap, so it would be easy (and cheap) to make and install.

semiconductors, similar to the ones used in solar panels, can also be used either indirectly to produce electricity in conjunction with catalysts for solar fuels production, or can be used as photoelectrodes to directly produce fuels from sunlight. All of the approaches have their own advantages and challenges both from a technical and cost perspective, requiring further materials discovery and research to address.

The Lewis Group, along with our partners and other scientists and organizations, is pursuing radically new designs that would make fuels from sunlight at a fraction of the price of the best solar fuels technologies (solar panels and electrolyzers) currently available. The key idea behind the new designs is combining the functions of solar panels and electrolyzers — conversion of light to electricity, followed by conversion of electricity to hydrogen — into a single, one-step process that would produce fuels directly from sunlight, resulting in simpler systems with low installation and materials costs, and therefore much lower costs for solar fuels.

However, reaching low enough costs by combining these functions requires intimate contact between the materials that convert light to electricity (semiconductors) with the strongly corrosive environment needed for an efficient electrolyzer. This causes semiconductors to corrode rapidly and to stop working. To address this problem, the Lewis Group is looking for new or non-traditional semiconductors that are stable in corrosive environments and is developing protective coatings that prevent the corrosion of semiconductors.

Common forms of commercial electrolyzers depend on expensive and scarce elements – platinum and iridium – to catalyze chemical reactions. The Lewis Group is discovering inexpensive materials – made from elements plentiful on Earth such as nickel, cobalt, and phosphorous – to replace these catalysts without reducing efficiency.

Additionally, scientists don't yet know how to produce carbon-containing fuels — such as natural gas (methane) or liquid fuels (methanol or ethanol) — efficiently from carbon dioxide and water in a solar fuels technology. The Lewis Group is discovering new catalysts to enable the generation of carboncontaining fuels.



A radically new design for a solar fuels technology might be analogous to artificial turf that can be rolled out and inexpensive to make and install.

These challenges are at the frontiers of solar fuels research: discovering new light absorbers to enable efficient, cheap, stable operation; discovering new catalysts to replace expensive materials that seamlessly mate with the light absorbers; discovering suitable membranes to provide for safe operation and to separate the products without introducing an explosion hazard; and insuring that all of the components are mutually compatible and function under the same operating conditions to form a complete system for solar fuels production. High-throughput experimentation, directed materials discovery, advanced computation and theory, and modeling and simulation tools at the system level are key ingredients in a broad solar fuels research program.

Where Can I Get More Information About Making Fuels from Sunlight?

- Check out the Lewis Group <u>Solar Fuels Research</u> page at <u>http://www.nsl.caltech.edu/solar-fuels/solar-fuels/research</u>
- Check out Who Makes Fuels from Sunlight at http://www.nsl.caltech.edu/who-makes-fuels-from-sunlight

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1. Verlage, E.; Hu, S.; Liu, R.; Jones, R. J. R.; Sun, K.; Xiang, C.; Lewis, N.; Atwater, H. A., A monolithically integrated, intrinsically safe, 10% efficient, solar-driven water-splitting system based on active, stable earth-abundant electrocatalysts in conjunction with tandem III-V light absorbers protected by amorphous TiO₂ films. Energy Environ. Sci. 2015, 8, 3166-3172. http://dx.doi.org/10.1039/c5ee01786f

Nathan S. Lewis is a Professor of Chemistry at the California Institute of Technology, Caltech. Dr. Lewis is an inorganic/materials chemist who is a globally recognized authority in artificial photosynthesis. Dr. Lewis has published over 400 papers, was cited over 4000 times in 2015, serves as the principal investigator on energy-related projects sponsored by the National Science Foundation, Department of Defense, and Department of Energy, and has supervised over 60 Ph.D. students who have gone on to careers in energy R&D. Prof. Lewis is the founding Editor-in-Chief of the journal *Energy and Environmental Science*, the leading scientific journal globally in energy R&D, and was named the #17 Agent of Change in America (and the top-ranked scientist) by Rolling Stone magazine in 2009, along with receiving numerous honors and awards from scientific and professional societies for his accomplishments.

Chairman Weber. Thank you, Dr. Lewis. Dr. Scherson, you're recognized for five minutes.

### TESTIMONY OF DR. DANIEL SCHERSON, PROFESSOR, CASE WESTERN RESERVE UNIVERSITY

Dr. Scherson. Thank you.

Chairman Smith, Chairman Weber, Ranking Member Grayson, and Members of the Subcommittee, I thank you for the opportunity to testify in today's hearing on innovation in solar fuels, electricity

Chairman Weber. Dr. Scherson, is your mike on? And put your mike-

Dr. Scherson. My apologies, sir. Chairman Weber. There you go, right in front of you.

Dr. Scherson. All right. Could I start again?

Chairman Smith, Chairman Weber, Ranking Member Grayson, and Members of the Subcommittee, thank you for the opportunity to testify in today's hearing on innovation in solar fuels, electricity storage, and advanced materials. My name is Daniel Scherson, and I'm the Frank Hovorka Professor of Chemistry and Director of the Ernest B. Yeager Center for Electrochemical Sciences at Case Western Reserve University in Cleveland, Ohio, and until a few days ago, President of the Electrochemical Society.

Electrochemistry, a 2-century-old discipline, has reemerged in recent years as key to achieve sustainability and improve human welfare. The scientific and technological domain of electrochemistry is very wide, extending from the corrosive effects of the weather on the safety and integrity of our bridges and roads, to the management of diabetes and Parkinson's disease, and to the fabrication of three-dimensional circuitry of ever-smaller and more complex architecture. In addition, electrochemistry is becoming central to the way in which we generate, store, and manage electricity derived

from such intermittent energy sources as the sun and wind. Among the most ubiquitous electrochemical devices ever invented are batteries. Mostly hidden from sight, batteries convert chemicals into electrical energy used to power cell phones and portable electronics, which are critical to the way we communicate and store information, as well as electrical vehicles, which are expected to mitigate the dangers posed by the release of greenhouse gases into the atmosphere.

I have been asked to focus my attention this morning on aspects of electrochemistry that relate to energy storage, which are expected to greatly impact not only the transportation sector but also the management and optimization of the electrical grid, which combined account for 2/3 of all the energy used in the United States. Scientific and technological advances in this area will bring about a reduction in operating costs, spur economic growth, and create new jobs and promote U.S. innovation in the global marketplace.

The advent of ever more powerful computers and advanced theoretical methods have made it possible to predict with increased accuracy the behavior not only of materials but also of interfaces. The latter play a key role in the chemical industry where there is a strong pressure to develop effective catalysts to increase yields and lower energy demands. This is also true in the area of electrocatalysis, which is critical to the optimization of electrolyzers and fuel cells, yet another class of electrochemical energy conversion devices.

In the area of transportation, any new developments aimed at augmenting reliability, safety, and comfort must be made without compromising performance. Today, batteries for electric cars cannot match already-established standards for range per tank of gasolinepowered vehicles. In simple terms, the energy a battery can store depends on the charge capacity and its voltage. So whereas the energy is dictated by thermodynamics, the power batteries can deliver

is given by the current times the voltage.

To illustrate, lithium-ion batteries rely on only a single electron per atom of electrode material to store energy and deliver power. One obvious solution to increase the energy is then to double or, better yet, triple the number of electrons per atom of storage material without decreasing its voltage. Although the viability of such a concept has been demonstrated for the case of magnesium, a divalent metal, using a purely empirical approach, its performance is still below that required for meeting the demands of the largest markets.

Theoretical work at the Joint Center for Electrochemical Storage Research, JCESR, DOE's energy hub led by Argonne National Laboratory, has unveiled new yet-to-be synthesized materials that display promising characteristics. Results have shown that the primary bottleneck resides in the mobility of divalent magnesium ion within the host lattice, which is greatly enhancing materials where the ions sit in energetically and unfavorable sites as compared to the sites along the path of migration. Such design rules have been validated in the laboratory for known materials, and arrangements have been made with partners, laboratories to synthesize these new promising materials.

Equally important is the search of new organic electrolytes exhibiting large voltage windows of stability, including ionic solvation. From an overall perspective, the problems that remain to be resolved towards achieving sustainability demand a fundamental understanding of the basic processes underlying energy conversion and energy storage at a microscopic level and the development of spectroscopic and structural probes with highly spatial and temporal resolution to monitor individual atomic and molecular events. Such knowledge can only come from new generations of scientists trained at our colleges, universities, and national laboratories, which will require increased research support from the government.

Thank you.

[The prepared statement of Dr. Scherson follows:]

### Written Testimony of Daniel Scherson Subcommittee on Energy Committee on Science, Space, and Technology United States House of Representatives June 15, 2016

Chairman Weber, Ranking Member Grayson, and Members of the Subcommittee, thank you for the opportunity to testify in today's hearing on Innovation in Solar Fuels, Electricity Storage, and Advanced Materials

My name is Daniel Scherson, and I am the Frank Hovorka Professor of Chemistry and Director of the Ernest B. Yeager Center for Electrochemical Sciences at Case Western Reserve University in Cleveland, OH, and, as of a few days ago President of The Electrochemical Society.

Electrochemistry, a two centuries old discipline responsible for the discovery of several chemical elements, has reemerged in recent years as key to achieve sustainability and improve human welfare. The scientific and technological domain of electrochemistry is very wide, extending from the corrosive effects of weather and other factors, which threatens the safety and integrity of our bridges and roads, to the management of such debilitating ailments as diabetes and Parkinson's disease, and to the development of copper plating processes, which have allowed fabrication of three-dimensional circuitry of ever smaller and more complex architecture. From an even broader perspective, electrochemistry is becoming central to the way in which generate, store and manage electricity derived from such intermittent energy sources as the sun and wind.

Among the most popular and indeed most ubiquitous electrochemical devices ever invented are batteries, which allow chemical energy to be converted into electrical energy. Mostly hidden from sight, batteries are the engines that power our cell phones and other portable electronics, which are critical to the way we communicate and store information. Battery powered cars will also contribute to decrease the release of green-house gases into the atmosphere and thus mitigate their adverse effects on the climate. I have been asked to focus my testimony this morning on aspects of electrochemistry that relate to energy storage, which are

expected to greatly impact, not only the transportation sector, but also, the management and optimization of the electrical grid.

Over the last two decades, the interplay between theory and experiment has experienced a rather radical change in balance. The advent of ever more powerful computers and advanced theoretical methods, have made it possible to predict with increased accuracy the behavior not only of materials, as I am sure will be addressed by my colleagues later in these proceedings, but also of interfaces. The latter play a key role in the chemical industry, where there is growing pressure to develop effective catalysts to increase yields, and lower energy demands. This is also true in the area of electrocatalysts, which are critical to the further optimization of fuel cells, yet another electrochemical device which, like batteries, convert chemical energy into electrical energy. At the pace we have witnessed over this past decade, it would not be surprising that in the next few years, theory will guide the search of new materials. Once identified, it will be up to experimentalists to devise and or implement methods for their synthesis and characterization. Long forgone will be the days of expensive and time consuming testing of compounds in the hope one of them may work. Transportation and the grid account for two thirds of all energy used in the United States. Scientific and technological advancements in these areas will bring about a reduction in operating costs, spur economic growth and create new jobs, and promote US innovation in the global marketplace.

In the area of transportation, any new developments aimed at augmenting reliability, safety and comfort, must be made without compromising performance. Today, batteries for electric cars cannot match already established standards for range per tank of gasoline powered vehicles. In simple terms, the energy a battery can store depends on the charge capacity and its voltage. Whereas the energy is dictated strictly by thermodynamics, the power batteries can deliver is given by the current times the voltage. To illustrate this point, lithium ion battery technology, responsible for the revolution in portable electronics and in transportation, relies on only a single electron per atom of electrode material to store energy and deliver power. Increases in the total energy then require for the size of the battery to be increased, which, in turn, increases the weight of the vehicle and thus the energy required to drive it. While Li-ion batteries have undergone a significant increase in energy density since their introduction in 1991, energy density is currently leveling off. One obvious solution

is to double or, better yet, triple the number of electrons per atom of storage material without decreasing its voltage and thus the energy that can be stored. Among novel chemistries currently being investigated, multi-valent (MV) intercalation is one of the very few that have the potential to supersede the energy density of Li-ion by multiples of two or three. In MV-technology, the Li $^{\dagger}$  ion is replaced by a divalent ion such as  $Mg^{2+}$ ,  $Zn^{2+}$  or  $Ca^{2+}$ , thereby moving twice the charge per ion transferred between electrodes. Hence, if one can establish that as many  $Mg^{2+}$  ions as Li $^{\dagger}$  ions can be stored in an electrode material, the charge storage capacity of cathodes per unit volume and weight will be doubled. In addition, Mg-ion technology may enable the use of a Mg metal anode which, with a theoretical capacity of 3800mAh/cc of storage density is among the charge-densest materials imaginable. Combined benefits of a Mg metal anode and a di-valent intercalant cathode are projected to combine to cells with two to three times the energy density of current Li-ion.

While proof of concept of rechargeable Mg batteries has been established, significant hurdles remain for it to become a viable high-energy-density energy storage technology. One of these is to find a suitable cathode material. In an intercalation cathode, ions insert upon discharge, to be released back to the electrolyte and anode upon charge of the battery. In order for charge and discharge to proceed at reasonable rates, diffusion of the MV-ion needs to be fast enough. While such fast diffusion at room temperature is rather common for mono-valent ions such as Li<sup>†</sup>, Na<sup>†</sup> and H<sup>†</sup>, the higher charge of divalent ions makes them interact stronger with the cathode structure and move much slower. Hence, finding good cathode materials among hundreds of thousands of possible compounds is akin to looking for a needle in a haystack. While materials with high MV-ion diffusivity are definitely out there –indeed proof of concept exists–finding them cannot simply done by trial and error, as each effort to synthesize, test, and characterize a target cathode compound, can take 6-12 months for a research group.

To find high energy density MV-ion cathode materials, the Joint Center for Energy Storage Research (JCESR), which comprises 14 partner institutions led by Argonne National Laboratory is integrating modern computational tools in a high-throughput computational search for the next generation battery materials to predict many of the relevant properties of candidate MV-ion cathode materials, including ion mobility. In such a search, tens of thousands of compounds are run

through a computational screening of successively more challenging property requirements with the objective of identifying a handful of candidate compounds for synthesis and testing. By combining such computational tools with synthesis and electrochemical testing, a more effective search for the next generation battery materials can be achieved.

A challenge to implement a complete high-throughput computational cathode search is that computational methods for predicting the mobility of an ion are extremely slow and computationally unstable. As a result, only "one-at-a-time" investigations are usually performed in theory groups. Developing new methodology that first identifies likely mechanism and migration paths, and then calculates the energy along those paths, has the potential to alleviate this issue to some extent, making a high-throughput search more likely in the future. While there used to be a generic believe that all MV-ion diffusion would be sluggish, the JCESR team has already identified the characteristics of low energy pathways in candidate materials, indicating that under certain conditions, MV diffusion can be more than fast enough for battery application. The key mechanism identified is to search for materials where the MV cation inserts in a coordination that is not its preferred environment (e.g. 4-fold for Mg<sup>2+</sup> or 6-fold for Zn<sup>2+</sup>). In such a case, the migration barrier can be kept low if the activated state along the diffusion path has a "better" coordination for the MV ion. An important consequence of this finding is the realization that good materials for one specific MV-ion are more likely than not to be bad for another: e.g. good Zn and good Mg diffusers are barely overlapping materials groups. This strategy has already born fruit in developing a novel cathode material, TiS2, with twice the energy density of the Chevrel cathode, the first functioning cathode for Mg batteries. While TiS2 does not have high enough energy density to surpass Li-ion technology it is an important validation of the search strategy towards even better cathode materials.

Also of importance is the search of new organic electrolytes that will display a large voltage window of stability to allow operation of higher potential electrodes. In particular, most known salts and solvents are incompatible with magnesium metal — causing the formation of a passive layer at the anode surface, and hence blocking reversible magnesium transport. The first working magnesium battery prototype utilized organometallic aluminum chloride, magnesium chloride-based salts which together with a THF solvent made possible a stable

electrolyte between 0-3 V vs magnesium and reversible stripping and plating of a magnesium metal anode. The only other salts that exhibit some promise are halides and borohydrides, in particular the recent carborane salt. However, today, there is no electrolyte that supports both reversible anode operations as well as the large electrochemical window necessary to fulfill the promise of high energy density multivalent energy storage. All magnesium electrolytes with higher anodic stability than 3 V exhibit decomposition reactions at the metal anode. Until recently, there was little fundamental understanding as to why it has been so difficult to find salts and solvent combinations that are stable against magnesium metal and the question of what makes magnesium electrochemistry so different as compared to Li has remained largely unanswered.

To answer this question, the recent revolution in computational materials software and rapidly increasing computing resources is being leveraged. Specifically, efforts at JCESR have led to the development of a rapid and accurate first-principles computational infrastructure for calculating properties of liquid solvent and salt molecules, within the high-throughput infrastructure of the world-leading Department of Energy-funded Materials (www.materialsproject.org). The Materials Project was launched at Lawrence Berkeley National Laboratory in 2012, as part of the President's Materials Genome Initiative, and has since calculated the properties of more than 66,000 solids as well as 21,000 molecules. This unique machinery coupled with the supercomputing facilities available at Argonne and Berkeley has made it possible to calculate, and hence screen, hundreds of molecules per week for the set of properties relevant for electrochemical applications. For magnesium electrolytes, electrolyte-relevant properties such as the solvation structure, the electrochemical window, ionic diffusivity etc for a broad range of salts and solvents are being rapidly elucidated. A number of extremely important novel insights were gained by this capability. First, it was learned that almost all multivalent electrolytes, in particular, magnesium-based ones, form contact ionpairs between the salt cation and anion in organic solvent solutions, even at moderate concentrations. This has fundamental impact on the transport, as well as the charge transfer properties of the electrolyte. The magnesium cations in solution now diffuse together with a negatively charged anion, which reduces the conductivity of the electrolyte and impedes the desolvation process at the anode. Furthermore, the charge transfer process of the magnesium cation at the anode metal interface involves two electrons, which includes a transient, highly reactive

intermediate Mg\* state, which puts a tremendous chemical 'pressure' on the accompanying anion and/or solvent molecules. In most cases, the close proximity of the anion with magnesium during the charge transfer reaction leads to irreversible decomposition of the salt, deposition of decomposition products on the magnesium anode surface and hence loss of active electrolyte. This scenario is fundamentally different from Li electrolytes, where the Li cation is primarily solvated by solvent molecules, and only needs one electron to complete the charge transfer process. The computational screening – and subsequent validation experiments performed within JCESR - confirmed that indeed, borohydrides and halide salts are – so far – the only known salts that are immune to decomposition while delivering and desolvating the magnesium cation at the anode interface. Hence, no

Using the insight of ion-pairing and its impact on the charge transfer process, we leverage our computational capability to uncover which anion or solvent bonds that weaken under the desolvation and charge transfer process. In the computer, we can artificially 'freeze' the charge transfer reaction and study the stability of each individual molecular bond of the solvating species, while exposed to the reactive Mg<sup>+</sup> transient cation. The knowledge of what constitutes the weakest links of the salt or solvent molecules allows us to perform target substitutions and modifications; to design in silico new molecules that are inherently more stable under the challenging electrochemical conditions posed by multivalent metal plating. As a result, we have now begun to design completely new salts, some of which are currently being made and tested within JCESR.

From an overall perspective, the problems that remain to be resolved toward achieving sustainability demand a fundamental understanding of the basic processes underlying energy conversion and energy storage at a microscopic level and the development of spectroscopic and structural probes with highly spatial and temporal resolution to monitor individual atomic and molecular events. Such knowledge can only come from new generations of scientists trained at our colleges, Universities and National laboratories, which will require increased research support from the Government.

### DANIEL A. SCHERSON Biography

Daniel Scherson was born in Santiago, Chile in 1951. He received his Licenciatura en Quimica (License in Chemistry) from the Faculty of Sciences, University of Chile in 1974, and later in 1979 a Ph.D. in Chemistry from the University of California, Davis, in the area the non-equilibrium nonlinear thermodynamics under the supervision of Prof. Joel Keizer. After completing his doctoral thesis, he held post-doctoral research appointments in the groups of Prof. John Newman at UC Berkeley, Dr. Phil Ross at the Lawrence Berkeley National Laboratory, Prof. Ernest B. Yeager at Case Western Reserve University and later at the Fritz Haber Institute with Profs. Dieter Kolb and Heinz Gerischer. In 1983, he joined the faculty of the Department of Chemistry at Case Western Reserve University, where he later became the Charles F. Mabery Professor of Research in Chemistry and, subsequently, the Frank Hovorka Professor of Chemistry. He has co-authored over 250 publications and 5 patents in experimental and theoretical areas of electrocatalysis, energy storage and energy conversion, and has advised 26 PhD students.

Over the years he has distinguished himself by combining theoretical principles with novel experimental strategies to develop and/or implement in situ spectroscopic methods covering a wide spectral range from infrared to synchrotron radiation to study, from a very fundamental viewpoint, problems of direct relevance to energy conversion and energy storage. Particularly noteworthy are his contributions in theoretical and experimental aspects of attenuated total reflection IR and UV vis spectroscopies in the presence of convective flow, and applications of synchrotron based techniques and Raman scattering to in situ studies of materials for batteries, fuel cells and supercapacitors, including actual operating devices. His interests also encompass the coupling of ultrahigh vacuum and electrochemical techniques, electrochemistry in ultrahigh vacuum, as well as the implementation of methods for the ultrafast monitoring of surface dynamics at solid electrode-liquid electrolyte interfaces. More recently, he has also become involved in the application of fundamental concepts of physical electrochemistry to the understanding of neural stimulation. Among his many contributions, Prof. Scherson applied in situ reflectance spectroscopy, X-ray absorption fine structure, atomic force microscopy and microgravimetric techniques to elucidate important aspects of the underlying physicochemical basis of the operation of nickel oxide electrodes in alkaline environments. In addition, his coupling of forced convection techniques and spectroelectrochemistry enabled new insights to be gained into the reduction of sulfur dioxide in aqueous electrolytes. More recently, he pioneered the use of Fourier transform infrared spectroscopy to the study of the reactivity of Li in ultrahigh vacuum environments and, based on the systematic use of this approach, helped unveil the mechanistic pathway of decomposition of linear and cyclic carbonates commonly used as solvents in lithium battery applications. In recent years, Prof. Scherson's attention has been focused on the application of ultrafast techniques for studies of molecular events at electrochemical interfaces, which culminated in the first real time second harmonic generation monitoring of a surface reconstruction induced by the applied potential in the submicrosecond regime.

He has been deeply involved in the activities of The Electrochemical Society (ECS), serving as Chair of its Physical and Analytical Electrochemistry and Battery Divisions. He was also Associate Editor and later Editor of the Journal of the Electrochemical Society. In recognition to his many scientific achievements he has received a number of prestigious awards including, the Vittorio de Nora-Diamond

Shamrock Postdoctoral Fellowship (1981), Max Planck Gesellschaft Fellowship (1982-83), IBM Faculty Development Award (1983-85), Japan Society for the Promotion of Science Fellowship (1993-94), David C. Grahame Award of the Physical Electrochemistry Division of ECS (2000), Humboldt Senior Fellowship (2002), Faraday Medal of the Electrochemistry Group of the Royal Chemical Society, UK (2004), Japan Society for the Promotion of Science Senior Travel Award (2007), and was made Fellow of the Electrochemical Society (2007).

Over the past few years he has organized a week long Workshop on Electrochemical Measurements sponsored by the Ernest B Yeager Center for Electrochemical Sciences to provide instruction to participants from academia, industry and National laboratories. As part of the Workshop participants have the opportunity to conduct actual experiments with the assistance of graduate students from Case. Lastly. Prof. Scherson is now serving in the Advisory Committees of the Joint Center for Energy Storage Research, (JCESR), led by G. Crabtree at Argonne National Laboratory, (ANL), and of three Energy Frontier Research Centers, (EFRC) led by D. Wesolowski, Oak Ridge National Laboratory, P. Fenter, Argonne National Laboratory, and S. Whittingham, Binghamton, NY.

Chairman Weber. Thank you, Dr. Scherson. Dr. Broholm, you are recognized for five minutes.

### TESTIMONY OF DR. COLLIN BROHOLM, PROFESSOR, JOHNS HOPKINS UNIVERSITY

Dr. Broholm. Thank you very much. Chairman Weber, Ranking Member Grayson, and distinguished Members of the Subcommittee on Energy, thank you very much for the opportunity to testify today on the topic of quantum materials.

Seventy years ago when amplification of an electrical signal by a transistor was first demonstrated, no one could have imagined that the average person in 2016 would employ billions of transistors in their energy and information-intensive lives. What will be the next materials-based technological revolution, and how can we ensure the United States once again leads the way?
Since its 1947 discovery of the transistor, Bell Laboratories, now

a part of Nokia, has shrunk and is no longer active in fundamental materials research. While the opportunities for groundbreaking progress from advanced materials have never been greater, the research now has a broad and fundamental character that no single

company can sustain.

The specific example that I'd like to focus on is quantum materials. Quantum mechanics has key effects in all materials, but the most dramatic departure from the familiar generally fade from view beyond the atomic scale. The Heisenberg uncertainty principle is, however, on display in elemental helium that fails to solidify upon cooling even to the absolute zero temperature. Instead, an astounding superfluid state occurs where atoms form a coherent matter wave that flows without any friction whatsoever.

We now find it may be possible to realize such counterintuitive properties of matter in a new class of quantum materials, of which

I shall provide a couple of examples.

Superconductivity is a low-temperature property of many metals, including aluminum wherein electrons form a coherent wave much as the atoms in superfluid helium. But because electrons carry charge, an electrical current can then flow with zero resistance. While presently available, superconductors require cryogenic cooling, we know of no reason that superconductivity like ferromagnetism should not be possible at much higher temperatures.

A practical superconductor would have enormous technological consequences, including the ability to generate, store, transport, and utilize electrical energy without resistive losses. There's much recent progress in the scientific understanding of a new class of superconductivity enhanced by interactions between electrons. While we do not have a winner yet, this fortifies our belief that a practical superconducting material will eventually be discovered.

The next topic is topological materials. The geometry of the wave function that describes electrons in these materials gives rise to revolutionary electrical properties. In a topological insulator, for example, all surfaces are electrically conducting even though the core or the center of the material is actually insulating. And this is a really appealing property considering that the surface transport must typically be engineered into electrical devices and is associated with significant resistive energy losses. In topological

insulators, a high-quality conducting surface occurs spontaneously, and there are many more fascinating properties of topological materials that indicate they will have transformative technological im-

Digital archiving of events from those of individual families to those that define our times is generally based on magnetic information storage. While hard disc storage densities now exceed 1 terabit per square inch, each bit still involves a very large number of atoms. By using wrinkles on a prevailing order within a quantum material to store information, it may be possible to dramatically increase the information storage density.

Finally, a new form of information processing called quantum computing has the potential to transform decision-making. One of the approaches now being pursued is to utilize so-called quasi-particles within a quantum material to carry and process information. While this is a long-term vision, it is as feasible now as an integrated circuit with 10 billion transistors must have seemed like in

1947.

Given the potential technological impacts, quantum materials are receiving huge worldwide attention. Dedicated research centers are proliferating, and I would argue that within the DOE as well, quantum material should be an area of high priority. The Basic Research Needs Report on quantum materials identifies four priority research directions that would accelerate scientific progress in

quantum materials and their technological deployment.

So as in much of the modern development of advanced materials, world-class tools are essential for this work. Such as the neutron sources at Oak Ridge Lab and the synchrotron and free electron laser-based light sources, these are absolutely essential to be able to sustain—to be able to do this kind of work. And while these are already excellent facilities that are having strong impacts, several are in urgent need of upgrades to sustain international leadership.

In the continuing quest to bend materials to satisfy our needs, it is inevitable that we should eventually employ the wave-like nature of matter for new functional materials and electronic devices. To do so requires a deep fundamental knowledge of interacting electrons in the quantum realm, versatile abilities to synthesize new materials from the atomic scale to bolt single crystals, and an array of experimental tools that probe structure and motion over broad range of length and time scales.

Sustained basic research efforts in quantum materials can ensure the United States leads the way as these materials transform a broad range of energy and information technologies. Thank you.

[The prepared statement of Dr. Broholm follows:]

### Statement by Collin Broholm to the Committee on Science, Space, and Technology Subcommittee on Energy of the US House of Representatives

June 15, 2016

Seventy years ago when amplification of an electrical signal by a transistor was first demonstrated, no one could have imagined that the average person in 2016 would employ billions of transistors in their energy and information intensive lives. What will be the next materials based technological revolution and how can we ensure the United States once again leads the way?

Since its 1947 discovery of the transistor, Bell Laboratories (now part of Nokia), has shrunk and is no longer active in fundamental materials research. Other companies that used to support long-term basic research now focus on short-term development work. While the opportunities for ground breaking progress from new advanced materials have never been greater, the research required for transformational progress has a broad and fundamental character that no single company can sustain for the required period of time.

The specific example I would like to focus on is quantum materials. If we can master the quantum realm these materials have the potential for transformative technological impacts. Quantum mechanics has key effects in all materials but wave interference, coherence, and tunneling, which are integral to quantum uncertainty usually fade from view beyond the atomic scale. A stark counter example is offered by elemental helium that fails to solidify upon cooling. Instead an astounding superfluid state occurs where atoms form a coherent matter wave that flows without friction. The ghostly wave function that describes the atomic scale thus becomes apparent at our length scale. We now find it may be possible to realize the counterintuitive properties of quantum mechanics in a new class of "quantum materials" and in the following I would like to provide a couple of examples.

**Superconductivity** is a low temperature property of many materials including aluminum wherein electrons form a macroscopic wave much as the atoms in superfluid helium. Because electrons carry charge, an electrical current can flow through a superconductor with zero resistance and no energy loss. Superconducting materials are already the basis for Magnetic Resonance Imaging and high voltage DC power transmission. While presently available superconductors require cryogenic cooling, we know of no fundamental reason that superconductivity – like ferromagnetism – should not be possible at much higher temperatures. A practical superconductor would have enormous technological consequences including the ability to generate, store, and transport electrical energy with no resistive losses. The impacts on the entire transportation sector would also be far reaching. There is much progress in the development and scientific understanding of materials where

superconductivity is enhanced as magnetism collapses and reasons to argue a breakthrough is possible.

In **Topological materials** the geometry of the wave function that describes electrons gives rise to anomalous electrical transport that is insensitive to atomic scale disorder. In topological insulators for example all surfaces of a sample are electrically conducting even though the core is insulating and topological protection ensures high electron mobility. This is an appealing effect considering that surface transport must typically be engineered into electrical devices and is associated with significant resistive energy losses. In suitable topological insulators high mobility spin polarized surface conduction can appear spontaneously.

Finally we turn to **magnetism and information**. Digital archiving of events from those of individual families to those that define our times is based on magnetic information storage. While hard disk storage densities now exceed 1 TB per square inch, each bit still involves million of atoms. By using collective quasi-particles such as skyrmions within a quantum material to store information, it may be possible to dramatically reduce this number and get closer to the information storage density of DNA. A new form of information processing called "quantum computing" has the potential to transform computing and decision making. One of the approaches now being pursued is to utilize collective particles within a quantum material to carry and process information. While this may be a reach today, it seems as feasible now as an integrated circuit with 10 billion transistors must have seemed in 1947.

Given the potential technological impacts, quantum materials are now receiving huge worldwide attention. Research centers for quantum materials are proliferating and I would argue that within the DOE as well, quantum materials should be an area of high priority. In the Basic Research Needs Report on quantum materials for energy relevant technology (see background material), we describe four priority research directions that would accelerate scientific progress in quantum materials and their deployment to improve energy efficiency and extend the information technology revolution.

As in much of modern development of advanced materials, world-class experimental tools such as the neutron sources at ORNL and the synchrotron and free electron laser based light sources are absolutely essential for progress. While these are excellent facilities that are having strong scientific impacts, several are in urgent need of upgrades to sustain international leadership.

In the continuing quest to bend materials to satisfy our needs, it is inevitable that we should eventually seek to directly employ the wave like nature of matter for new functional materials and electronic devices. To do so requires a deep fundamental knowledge of interacting electrons in the quantum realm, versatile abilities to

synthesize new materials from the atomic scale to bulk single crystals, and an array of experimental tools that probe structure and motion over a broad range of length and time scales. A sustained basic research effort in quantum materials is required to accelerate their technological deployment and ensure the US like in the solid state electronic revolution that started seventy years ago, can also lead the way as quantum materials transform a broad range of energy and information technologies.

The testimony represents the opinions of Collin Broholm and not necessarily the viewpoint of the Johns Hopkins University.

COLLIN LESLIE BROHOLM is the Gerhard H. Dieke Professor in the Department of Physics and Astronomy at the Johns Hopkins University. He earned his Ph.D. from the University of Copenhagen in 1988, was a post doc at AT&T Bell Laboratories from 1988-1990, and joined Johns Hopkins in 1990. Dr. Broholm is interested in anomalous forms of magnetism, superconductivity, and their interplay. Of particular interest are crystalline materials where quantum effects are enhanced on account of competing interactions (frustration) or low dimensionality. The main experimental tool is neutron scattering and Dr. Broholm is involved in development of the corresponding instrumentation. He has built two spectrometers at the NIST Center for Neutron Research and has served on committees overseeing instrumentation development at National facilities for Neutron Scattering. Dr. Broholm received the Presidential Faculty Fellowship in 1994, became a fellow of the American Physical Society in 2004, and received the Sustained Research Award of the Neutron Scattering Society of America in 2010. He was selected as a Gordon and Betty Moore Foundation experimentalists in quantum materials in 2014. Dr. Broholm co-founded and directs the Johns Hopkins Institute for Quantum Matter.

### **Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology**

Draft Workshop Report 6/6/16 4:47 PM

### BASIC RESEARCH NEEDS WORKSHOP ON QUANTUM MATERIALS FOR ENERGY RELEVANT TECHNOLOGY

Report of the Office of Basic Energy Sciences Workshop on Quantum Materials

Chair:

Collin Broholm, Johns Hopkins University

Co-chairs:

Ian R. Fisher, Stanford University

Joel E. Moore, LBNL/University of California-Berkeley Margaret Murnane, University of Colorado-Boulder

Panel Leads:

Superconductivity and charge order in quantum materials

Adriana Moreo, University of Tennessee-Knoxville John Tranquada, Brookhaven National Laboratory

Magnetism and spin in quantum materials
Meigan Aronson, Texas A&M University
Allan MacDonald, University of Texas at Austin

Transport and non-equilibrium dynamics in quantum materials

Dimitri Basov, University of California-San Diego

Jim Freericks, Georgetown University

Topological quantum materials

Eduardo Fradkin, University of Illinois at Urbana-Champaign

Amir Yacoby, Harvard University

Heterogeneous and nano-structured quantum materials

Nitin Samarth, Pennsylvania State University

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### **Executive Summary**

Imagine future computers that are able to perform calculations not feasible with the most powerful supercomputers today and at a fraction of the cost in energy and time. Imagine electronic devices so efficient they use practically no electricity. Imagine electricity being generated, stored and then transported across the national grid with nearly no loss of energy. Imagine ultrasensitive sensors and detectors with extraordinary performance for the military and manufacturing. Imagine that we understand how to alter electronic, magnetic, optical and thermal properties of materials in the blink of an eye to carry out the functions we want. The key to attaining these technological possibilities in the 21<sup>st</sup> century is a new class of materials largely unknown to the general public at this time but destined to become as familiar as silicon. Welcome to the world of quantum materials - materials in which the extraordinary effects of quantum mechanics give rise to a plethora of exotic and often incredible properties.

Just as the discovery of semiconductors revolutionized computation and information storage, and ushered in today's hundred-billion dollar electronics industry, quantum materials have the potential to revolutionize energy and energy-related technologies, as well as the storage and processing of data, with possible economic ramifications of staggering proportions. Even now new quantum materials are emerging that feature unprecedented capabilities. One quantum material just entering the public radar is "graphene" - a sheet of carbon just one atom thick. Not only is graphene 200 times stronger than steel while weighing less than paper, electrons race through its two-dimensional plane 100 times faster than they move through silicon. While graphene has already been identified as a potential superstar by the electronics industry, new quantum materials are emerging to challenge it. For example, two-dimensional (2D) transition metal dichalcogenides (TMDCs) are more device-ready than graphene, and offer other advantages for high-speed, low-power electronics. Additional breakthroughs are being seen in materials known as "topological insulators" where novel properties are found in electronic states that only exist on the material's surface. From TMDCs and topological insulators, to materials that display other extraordinary effects such as "quantum spin liquids" and high temperature superconductivity, we may be seeing the dawn of a new era of quantum materials.

To realize the tantalizing potential of quantum materials, there is much basic scientific research to be done. Recognizing the high potential impact of quantum materials, nations around the world are already investing in this effort. We must learn how the astonishing properties of quantum materials can be tailored to address our most pressing technological needs, and we must dramatically improve our ability to synthesize, characterize and control quantum materials. To accelerate the progress of quantum materials research, the U.S. Department of Energy's Office of Science sponsored the "Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology," which was held near Washington, D.C. on February 8 - 10, 2016. Attended by more than 100 of the nation's leading scientific experts in the synthesis, characterization, and theory of quantum materials, the workshop identified four priority research

directions (PRDs) that will enable us to better understand quantum materials and harness their rich technological potential.

### Control and exploit electronic interactions for the design of materials with novel functionality

One of the effects of quantum mechanics is spontaneous "quantum fluctuations" of physical quantities which can break down conventional order in solids and usher in entirely new forms of electronic order. The resulting material properties, coupled to an extreme sensitivity to external perturbations, hold promise for novel functionality that could impact technologies ranging from power management and transmission, to platforms for quantum computation, to the design of novel sensors.

### · Harness topological quantum states for ground breaking functionalities

Topological materials are a newly discovered class of quantum materials with distinct electronic properties in a protected surface region. Like graphene, the 2D electronic nature of topological materials offers potential game-changing advances in the energy and electronics industries because of an ability to support switchable electrical currents on their surfaces with dramatically lower energy loss.

### Drive and manipulate quantum behavior (coherence, entanglement, and transport) for transformative technologies

Nano-structured quantum materials can be externally manipulated beyond thermal equilibrium using new techniques for ultrafast, coherent excitation. The formation of quasiparticles with exotic names such as skyrmions, magnons and spinons, and the seemingly magical qualities of quantum effects such as coherence and entanglement in these materials offer a pathway to ultrafast, ultra-energy efficient computing with seamless linkages to optical communications.

### Design revolutionary tools for synthesis, characterization, and modeling to accelerate discovery and technological deployment

The development of new methodologies and tools will accelerate the discovery of new quantum materials, and advance the ability to probe, predict and exploit their remarkable properties.

Detailed discussions of the four PRDs along with guidelines and recommendations for achieving their objectives are provided in chapter 2 of this report. Chapter 3 includes the detailed background information on quantum materials developed as part of the workshop. The full report is available through (information to come) or can be accessed on-line at (Website url to come).

### 1. Introduction

### Those who see things grow from the beginning will have the best understanding of them . . . Aristotle

Every day of your life you encounter thousands of different materials. The text you are now reading is made from either ink on a paper substrate or a liquid crystal sandwiched between two layers of glass. The clothes on your back, the containers that hold your food and beverage, the buildings that give you shelter, the vehicles that transport you, the energy systems that power them and the roads they travel, the tools with which you work and the devices that inform or entertain you – all reflect the ubiquity of engineered materials in modern life.

At an accelerating pace stretching from the pre-historic age of stone tools to the age of bronze alloys, to the transformation of iron into steel, to zone-refined silicon for electronics, the progression of human society is inextricably linked to its ability to make and use materials. As we continue to bend materials to satisfy our needs, it is inevitable that we should eventually reach the atomic scale. There, as matter becomes wave, we find quantum phenomena such as interference, tunneling, quantum fluctuations, quantum entanglement, and topological effects that are perhaps even more counterintuitive and surprising to us than the strength of bronze to our predecessors. Based on our improved understanding and control of interacting electrons at the atomic scale, "quantum materials" seem poised to transform an array of critical technologies, particularly those related to information and energy.

Before the advent of quantum mechanics, many properties of solids seemed so magical that Thales of Miletus in the 6<sup>th</sup> century BCE ascribed a soul to the magnetic lodestone (Fe<sub>3</sub>O<sub>4</sub>). In the ensuing millennia, inventive navigators took advantage of the lodestone in compasses even if a proper understanding of how a solid's electrons become magnetized had to wait until the 20<sup>th</sup> century. The strongly quantum-mechanical nature of electrons in many solids leads to their being called quantum materials, and leaps in our understanding of these materials are now positioned to enable technologies as revolutionary as the compass was in its day.

Solid-state magnetism is based on the spin of the electron, which also underlies new approaches to computing. Spin is the intrinsic rotational momentum of a quantum particle – here an electron, which is quantized to spin up or down (corresponding to two senses of rotation). A modern hard disk is based on magnetic regions that are tiny, with more than a trillion bits per square inch, but each region still includes many spins. Improving our control of magnetism at the single-spin level and finding new types of magnetic ordering in quantum materials will enable improved computer memory and logic devices to extend the information technology revolution.

Quantum materials may enable fundamentally new approaches to computation, such as quantum or neuromorphic computing, to progress from fantasy to reality. Quantum computing has the

potential to render trivial certain critical mathematical tasks that are now practically impossible even on the world's fastest supercomputers. The blinding speed and awesome power of quantum computing would be made possible by the weird but demonstrably real effects of quantum mechanics. Today's information technologies largely rely on the electrical charge of electrons to store and process individual "bits" of information as either a one or a zero. Under quantum computing, information would be processed and stored in "qubits" that in a sense behave as both a one and a zero to enable massively parallel computation. Advances in our understanding of quantum materials might also enable the construction of neuromorphic computers that mimic the processing approach of a human brain by learning and adapting as they interact with the world.

Even current "classical" computing is in a position to be revitalized by the development of quantum materials. The portable electronic devices, upon which we so heavily depend in our daily lives –cell phones, tablets, laptops, etc., - consume a substantial amount of energy estimated at 10-percent of the world's total electricity generation. As Information and Communication Technology (ICT) devices continue to proliferate, this consumption will continue to grow and the strain on the global grid system will increase. Quantum materials, with their potential for enabling smaller and far more energy-efficient ICT devices, could do much to relieve this strain.

One of the most dramatic phenomena in quantum materials is superconductivity- the ability of a material through the correlation of its electrons to support electrical current flow with zero resistance, meaning no energy is lost to heating or other inefficiencies. While superconductivity is a property of many metals, it typically occurs in metals only near the absolute zero of temperature (-273 Celsius). Many of the most powerful and compact magnets in the world, used to channel high-energy particles in colliders or to diagnose disease through Magnetic Resonance Imaging (MRI), are based on superconducting materials, because a superconductor can carry enormous electrical current densities that would melt even a good conductor like copper.

In the late 1980s, scientists learned that some quantum materials superconduct at relatively high temperatures even though their room temperature state is not nearly as conductive as an ordinary metal. These "high-temperature superconductors" are now being used to bring electrical power more efficiently to high-rise buildings and in major power cables in Seoul. At the demonstration level, superconductors have been used to support and propel a train at 375 mph in Japan, and to support a fusing plasma so hot that no material can contain it. A more widespread application of superconductivity has the potential to save tens of billions of dollars in energy transmission, generation, and storage losses. By enhancing the correlations between electrons so superconductivity can be sustained at even higher temperatures, quantum materials could transform our energy distribution systems, the medical and scientific applications of strong magnetic fields, and potentially the entire transportation and energy production sectors.

While ferromagnetism has been known to man for more than 2500 years and superconductivity was first observed a century ago, other classes of quantum materials were discovered much more recently. Topological quantum materials have remarkable properties whose understanding took

off in the past decade. Topological insulators are an example: these are materials that are insulating in bulk, but every surface supports an atomically thin conducting layer. As artificially created thin conductors are the basis of special transistors used in cell phones and other applications, the idea that a material naturally creates such layers is quite appealing. Two other directions with great progress in recent years are the manipulation of quantum materials at extremely short time scales (well under a trillionth of a second), and their manipulation in space at the atomic scale.

In recognition of the tremendous scope and scale of the transformative opportunities offered by quantum materials, the U.S. Department of Energy's Office of Science sponsored an intense two-day workshop on the subject, which was held near Washington, D.C. February 8 - 10, 2016. The "Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology" was attended by more than 100 of the nation's leading scientific experts in the synthesis, measurement and theory of quantum materials. Attendees were organized into panels that examined the current state of the field in such key areas as superconductivity, quantum magnetism, transport and non-equilibrium, topological materials, heterostructured quantum materials, and the "tools" needed to synthesize, probe, and model quantum materials. From these panels, four priority research directions (PRDs) were identified, based on the compelling nature of fundamental questions and the potential for future energy-relevant technologies.

### PRD1: Control and exploit electronic interactions for design of materials with novel functionality

Many of the remarkable properties of quantum materials result from strong interactions among their constituent electrons and the rich variety of ordered states that emerge as a consequence. These properties include an extreme sensitivity to perturbations, affecting electronic, magnetic, optical and thermal properties; quantum entanglement (in which an action on one electron impacts another electron even if the two are separated by a substantial distance and do not interact); and superconductivity. To assess the utility of these materials for applications, and enhance their potential functionality, fundamental research is required that is directed towards understanding the organizing principles that govern electron dynamics in the presence of strong quantum fluctuations. Looking beyond the standard paradigms of simple metals and semiconductors, how are strongly interacting electrons organized in quantum materials, and how can this be controlled for energy-relevant technologies? Research thrusts under this PRD specifically target a comprehensive understanding of complex phase diagrams, including the interplay of collective modes with quasiparticle dynamics, and the discovery and characterization of new electronic phases. This will require the development of new methods to expose quantum entanglement as well as the means to understand and control the effects of quenched disorder. A central but still poorly understood concept in all of these areas is that of the quantum phase transition in metals. Significant advances in these areas could lead to improved superconductors

for power applications, improved materials for information storage and processing, and new materials for sensing and quantum computing.

### PRD2: Harness topological quantum states for groundbreaking functionalities

In topological materials the geometry of the quantum-mechanical "wave function" that describes the material's electrons has complex structure with some simple and important consequences: an example is that a material's surface can behave fundamentally differently from the bulk. Topological insulators for example are electrically insulating in the bulk but have atomically thin conducting layers on every surface. The area of topological materials has seen remarkable and unexpected progress in the past decade, enabled by close connections between experimental and theoretical work.

Much of the scientific excitement and potential utility of topological quantum materials can be traced to two properties that have the potential to provide groundbreaking electronic functionalities. The first is dissipationless electron transport - the ability to support large, switchable electric currents without energy loss. The dissipationless transport of electrons in a topological quantum state is similar to the transport of electrons in a superconductor, so that these materials present exciting new opportunities for applications of quantum transport. Harnessing topological quantum states as called for in PRD2 offers a new approach to increasing the energy efficiency of current computing and thermoelectric devices, as well as creating new kinds of devices, e.g., based on spin transport.

The second unique property of topological quantum states is that they can host electron-derived quasiparticles with significantly different properties than the original electrons. Quasiparticles can, for example, carry fractional charges so that it takes several of them to equal the charge of an electron. Thus within the confines of the material the electron has been fractionalized. In two-dimensional systems, fractionalized quasiparticles can be non-abelian, meaning that the physical exchange of two identical particles fundamentally alters the underlying quantum state. Quasiparticles in topological quantum materials offer new approaches to the computing process itself, including the creation of robust quantum computers that are desensitized to noise and disorder. PRD2 focuses on the scientific effort required to improve topological materials so their dissipationless transport and fractional quasiparticles can be the basis for amazing new electronic devices.

### PRD3: Drive and manipulate quantum behavior (coherence, entanglement, and transport) for transformative technologies

Today's silicon-based information technologies are approaching physical limits set by dissipation, density and speed. Quantum materials, by comparison, offer a staggering array of

new electronic functionalities that promise to extend and expand current information technologies far beyond the capabilities of silicon. The potential technological bounty of quantum materials stems from the exotic quasiparticles they can harbor - magnons, spinons, visons, skyrmions, magnetic monopoles, etc., - which, within the material, are as real as the electrons and photons that drive the internet. These quasiparticles boast quantum behaviors coherence, entanglement and transport - the exploration of which in nano-structured quantum materials provide abundant opportunities for fundamental discoveries that enable radical new low-power information storage and processing. PRD3 focuses on exploring the transport and non-equilibrium properties of quantum materials, and the heterogeneous and finite-sized structures that reveal fundamental properties and can be the basis for transformative technologies. Stimulating quantum materials with femtosecond light pulses can, for example, create metastable states of matter with specific electronic functionalities that do not exist in equilibrium. Desirable properties, such as superconductivity, may be enhanced by exciting specific vibrational states (phonons), and magnetic bits in nanostructures may be individually switched with spatially patterned optical driving fields. The rich interactions between light and quantum materials offer outstanding opportunities to transfer information from fiber-optical encoding to quasiparticle assemblies for information processing within a quantum material. Nano-structured quantum materials thus open the possibility of a new class of ultra-fast and energy efficient computing with seamless linkages to optical communication systems.

### PRD4: Create revolutionary tools for synthesis, characterization, and modeling to accelerate discovery and technological deployment

The remarkable properties of quantum materials that are generating such keen scientific interest - including the ability to alter their electronic, structural or magnetic state through external stimuli, or transport spin and charge with extreme efficiency - also pose immense challenges to the experimental and theoretical work that is required to understand and exploit them. PRD4 calls for development of the necessary tools to address these challenges, affecting the synthesis, characterization and theoretical treatment of quantum materials. Key challenges include establishing appropriate methods to grow and manipulate complex and nanostructured quantum materials with desired purity and control of dopants and defects from a single atomic layer on up to bulk crystals. Issues addressed by PRD4 encompass new in-situ characterization and feedback techniques, and the discovery of materials with improved properties based on these new techniques; characterizing quantum materials and learning how to manipulate their properties on all length and time scales relevant to function, including development of appropriate tools to reveal the often subtle forms of emergent and topological order that such materials can harbor: and predicting the fundamental properties of quantum materials, including tendencies to emergent order, and their behavior far from equilibrium and in the presence of disorder. Progress in these areas will enable the science described in the other PRDs. These new capabilities will also have a broad impact across wide ranges of materials with potential applications in energy and computational sciences, nanotechnology, nanomanufacturing and nanoengineering.

Achieving the objectives of the four PRDs presented in this report will require a substantial investment of federal funds but the potential rewards in terms of strengthening our nation's economy and energy security are as stunning as the properties of quantum materials themselves. Research into quantum materials has become a worldwide enterprise amongst all of the technologically advanced nations because there are billions upon billions of dollars to be realized in the next generation of information and energy-relevant technologies.

In his seminal 1959 lecture, "There's Plenty of Room at the Bottom," physicist Richard Feynman called out the vast potential of manipulating matter at the atomic scale. Nearly 60 years later, with many of his ideas now being applied to hundreds of millions of smartphones, we find the prospects are even more exciting than perhaps envisioned by Feynman: the unique properties of the quantum realm can be exploited in quantum materials to solve problems surrounding energy and information that before seemed utterly intractable.

### **Basic Research Needs Workshop Energy Relevant Technology** on Quantum Materials for

iair: Collin Broholm, Johns Hopkins University

Co-chairs: Ian R. Fisher, Stanford University

Joel E. Moore, LBNL/University of California-Berkeley

Margaret Murnane, University of Colorado-Boulder

### **Basic Energy Sciences Leads:**

Linda Horton, Office of Science, Department of Energy

Jim Horwitz, Office of Science, Department of Energy



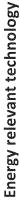
## Quantum Materials

### Quantum mechanics beyond the atom

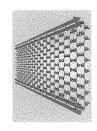
- Quantization, quantum fluctuations, coherence, & tunneling at mesoscopic or macroscopic length scales
- Superconductivity, BEC, Quantum spin liquid, Topological insulators, Dirac and Weyl materials, spin-orbital liquid

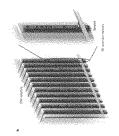


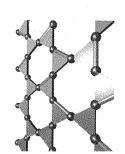
Discover, Create, classify, understand, & control qualitatively new quantum states of matter

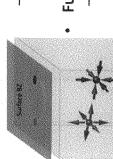


- Lossless transmission, generation & transduction
- Novel material responses for energy efficiency and sensing
- Energy efficient information storage & processing
- Quantum information processing based on collective quasi-particles









2,000

10,000

# A Focus on Quantum Materials



Citations in Each Year

Papers: 4739 Citations: 105k H-index: 132

- Copper; then iron superconductivity
- Richness of quantum magnetism
- Surprising impacts of topology
- Topology & interactions
- Public & Private funding
- Univ. & Gov. Labs. start quantum materials groups
- Network grants in North America, Asia & Europe
- Moore foundation invests \$90M (EPIQS program)
- DOE: Basic Research Needs Workshop

Multiple Manual Control of the Manual Contro

# Elements of Quantum Materials Research

- **Materials Synthesis**
- **Exploratory synthesis**
- single crystal growth
- Nanostructured
- **Experimental work**
- Multifaceted characterization
- Advance the experimental methods

- Laboratory and facility scale experiments
- Theory & modeling
- Interacting quantum systems (analytical field theory)
- Numerical methods for correlated electrons
- Density functional theory and extensions

## 

• Identify basic research needs and priority research directions for quantum materials with a focus on new, emerging areas with potential for transformative scientific advances and for impact on energy technologies.

## Questions to be addressed include:

- What distinct materials phenomena can arise when ordered electronic states are suppressed by quantum fluctuations?
- What experimental and theoretical methods are needed to advance the understanding of quantum materials?
  What roles can beterogeneity and interfaces play in their
  - What roles can heterogeneity and interfaces play in their function?
- What technological opportunities particularly in the areas relevant to energy – arise from quantum materials and how can this potential be realized?

### An opportunity to:

 Accelerate and coordinate progress in our understanding of quantum materials and their applications for energy relevant technology

# Five Panels – A universe of materials

<b>/</b>	<b>Superconductivity</b> and charge orders A. Moreo in quantum materials	A. Moreo J. Tranquada
7	2. Magnetism in quantum materials	M. Aronson A. MacDonald

dynamics in quantum materials	J. Freericks
	E. Fradkin
	A. Yacoby
quantui	<b>4. Topological</b> quantum materials

<b>ostructured</b> N. Samarth	S. Stemmer
5. Heterogeneous & nanostructured	quantum materials

## Cross-cutting panels: Tools of the trade

### A. Synthesis [lan R. Fisher]

- Bulk; powder, crystal
- Nano-structured, heterogeneous

## B. Instrumentation [M. Murnane & C. Broholm]

- Spectroscopy (photons, x-rays, neutrons, electrons) - Imaging (photon, x-ray, STM, neutron)
  - Extreme conditions (B, P, T,...)
- Transport
- Thermomagnetic methods

## C. Theory and Modeling [J. E. Moore]

- Ab-initio (LDA+U, DMFT)
- Analytical
- Exact numerical





## Plenary Presentations

- Fundamental Science
- Louis Taillefer
- Subir Sachdev
- Harold Hwang
- Alessandra Lanzara

















- Peter Littlewood
- Stuart Parkin

▼ Design revolutionary tools for synthesis, characterization, &

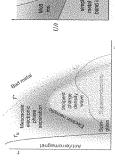
## Priority Research Direction

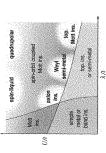
Harness topological quantum

states for disruptive

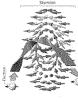
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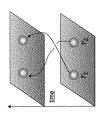


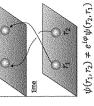


entanglement, & transport) for V Drive & manipulate quantum transformative technologies behavior (coherence,

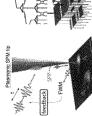


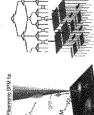


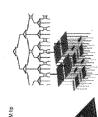








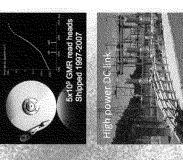


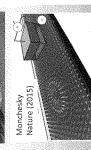


# 1. Control & Exploit Electronic Interactions for Design of Materials with Novel Functionality

## Extraordinary materials properties when we marshal interacting electrons

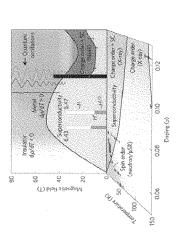
- Adaptable and responsive materials
- Efficient optical, electric, thermal switching
  - Detection/sensing
- Thermo-electrics solid state refrigeration & energy scavenging
  - Neuromorphic computing
- Practical Superconductivity
- Energy distribution: generation, transmission, storage
  - Transportation: Levitation & Propulsion
- A fabric for collective particles
- Quantum computing (non-abelian anyons)
- Fast & efficient communication (magnons, skyrmions)





## intertwined order in metallic quantum materials A. Understand & control competing, coexisting &

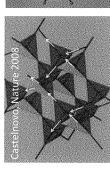
- Interplay between ordered phases of conducting systems
- Quantum criticality in metals
- The physical origins of strange metals
- The roles of disorder

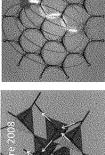


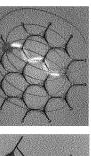
### B. Predict, realize, & probe strongly correlated quantum magnets

Metallicity





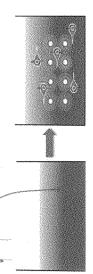






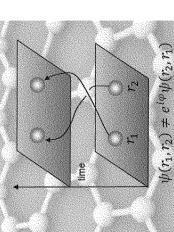






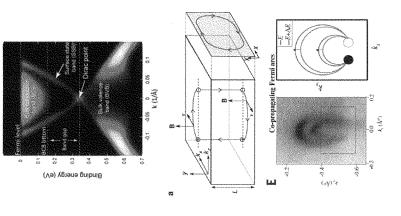
### for groundbreaking Functionalities Harness Topological

- **Topologically Protected Transport**
- Energy efficient surface transport
- Reduced dissipation in electronics
- Neuromorphic computing
- Fractional quasi-particles
- Solid state quantum computing - Information storage
- communication



# A. New Topological Quantum Materials

- Non-Interacting Topological Insulators, and Dirac and Weyl semimetals
- Topological Superconductors
- Interacting topological insulators
- Topological phases in strongly-correlated systems
- · Fractionalized topological phases in 3D
- Topological magnetic systems
- Robust topological quantum phenomena

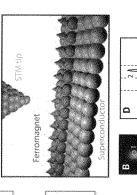


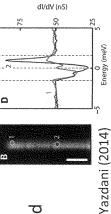
correlated TI SmB<sub>6</sub>

Neutrons probe

### Fuhrman 2015 New methods to probe & manipulate topological states <u></u>

- Topologically sensitive probes
- Transport in extreme magnetic fields: topological states in the quantum limit
- Correlated topological materials probed by symmetry-specific probes
- Fractional quantum magneto-electric effect
- Engineering non-abelian statistics and Majorana fermion zero-modes
- Engineering topological phases by proximity coupling
- Engineering states with parafermions and other exotic excitations





- 3. Drive & Manipulate Coherence, Entanglement, & Transport for Transformative Technologies
- Nanostructured functionality
- at the interface between quantum materials
- In confined quantum materials
- In artificially layered structures
- Quasi-particles transport
- Low-loss transport
- Coherent transport
- Out of equilibrium
- Writing bits with photons
- Switched quantum matter

### exploit quantum coherence & entanglement A. Employ nanoscale structuring to elucidate &

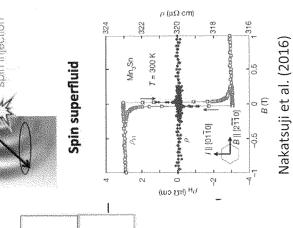
- Control the character of electrons in quantum materials
- Use electrostatic gating to adjust the electron density without disorder.

4

- Use layered structures such as moiré solids for rational design of bandstructures and their filling.
- Tune electronic interactions through nano structuring
- Confine electrons to surfaces where it is easier to modulate anisotropic interactions.

## B. Understand transport in quantum materials & expose the technological potential

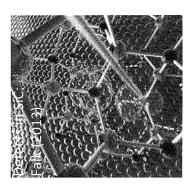
- Spin-orbit torques to read and write information
- Topological magnon band structures for quantum transport
- Store and transport energy and information in antiferromagnets
- lossless transport through magnetic condensates
- Skyrmions for information storage and transport
- Valley index quantum transport
- Transport in moiré patterned solids



## materials, harnessing coherence & entanglement C. Dynamically visualize and manipulate quantum

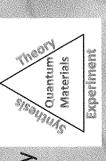
- Access metastable states of matter
- Explore thermalization of interacting quantum matter
- Create novel states of matter driven by the strong time dependent fields of pulsed light.
- Form entangled states between defects in pristine solids, which act as isolated atoms
- New theoretical methods to understand and control interacting quantum materials in the time domain.

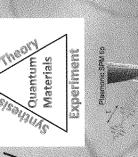


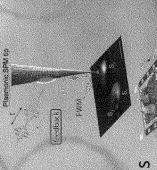




Progress in all PRDs driven by ability to make, measure, and model







Impacts on applications

 New quantum materials faster - Diagnose operating device

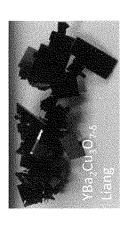
strongly interacting quantum systems - Predict behavior of heterogeneous

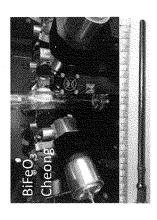
## Enhanced synthesis of quantum materials; from bulk crystals to single atomic layers

- Establish generalized rules of assembly for complex materials
- Towards materials by design
- New methodologies and new tools
- Establish methods to tailor local structure

Extend the physical regimes for synthesis

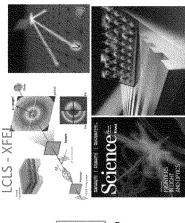
- Access kinetically trapped compounds
- Expand the scope of exploratory synthesis
- experimentally driven exploratory synthesis
- Accelerated discovery of new materials



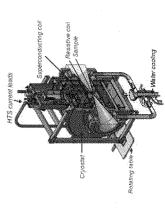


## New windows into quantum materials മ

- Enhanced efficiency, speed and resolution for spectroscopic probes of response functions with THz to X-ray light, neutrons & electrons
- Real-time and real-space imaging to capture quantum materials in situ and in operando
- Multi-dimensional spectroscopies from THz to multi-keV.
- Probe solid state quantum entanglement in spin and orbital sectors
- Access to new phases of matter using extreme electric and magnetic field, stress, and pressure
- X-ray and neutron scattering under extreme electric and magnetic field, stress, and pressure
- Big Data: Better algorithms and data sharing approaches



High Harmonic soft x-rays



2D MERA

D MERA

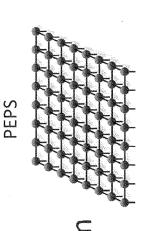
## quantum materials beyond 1-electron paradigms C. Develop efficient theoretical methods for

 Tensor Networks (DMRG, PEPS, MERA)



Simulate lattice gauge theories

Interacting quantum matter far from equilibrium



### 

- the atomic scale where quantum physics drives function In the quest to shape materials to our needs we reach
- Basic science can unlock the potential of quantum materials for energy and information
- The science is transforming our understanding of matter with broad impacts on physical sciences
- As we master the quantum realm technology is transformed



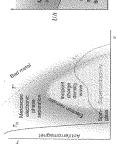
## **Priority Research Direction**

Warness topological quantum

states for disruptive

functionalities

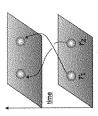
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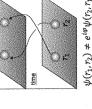


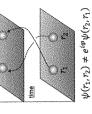
entanglement, & transport) for Volve & manipulate quantum transformative technologies behavior (consence,









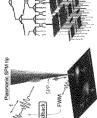


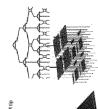


modeling to accelerate discovery

 → Design revolutionary tools for the property tools. The property tools for the property tools for the property tools for the property tools. The property tools for the property tools for the property tools. The property tools for the property tools for the property tools. The property tools for the property tools for the property tools. The property tools for the property tools for the property tools. The property tools for the property tools for the property tools. The property tools for the property tools for the property tools. The property tools for the property tools for the property tools. The property tools for the property tools for the property tools. The property tools for the property tools for the property tools. The property tools for the property tools for the property tools. The property tools for the property tools for the property tools. The property tools for the property tools for the property tools.

2. \*\*The property tools for the property too synthesis, characterization, &





Chairman WEBER. Thank you, Dr. Broholm. Dr. Hallinan, you're recognized for five minutes.

### TESTIMONY OF DR. DANIEL HALLINAN JR., ASSISTANT PROFESSOR, FLORIDA A&M UNIVERSITY—FLORIDA STATE UNIVERSITY COLLEGE OF ENGINEERING

Mr. HALLINAN. Good morning. Thank you for the opportunity to

testify in today's hearing.

I'm here to speak to the importance of the Department of Energy's national light sources to research and to the technological challenges of the nation. I will also briefly address the impact of the proposed upgrades on research capabilities and U.S. scientific competitiveness. I thank the Committee for its long-standing and ro-

bust support of national light sources and energy research.

Synchrotron light sources are large-scale facilities. These clearly are not possible—practical for individual academic or industrial labs, let alone at home. However, they enable high-impact research that would not be possible otherwise, and they advance our scientific understanding of matter across length scales from the atomic to that which we can see with our own eyes. They provide insight into dynamics from ultrafast making and breaking of chemical bonds to structural relaxations that take longer than a year. They allow us to map in three dimensions the composition of materials that are poised to address energy and water needs of the country and the world.

So my personal experience with synchrotron light sources began during my postdoctoral fellowship at Lawrence Berkeley National Laboratory where I used four of the beam lines of the Advanced Light Source, and I worked with beam line scientists there. Now as an Assistant Professor at Florida State University, my group continues to collaborate with scientists at Berkeley Lab, but we also use, due to uniquenesses, some beam lines at the Advanced Photon Source of Argonne National Lab. FSU, Florida State University, recognizes the value of the travel to do this research, and they support it.

So this schematic that you see on the monitors I'm going to use just to explain to you briefly how the synchrotron light source actually works. So electrons are accelerated to near the speed of light around this ring, and in order to get them to curve around the ring, magnets are used. And when the magnets curve the electrons, x-rays are released tangentially, and you can see those x-rays then go to experiment stations. And there are many experiment stations located all around this ring. So they are—and there are many different types of experiments that can be done with these x-rays.

So you can categorize those experiments into three main types, and that's scattering, microscopy, and spectroscopy. So with scattering, x-ray scattering allows us to do is to look at both length and time scales of a very wide range of length and time scales of complex materials. Microscopy allows us to look inside materials so we can get inside something you couldn't see inside of with optical light and very small length scales and we can see the composition in there. And then spectroscopy specifically gives us the composition of materials. So, for example, we can watch the chemical

changes that occur as we charge and discharge a battery that occur

in the electrode, for example.

So just some statistics about these user facilities, there are many thousands of researchers that access the light sources across the nation each year at no charge, but this access is based on a competitive process. And the competitive process is to ensure that sound and impactful science is being conducted. The researchers come from a wide range of fields and generate thousands of research publications each year, contributing significantly to the nation's innovation-based economy.

And the most exciting thing to me is that these synchrotron light sources enable numerous scientific discoveries that wouldn't be practical without the facilities. And this practical uniqueness of each facility is the primary reason that they continue to be an inte-

gral part of my research program.

So I'll mention two areas of my personal research that they impact. So the first is safer, longer-lasting batteries. With batteries, we could increase dramatically the efficiency of our transportation. These electric vehicles are much more efficient than internal combustion engines. But commercial lithium-ion batteries now are not inherently safe. They have a flammable liquid electrolyte. There are engineering controls to protect against that, but they're not inherently safe, so that's why we're interested in polymer electrolytes. And these polymer electrolytes can not only enable safer batteries but they're compatible with some advanced electrode materials. But their dynamics are somewhat limited, and so we're studying the dynamics and the structure of polymer electrolytes for batteries.

The other area that I'm really interested I'm just going to touch on for a moment is energy-efficient water generation. So polymer electrolytes, polymers with charge in them are actually promising materials for generating more energy-efficient water from desalination, for example. But in order to do that, the structure of the polymer is very important, and that structure is a function of the water content and the salt concentration in the polymer. So we're using these—some of these x-ray facilities to study the structure as a function of salt and water in these polymers.

So in closing, for those of you who have not had the opportunity to visit one of these facilities, I would like to impress upon you the scale. So as you saw in that schematic, these things can be the size of a baseball field or even larger than the size of a whole baseball stadium depending on the facility, and they have hundreds of personnel, highly trained personnel, who work as a team to keep these things operating consistently and safely. There are a lot of safety concerns.

So this was really inspiring to me to see this many people working together on science. And I think it's a testament to what we have achieved, but new opportunities do await with the most recent synchrotron breakthroughs, and I encourage you to continue to robustly support the operating budgets of these facilities, as well as the proposed upgrades.

I thank you for your time, and I'm happy to answer any questions you might have.

[The prepared statement of Dr. Hallinan follows:]

### **Congressional Testimony**

### Committee on Science, Space and Technology Subcommittee on Energy U.S. House of Representatives

June 15, 2016

Daniel Hallinan Jr., Assistant Professor
Chemical and Biomedical Engineering
Florida A & M University – Florida State University College of Engineering

### Summary

I am here to speak to the impact of the Department of Energy Office of Science's national light sources on research and national needs primarily as it relates to energy storage and advanced materials. Synchrotron light sources are large scale facilities that are not practical for individual academic or industrial laboratories to operate. However, these facilities, funded by the DOE Office of Sciences Basic Energy Sciences program and operated by national laboratories, enable high-impact research by academic groups and industrial users, research that would not be possible otherwise. They advance our scientific understanding of matter across length scales from atomic to that which we can see with our own eyes. They provide insight to dynamics from the ultrafast timescales of the making and breaking of chemical bonds to slow mechanical fatigue processes that take more than a year. They allow us to map, in three dimensions, the composition of materials that are poised to address energy and water needs of the country and world.

My experience with synchrotron light sources began with my postdoctoral work on block copolymers for lithium batteries at Lawrence Berkeley National Laboratory. Block copolymers form structures on the scale of 100 nanometers, about 1,000 times smaller than the thickness of a human hair. These structures of block copolymers address safety concerns of lithium batteries — a major challenge in the broader distribution and utilization of energy storage technologies. However, the structure is so small that it cannot be viewed under a standard microscope, which is why we turn to synchrotron light sources. X-rays generated by light sources have short wavelengths, smaller than the wavelengths of light, that make it possible to measure nanometer scale structures such as those in block copolymers. I conducted experiments and worked with beamline scientists at four beam lines of the Advanced Light Source at Berkeley Lab and one beam line at the Stanford Synchrotron Radiation Lightsource.

As an independent investigator, my group still works with scientists at Berkeley Lab, but we now also use several beam lines at the Advanced Photon Source at Argonne National Laboratory. This makes it possible to perform time-resolved experiments (similar to movies) of the dynamics of block copolymers and polymer nanocomposites (mixtures of polymers and small particles) that are relevant for lithium batteries. With proposed upgrades it will be possible to look at essential dynamics occurring over smaller length scales that are simply inaccessible now.

We are now interested not only in materials for lithium batteries, but also in membranes for water purification. In both of these areas, identified as grand challenges by the National Academy of Engineers, heterogeneous polymers are promising materials — understanding dynamics in them is crucial to enabling technological solutions to these challenges. It is only with these exceptionally bright light sources (one billion times that of the sun and slated to increase by a factor of at least 100 with proposed upgrades) that rapid experiments on extremely small length scales are possible to further our understanding of advanced materials, such as block copolymers, for energy storage and water purification.

My work has touched on only a small fraction of the types of experiments that can be conducted at light sources. The capabilities are crucial for a vast range of technologies of national importance. These include characterization of both hard and soft materials for energy generation and storage, investigation of electronic and photonic materials for sensing and computing, and a wide-range of biological applications. It is imperative that these facilities receive robust funding for operations, and also receive the funding necessary for upgrades that will allow them to address the critical science challenges that our nation must solve going forward.

### Statement

Chairman Weber, Ranking Member Grayson, and Members of the Subcommittee, thank you for the opportunity to testify in today's hearing on Innovation in Solar Fuels, Electricity Storage, and Advanced Materials. I am here to speak to the impact of the Department of Energy's national light sources on research and national needs primarily as it relates to energy storage and advanced materials. I thank the committee for its long-standing and robust support of our national light sources. I understand that there are upgrades proposed for some of these light sources. Although I strongly support upgrading the nation's portfolio of light sources, based on my personal area of expertise, I will not speak in detail about the upgrade proposals. Rather, I will emphasize the importance of these national light sources and explain how the upgrades would advance U.S. research capabilities.

My interest in alternative energy began in the mid 1990's, when I was first exposed to hydrogen fuel cells by my undergraduate Chemical Engineering advisor, Professor Javad Tavakoli, at Lafayette College. Eventually I was led to graduate school at Drexel University with Professor Joe Elabd, where I became an expert in polymers and in time-resolved experiments. Based primarily on his reputation, I acquired a postdoctoral fellowship at Lawrence Berkeley National Laboratory with Professor Nitash Balsara. In order to enable safer, longer lasting batteries, we demonstrated a completely solid battery using block copolymer electrolytes. I am now an assistant professor in Chemical and Biomedical Engineering at Florida State University, where my group uses synchrotron light sources to study structure and dynamics in heterogeneous polymer materials for lithium batteries and water purification.

A battery contains two electrodes separated by an electrolyte. Electrolytes are essential for battery operation because they conduct ions (charged molecules) between the electrodes when a battery is charged or discharged. Commercial lithium ion batteries contain liquid electrolyte that can explode and burn if abused. Although there are engineering controls for safety, commercial lithium ion batteries are not inherently safe. Examples of this abound, a high-profile and recent one being the overheating of lithium ion batteries in Boeing Dreamliners. In addition, liquid electrolyte is not compatible with many of the advanced battery electrodes that have been developed in recent years.

Polymers, on the other hand, are large molecules. Examples include plastic, rubber, plexiglass, wood, and DNA. It is possible to connect dissimilar polymers together to form a block copolymer. These are amazing materials. The two polymers try to separate like oil and water, but the connection prevents complete separation. As a result, intricate structures are formed on molecular length scales. The nanotechnology that has revolutionized our technological landscape since the turn of the century relies primarily on properties of materials that emerge from interfaces, i.e. interactions between different materials. Block copolymers are a prime example of

a nanomaterial because they can combine the ion conduction property of one polymer with the strength of another polymer, which is not possible with simple mixing.

Block copolymer electrolytes hold promise for developing safer batteries that can last ten times longer between charges than existing batteries.<sup>1</sup> They are amenable to flexible laminar cell construction, which holds the potential for significant cost savings.<sup>2</sup> The ability to combine disparate properties into a single material makes block copolymers of interest for water purification as well, where a strong material is needed that can conduct water but not contaminants. For successful operation of block copolymers in these technologies the structure and the dynamics of the material is important. The structures in these materials are extremely small, about 1,000 times smaller than a human hair. It is quite challenging to image on this scale with a microscope, especially a soft material such as a polymer. Therefore, we turn to synchrotron x-rays, found at our nation's light sources, which can be used in a variety of ways to determine the structure, dynamics, and composition of a material.

### Synchrotron Light Sources

A schematic of a synchrotron light source is shown in Figure 1. It is overlaid on a baseball diamond for scale. This is roughly the size of the Advance Light Source in Berkeley operated by Lawrence Berkeley National Laboratory, which specializes in soft (low energy) x-rays that make it possible to map the composition of elements in a material on an extremely small length scale. The Advanced Photon Source in Chicago, operated by Argonne National Laboratory, is nearly six times larger and produces hard (high energy) x-rays that enable time-resolved experiments again on extremely small length scales. The National Synchrotron Light Source II at Brookhaven National Laboratory is a medium-energy light source. There are also synchrotron sources operated by SLAC National Accelerator Laboratory. These facilities are all supported by the Department of Energy, although an additional U.S. synchrotron facility is operated by Cornell University under National Science Foundation funding. Each of these light sources has unique expertise and capabilities that provide access to complimentary experiments and imaging characteristics.

A synchrotron generates x-rays by accelerating electrons to near the speed of light and then bending them with magnets around the ring depicted in Figure 1. As the electrons pass through the magnets they emit radiation (light) over a wide spectral range including infrared (energy less than visible), but primarily as x-rays. Many experiment stations are situated around the ring achieving a wide variety of experiment types available at each facility. Access to these facilities is free and competitively awarded. The demand for these experiments requires that they operate around the clock. In order to maintain the research innovation that drives the success of U.S. technology in the competitive world economy, it is important to implement technological upgrades to the synchrotron light sources themselves. Doing so will allow U.S. researchers like myself to continue to perform cutting-edge research domestically.

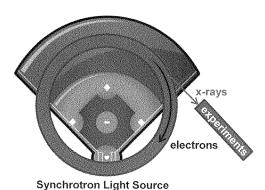


Figure 1. Schematic of a synchrotron light source overlaid on a baseball diamond for scale.

The wide range of energies achieved by the aforementioned Department of Energy light source user facilities make possible an immense range of unique experiments. They can be categorized into three main types: scattering, microscopy, and spectroscopy. Scattering can probe structure and dynamics of complex materials across an immense range of length and time scales. Microscopy provides a three dimensional look inside materials. Spectroscopy determines the make-up of a material. The most powerful experiments are combinations of these three experiment types. These experiments are applied at our nation's light sources by thousands of researchers each year in the fields of materials, chemical, and life sciences, as well as physics and geological sciences. This research also generates thousands of research publications each year contributing significantly to the nation's technology and innovation-based economy. Most exciting to me are the numerous scientific discoveries that would not be possible without these facilities. For example, a new form of matter has been discovered called topological insulators. The most-prescribed drug for HIV, the fuel injectors at the heart of modern gas engines, the battery for the Chevy Volt electric car – all of these crucial discoveries, plus thousands more, were made possible by these user facilities.

With upgrades to these facilities other barriers will come down, making it possible to see structural changes at the atomic level that happen before a steel girder starts to crack, before a healthy brain succumbs to Alzheimer's, and before an electric car's battery begins to fail. Researchers will be able to observe individual atoms moving and reacting — in real time, deep inside real samples, organisms and systems. Researchers will be able to observe every aspect of battery function and failure at every length scale, gleaning atomic-level information to speed development of the safe, reliable, powerful and affordable next-generation batteries we need to transform energy storage for transportation and the power grid.

### Longer Lasting Batteries

The interface between electrolyte and electrode is a crucial component of a battery that for the most part dictates the lifetime of a battery. In order to study the products that form at these interfaces my laboratory has developed new techniques for coating electrode surfaces with nanoparticles. These nanoparticles can be finely tuned to control both optical and electrical properties of the interface. These properties are controlled by the spacing and size of the nanoparticles. As shown in Figure 2, we have used x-ray scattering to measure both particle size and particle spacing. X-ray scattering provides quantitative measurement of a large sample but can detect extremely small differences in spacing, which are important for controlling properties. These nanoparticle coatings will be used to examine the products that form on the surface of advanced electrodes in contact with liquid or polymer electrolyte. Our project has the potential impact of increasing battery energy density by 50 to 100%. In addition, we will gain better understanding of chemical changes occurring in operating batteries. Without x-ray scattering we would enter this research rather blindly without good understanding of the structure of our materials.

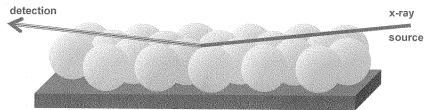


Figure 2. Schematic of x-ray measurement of nanoparticle size and spacing.

### Advanced Materials

The fuel economy of conventional vehicles has increased by 5% since 2000<sup>3-4</sup> due, in part, to transition from steel to aluminum bodies. There is now interest in transitioning to much lighter nanocomposites that can further improve fuel efficiency not only in automobiles but also in aircraft.<sup>5</sup> Designing stronger, lighter polymer composites requires understanding the adhesive properties of the polymer within the material, which depend on polymer dynamics. Even greater improvements in transportation efficiency can be achieved by replacing conventional engines with battery-powered electric motors.<sup>6</sup> Realizing this requires improving both battery lifetime and rate capability. Lifetime is limited by adhesion between polymer electrolyte and the battery electrodes. Rate capability is limited by the ion conductivity of the polymer electrolyte, which like adhesion is coupled to polymer dynamics. Therefore, we are investigating dynamics in block copolymer electrolytes and polymer nanocomposites using time-resolved x-ray scattering techniques.

### Energy Efficient Water Purification and Desalination

The National Academy of Engineering has identified access to clean water as a grand challenge in the 21<sup>st</sup> century<sup>7</sup>. By the year 2040, 6 billion of the projected 9 billion people on the planet will live in water stressed regions<sup>8</sup>. In order to supply potable water in these regions, water either needs to be reclaimed and purified or desalinated. Polymer electrolyte membranes are integral to energy efficient water desalination and water reclamation. The cost and energy requirements of these processes depend on the rate at which water is transported through the membrane and the efficiency with which salt and contaminants are rejected<sup>9-10</sup>. A common problem in water purification is membrane fouling<sup>11-12</sup>, in which microbes adhere to the membrane surface blocking water molecules from permeating the membrane and increasing both cost and energy consumption. Heterogeneous polymer electrolyte membranes can potentially address these problems. The structure of these materials is a function of water content and salt concentration. We are investigating the evolution of this structure using x-ray scattering and the resulting effect of structure on water transport and fouling. By developing membranes with selectivity for water over salt and contaminants that are resistant to fouling, a significant impact can be made on energy efficient generation of fresh water.

### Human Health

Although not a topic of my research, human health is a significant national concern that is greatly impacted by synchrotron light sources. Alzheimer's disease is now our nation's 6th leading cause of death. High brightness and tight focus enabled by synchrotron upgrades will make it possible to observe the initial processes that cause brain proteins to start to deform – processes that occur too quickly for current technologies to capture, and that must be understood before we can learn to interrupt (or even prevent) Alzheimer's and related brain diseases.

I had the opportunity to tour a second generation light source (the Bevatron) before it was demolished. Toward the end of the tour, the tour guide pointed out an area where there had been curtains and they brought in patients for cancer treatment. This work was initiated by Ernest Lawrence, Nobel Prize winner and founder of Lawrence Berkeley National Laboratory, and his brother, who was a physician, at an even earlier facility. The scene, something like a large warehouse with a massive concrete ring in the center (the synchrotron) and an examination area for patients in gowns struck me. This image speaks not only of the importance of the work that goes on at these facilities (the technique in question is used today to treat cancer that is not responsive to other treatments), but also of the scale (these are facilities that require federal funding and are appropriately housed at national laboratories). It is imperative that these facilities receive robust funding for operations, and also receive the funding necessary for upgrades that will allow them to address the critical science challenges that our nation must solve going forward

### Biography

My given name is Daniel Thomas Hallinan Jr. I am originally from Pennsylvania, where I attended Catholic schools through high school. In 2001, I received a Bachelor of Science degree in Chemical Engineering and a Bachelor of Arts in Philosophy from Lafayette College. After a hiatus from academics, I returned to Drexel University where I received a PhD in Chemical Engineering in 2009, studying the transport of ions and water in polymer electrolyte membranes for hydrogen fuel cells under Dr. Yossef A. Elabd. Having discovered the reward of teaching, I continued on the academic track with a postdoctoral fellowship at Lawrence Berkeley National Laboratory (LBL). There I studied block copolymer electrolytes for lithium batteries in Prof. Nitash P. Balsara's laboratory, conducting a variety of hard and soft x-ray scattering, tomography (3D imaging), as well as some x-ray spectroscopy at the Advanced Light Source of LBL. Now as an independent investigator at Florida State University (FSU), my students and I use several beamlines at the Advanced Photon Source (APS) of Argonne National Laboratory. FSU recognizes the importance of user facility research and supports our travel to the APS. With the hard x-rays of APS we are able to examine block copolymer and nanoparticle dynamics. Experimental measurement of local dynamics in heterogeneous polymer materials is unprecedented. These measurements promise to unravel intriguing observations of kinetic properties in nanostructured polymer materials that are significantly different from those in the bulk materials. We are eager to investigate faster processes on shorter length scales that will be made possible by the proposed upgrades.

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Chairman Weber. Thank you, Dr. Hallinan.

I now recognize myself for five minutes, although that's not

enough time for questions.

Dr. Lewis, you mentioned in your testimony that multidisciplinary teams of researchers can serve as a useful mechanism to advance to artificial photosynthesis research. Do you think that that model is the preferred approach to this science compared to individual investigator labs? And then I'm going to have you weigh in on it also, too—well, I'll come back to you. Go ahead, Dr. Lewis.

Dr. Lewis. Thank you for the question. I think we need both. We need individual investigators still exploring all sorts of possibilities, and then we need teams of people because solar fuels is much like building a battery. If you have one piece, a catalyst, or you have another piece, a light absorber, and they don't work together or they're not safe operating together, then you still don't have anything that's relevant in the end.

So this is where you need the teams of people. You need the teams of people to think at the systems level to make sure that we're all rowing our oars in concert toward the same end goal, and that's best done by having engineers, chemical and mechanical engineers, by having applied physicists, by having chemists all at least talking to each other on a regular basis and working toward the same end goal, whether they're all in one facility or distributed in different facilities by videoconferencing is less important than that they all are on the same page.

Chairman WEBER. How often do they talk to one another and in what format? And I think you may have answer part of that ques-

tion, videoconferencing. How often does that take place?

Dr. Lewis. It depends on the facility. In Energy Frontier Research Centers, and Energy Innovation Hubs that I've been affiliated with on some cases every day, in some cases every week, but certainly more often than every month. A lot of it is in person, and for remote sites, routinely by video.

Chairman Weber. Dr. Scherson, I have the same question for you regarding how to achieve those potential breakthroughs in

electrochemistry.

Dr. Scherson. Yes, well, certain aspects of my answer will follow what Professor Lewis was referring to. In a battery we have two electrodes and we have an electrolyte in between. Each of these components needs individual attention. Solving 2/3 of the problem does not solve the problem of coming up with a viable device. So it's absolutely essential to engage people with knowledge in physics so that we can understand how ions migrate through lattices. We need to involve our chemists that are going to give us insight into how ions solvate and migrate through the electrolyte and engineers that will have to teach us how to assemble the device, and finally, I guess that technoeconomic models are also necessary in order to decide whether certain technology is viable or not in the market-place.

Chairman Weber. I just want to know if you can explain that to my wife so she can keep her cell phone battery charged more often. If you could put that in layman's language for her, that'd be

helpful.

So let me follow up then for you both. So we've been scrutinizing the entire DOE research and development portfolio in this Congress, and I've never heard of EERE supporting any R&D in these areas. What are the research challenges to enable artificial photosynthesis in multivalent systems to transition into that technology that is ready for the private sector to commercialize? And could DOE's EERE applied research programs support that work, Dr. Lewis?

Dr. Lewis. Thank you. That's a very important question and also programmatic aspects. EERE does support work on not solar fuels but related systems where there's corporate activity such as electrolyzers or fuel cells. That being said, they can leverage that investment they've already made where there's common ground because a solar fuel system just works as a fuel cell in reverse.

So the same kind of structures, the same kind of implementation that EERE is learning from and developing could well be applied and should be applied in translational research to build systems like the bubble wrap vision that we might have for a solar fuels generator to take the pieces that are developed by the Office of Science and to constrain them into the useful sets that are in a system that could be deployed. That would be very important as a role for EERE.

Chairman Weber. Dr. Scherson?

Dr. Scherson. Yes. In fact, the same role would apply to the field of batteries. There are situations where developments are made and people get excited and then they go and try to make a viable device, and to find that certain questions were not answered properly. And so I think that the involvement of the government of the basic research becomes essential in order to migrate from the very basic research into industry. This is a role that EERE should play.

Chairman WEBER. Thank you. I'm out of time. I'm now going to recognize the Ranking Member here with us, Dr. Mark Veasey.

Mr. VEASEY. Well, thank you very much.

And I wanted to ask some questions about energy storage for Dr. Hallinan and Dr. Scherson. I know that you're both working on innovations in electrical energy storage. I wanted to know if you could speak about your research and how it may lead to breakthroughs in developing new battery technologies.

Dr. Scherson. If I may start?

Mr. VEASEY. Yes, please.

Dr. Scherson. Well, the components of a battery are numerous. In fact, very simply, if you take a cathode of the lithium-ion battery that powers your cell phone, you will find that it is composed of little tiny particles that are all electrically interconnected by yet another component, and so the key is to be able to isolate each of the components of the battery and try to understand their properties, their intrinsic properties. So in my research group, we are looking at single particles of a cathode or anode and trying to investigate the dynamics, for example, of ion insertion into the materials. That's important when you charge or discharge. We are taking particles of the anode and trying to understand how the anode reacts with the electrolyte, forming a passive film that is required for the operation of the battery.

So in essence, we need to understand the individual components and then understand how the assembly of these components will make a device that is going to fulfill the purposes for which it was intended.

Mr. Veasey. Another question I wanted to ask you was about energy storage. As we know, there are many challenges that we face when it comes to energy storage in the area of wind and solar, particularly if we want to be able to provide a certain amount for our energy grid and portfolio. Do you have—anything else of—just about the challenges that may remain that we may not be aware of?

And then also I wanted to ask you, do you think that if we're able to overcome some of the storage challenges and issues, will that allow us to be able to even use wind more efficiently? I don't know if you've ever been to a wind farm in Texas. We provide a lot of wind in the State of Texas, but they do take up quite a bit of space to get the wind from West Texas into the Dallas-Fort Worth metroplex, for instance. You're talking acres and acres and acres. If you could just briefly touch on that, I definitely would appreciate it.

Dr. Scherson. Well, in fact, I have not been in Texas at those facilities, but I've been in Spain where there is a heavy use of wind. So the trick here is to convert the wind energy into, let's say, another kind of energy, so one way is to store it electricity. So you may ask what kind of devices are there available in order to store this electricity for use when the wind is not blowing?

So there are batteries, right? There are also some other devices that are called redox flow batteries, which is like a battery but then you have these enormous amounts of liquid that get passed through the electrodes and then you can store power in that fashion. In fact, the Swiss Government is investing lots of money in implementing such an approach.

The other possibility is to convert that electrical energy into chemicals that can be stored and then used at a later time.

So just to give you an idea of the numbers. In your car you have the lead acid battery, and that will give you, let's say, 100 units. So if you were going to move the technology into lithium-ion, then you will get 250 units. So if we can transition that into magnesium, which is one of the divalent metals that is being explored at JCESR, then you can increase that number up to 700.

And then lastly, if you go to the limit you could have three electrons per atom of charge storage, you can get easily to 1,000. So you can see by transitioning from today's technology with lead acid, we can get about an order of magnitude more efficient energy storage by moving into these multivalent ion systems.

Mr. HALLINAN. Could I make a comment?

So there are other ways also to increase the capacity of energy we can store. And as has been mentioned, if we increase the voltage of—the energy that's stored is the product of the capacity times the voltage. So we can—to increase the energy, we can increase the capacity, which we can do by going to multivalent ions or going to other electrochemistries. Lithium air batteries is this holy grail that takes us an order of magnitude higher in battery capacity en-

ergy storage. But then we can also just go to higher voltage, make

the voltage of the battery higher.

And in order to do those things, in addition to moving electrons through the electrodes, we also need to move ions from one electrode to the other, and that's where polymer electrolytes come into play because for—especially for lithium air batteries, we—it's essential to have a solid electrolyte, that a liquid electrolyte is not even a possibility for these advanced technologies.

But we need to address the slow dynamics of polymer electrolytes, and so I think if we can really make that breakthrough, we are really looking at either—between using multivalent ions and using new cathode chemistries, we're looking at an order of magnitude or even more increase in energy density in theory. I mean, it is a challenging problem, but it's theoretically possible.

Mr. VEASEY. Thank you, Mr. Speaker. I yield back.

Chairman WEBER. Well, not only did you get a promotion to doctor, I got a promotion to speaker.

Mr. VEASEY. That's right.

Chairman Weber. So the Chair now recognizes Mr. Brooks of Alabama.

Mr. Brooks. Thank you, Mr. Speaker.

Dr. Lewis, you pointed out that your lab has demonstrated a functional solar fuel system. Can you elaborate on the fundamental chemistry and materials research needed to discover new molecules and materials and why that research is needed if you have already demonstrated at least one version of a solar fuel system?

Dr. LEWIS. Certainly. Thank you for that question. Demonstrating one version of a solar fuel system is, in our view, like the early flight of a Wright brother is we can get off the ground that we can't fly very far. We need pieces, we need materials that are as to an aircraft a jet engine is to that Wright brother's air-

plane in the first place.

We need to simplify the system so that it doesn't have many socalled junctions. We need to get catalysts that don't use precious expensive metals like platinum or iridium. We've made lots of progress there, but we still have a ways to go in order to get all of these pieces and we need all out of easily manufacturable simple things that you or I can do in our garage as opposed to having to have very esoteric laboratory preparations of them using expensive materials. And they also all have to be compatible with each other and last for 20 years, not 20 minutes. So we've demonstrated it's possible, but we still need to do a lot of fundamental materials science and chemistry development to get it to be practical.

Mr. Brooks. Okay. A follow-up in that regard, has the Department of Energy's Energy Efficiency and Renewable Energy Office provided adequate support for transitional or early-stage research and development for artificial photosynthesis or for that matter a

functional solar fuel system?

Dr. Lewis. To my knowledge, EERE has not had a significant program yet in solar fuels. They do have related programs in consuming that fuel, and there are lessons to be learned. They should be trying out systems like our potential concept of bubble wrap that would concentrate the sunlight just like the bubble wrap we

receive onto small areas minimizing the amount of material that

we would need, and letting us use more costly material.

There are other designs that are much more amenable to reduction to practice that are beyond the Office of Science's typical charter that would logically be built in EERE's domain so that we can solve problems that are problems and not solve that are not problems, learning from experience in a synergistic effort.

Mr. Brooks. All right. This next question will be for each of you, and we'll start with Dr. Hallinan and move to my left, your right. How is the United States faring against international competition in foundational energy research? And each of you have talked about different subject matter, so if we could, your answer be di-

rected to your areas of expertise. Dr. Hallinan?

Mr. HALLINAN. Thank you. So these upgrades—the proposal—the upgrade proposals, they address mainly being able to look at complex materials in much smaller length scales and much faster times. And this is a new breakthrough in synchrotron science. It's already being implemented in Sweden, and there are plans to implement it in Brazil. So in that regard I would say regarding the upgrade to our synchrotron light sources, the United States is a little bit behind.

I think that really to look at polymer dynamics at the scale and at the rate that we need to, which is smaller than we can do now and is faster than we can do with our existing facility, so I do think the upgrades are important in addition to maintaining our competitiveness from a research standpoint.

Mr. Brooks. Thank you.

Dr. Broholm. In my area of quantum materials, I think that the United States has a very lively program, and it is—has been characterized I think now by a stronger component of materials synthesis, which is a really key part of development of quantum materials. I think comparing to other developed countries sometimes one sees that looking, for example, to Europe a more kind of organized approach to some of these topics, but I think sometimes it's difficult to say whether the organizer as opposed to the thousand points of light is the better approach. I think things are going pretty well.

If I could say about the facility upgrades, maybe we'll return to it later, but the—in terms of the neutron facilities, the spallation source is presently the world's most intense source of neutrons, pulse neutrons, but the European community is now building a spallation source in—also in Sweden, which will be a 5 megawatt source. And there's quite some concern in the—in—among scientists who use neutron scattering that this facility will in fact surpass the spallation neutron source, and we believe that an upgrade is very important in order to sustain leadership in that area.

Mr. Brooks. I don't know if the Chair will permit, but I've got two more witnesses. Can they respond?

Chairman Weber. Yes.

Mr. Brooks. Dr. Scherson?

Dr. Scherson. Thank you. Yes, the only example that comes to mind that I'm fairly acquainted with is in Japan where they have tried to emulate the EFRCs and hubs programs that DOE is supporting in this country. The amount of financial support is lower

than the one that the government here provides for these multi-

disciplinary centers.

One difference that perhaps may be considered is the integration of industry into the program. So now you have the beginning from the basic knowledge to the end user, and that has proven to be of value so that by going from one extreme to the other one, this conversation makes it possible to take the good ideas and then migrate them very quickly into the marketplace.

Mr. Brooks. Dr. Lewis?

Dr. LEWIS. Thank you. Two points to speak to on this, one is I did mention that in solar fuels there are burgeoning efforts now, very substantial, in Korea, Japan, China, Sweden, Germany, and the EU, and I'd say either individually or collectively they're defi-

nitely on par with what we are doing in the United States.

The second perspective is I'm the editor-in-chief of the preeminent journal in this field, Energy and Environmental Science, and that's a global journal. It's turning down 90 percent of the articles that are submitted so it's very selective, and over half of those articles that appear in this field are from China, Japan, Korea, and our competition.

We still have leadership, intellectual horsepower, but I think we're at a crossroads here, and we need to really understand that there are other nations who see opportunity for the scientific effort, and we have to make a decision as to whether or not we're going

to continue to lead, and I hope that's a positive decision.

Mr. Brooks. Thank you for your insight.

Mr. Chair—Chairman, thank you for the additional time.

Chairman WEBER. Thank you. The Chair now recognizes the

Ranking Member.

Mr. GRAYSON. Thank you. Dr. Lewis, I want to ask you some questions about something that sort of sounds like an oxymoron, which is artificial biological photosynthesis. I realize that your own specialty is physical analogs to photosynthesis, but it sounds like you're knowledgeable about biological alternatives as well. So I have a few questions for you.

Biology is the most fruitful means of producing ends, concrete results that we know of. We can do far more with biology-or biology does far more for itself than we see through physical processes or chemical processes. The fact that I'm looking at you right now is an example of that. Biology created the eye and the brain. That process is what comes through the eye, both remarkable accomplishments that we have no physical or chemical analog for.

So given that fact, is it reasonable to be hopeful that we can come up with artificial photosynthesis based upon biology itself?

Dr. Lewis. Certainly it's reasonable to be hopeful. There are various methods by which this is practiced. One would be to de-bottleneck photosynthesis, which is fundamentally inefficient. The plant should be black, not green, to get all the colors of the spectrum. It actually saturates its productivity the tenth the light intensity of the sun to protect itself from radical damage in the shade of the

There are lots of molecular links in biology that deregulate systems so that they can be stable and reproduce and do other things that a science approach to un-bottlenecking and making plants more optimal for energy conversion as opposed to everything else could be very fruitful.

There's also people and scientists that are trying to take biological enzymes, pull them out of the biological system, and couple them to the manmade systems. And so you can see how a crosscutting effort that would try to take the best of both worlds should also be explored. And this would involve a strategic collaboration between many different parts of our biological, physical, and chemical research enterprise to find the best of all worlds in this end use.

Mr. GRAYSON. All right. So one possibility is what you refer to as un-bottlenecking. What are some of the possible approaches there? Are you referring to genetic engineering? Are you referring to some kind of forced evolution? What are people actually doing on this?

Dr. Lewis. Right. They're both. Traditionally, we called it breeding where we breed crops——

Mr. Grayson. Right.

Dr. Lewis. —for fitness, but it would be through genetic engineering and directed evolution toward—the molecular part is the coupling between Photosystem I and Photosystem II. That has to move a molecule, a quinone, and that's a slow process. And so if you could instead introduce a wire, a molecular wire that would move the electrons without moving the molecule, you could de-bottleneck inherent photosynthesis, and there's lots of interest in that, but probably should have much more attention at the research level.

Mr. Grayson. Well, that's an interesting question itself. Do you have any information about, let's say, Exxon doing research like this? Are there private enterprise efforts that are being conducted along these lines, or is it being left to the government to try to develop this?

Dr. Lewis. My knowledge is that there are enterprises thinking about manipulating algae, for instance, but not so much in the private sector and the energy companies for certain. And I think it is now left to the government as very early stage maybe appropriately because it is a complex system, and we still have to do research. It's not just taking tools that we understand and engineering them, but it's somewhere in that mix.

Mr. GRAYSON. Well, given the upside here, the fact that you're basically talking about being able to create an artificial fuel, transportation fuel, artificial oil, maybe artificial natural gas, and that has an enormous effect on the economy. That's roughly ten percent of the entire world economy right now. Given the upside here, why do you think that there isn't more effort in the private sector to accomplish this?

Dr. Lewis. I think it's pretty simple. The rate of return and the capital needed to invest in energy systems is typically 10 to 15 years, and when you're reporting to your stockholders every quarter, you can't justify a long-term program to return capital when you have to report everything every quarter to your stockholders.

Mr. Grayson. So in the short time that we have left, can you tell us specific examples of artificial biological photosynthesis that are

being conducted right now or at least efforts that are being made in that direction?

Dr. Lewis. Absolutely. There are laboratory experiments that have taken enzymes that feed on hydrogen that then convert them with carbon dioxide into selective liquid fuels like isopropanol. And so we have a recent demonstration of that, in fact, out of Harvard that has shown that this is possible. That's an important first advance. We still have to then reckon with how long will those enzymes last. Will they be robust enough to be put into a system? How can we make them scaled up and cheap enough to deploy at large-scale? But there is this strategy of—at the research level taking the best pieces from wherever they are and then combining them into the best system, and that's certainly a good approach.

Mr. GRAYSON. Last question, is there any experiment so far to date regarding artificial biological photosynthesis that has actually resulted in the recovery of a fuel that had more energy content than what you put into it, what we call in the—in an analog of fu-

sion we'd call that ignition.

Dr. Lewis. Exactly.

Mr. Grayson. So is there something like that that exists already

for artificial biological photosynthesis?

Dr. Lewis. Probably not yet. Maybe, maybe in some limited circumstances, but of course that's the goal is to get the energy payback more than the system energy put in, but that's certainly where we want to be.

Mr. GRAYSON. All right. Thank you very much. I yield.

Chairman WEBER. I'm going to follow up on that, Dr. Lewis, if I can. That's a fascinating conversation. You said plants need to be black instead of green. Somebody earlier said they pick up the red rays and the blue rays and this is Democrat and Republican. It's

bipartisan, you know.

And so in following up with your discussion with my good friend Mr. Grayson, you're talking about algae that had a—a plant should be black and then you said that you needed a wire to like move the electrons in some of those plants? Are you seeing articles about this particular process in this very prestigious journal known as the Energy and Environmental Science? I happen to know the editor. Right.

Dr. LEWIS. Yes, I'm seeing them, and I don't have time to read every article, but—

Chairman WEBER. Okay.

Dr. Lewis. —we do see them in many constructs. The wire isn't a wire like we think of a copper wire with insulation. It's at the molecular scale. It's molecules that—

Chairman Weber. Something that moves the——

Dr. LEWIS. —electrons— Chairman WEBER. Right.

Dr. Lewis. —between these sites in a way the biological system wouldn't do itself. And you really do want a solar converter to look black to the human eye so that it does have a red component and a blue component and therefore harvests all of the sunlight. Plants are not optimal for energy conversion machines because they look green. That means that they're wasting some photons. They had other evolutionary constraints and design that when you build an

aircraft you don't make it out of feathers if you want it to fly faster. You're inspired by that, but we know we can do better.

Chairman Weber. Right. And the landings are brutal.

Dr. Lewis. The landings are brutal.

Chairman Weber. Yes. All right. Thank you. I'm going to—I yield to the gentleman from California, Mr. Knight.

Mr. KNIGHT. Well, you only get one landing if you make them out of feathers.

Dr. Lewis, thanks for coming. I appreciate you being here. You mentioned that artificial photosynthesis could benefit from modeling and simulation using high-performance computation systems. Is that something that the research community has begun to discuss with DOE?

Dr. Lewis. I believe so but not in such an organized fashion as to establish a separate program for high-performance computing applied only to this problem. But there are specific examples. I'll give you three briefly. We discovered a nickel gallium alloy just recently in our laboratory that selectively takes energy-efficient carbon dioxide and makes interesting carbon-coupled liquid and gaseous products. That was predicted by theory before we did it experimentally.

Now, it turns out that the theory got the energy efficiency right but it got the carbon products wrong. They predicted methanol. Well, that's because the theory was done in an ideal surface with perfect atoms, and the real sample we made had all sorts of nooks and crannies and edges that then we have to iterate back to tell the theorists, well, now you've got to predict what the real-world samples are. But they got it close enough to tell us where to look.

The second point is that theory has predicted out of 19,000 metal oxides, 200 that might be stable light absorbers under our conditions. We don't yet know how many of them can made—can be made outside of the computer and exist, but now we're looking there to try to have a guide from high-performance computation into where the experimental work should begun and then refine it. So that would be the optimal way in my view to not have the world just abstracted in computer. We have to build it, we have to make it, and then we have to find out where the theory is right and wrong and then iterate back and forth until we get to where we need to be.

Mr. KNIGHT. Just like any test or experiment, you've got to have a theory and then you've got to actually see the ability to see it practically work.

I want to go to Dr. Hallinan about the batteries. And Mr. Veasey was talking about Texas. Well, in California we have quite a bit of photovoltaics and solar and wind and all kinds of renewable energy products there in the Mojave Desert. Our biggest problem is battery storage. Our biggest problem is the wind is not always blowing and the sun is not always shining. And so if we want to move to our new RPS, which is our renewable portfolio standard of 50 and then 60 and 70 percent, we might get to that line where we can't go any higher. We've got to burn something because, like I said, the wind's not blowing and the sun's not shining, so we've got to burn something to keep the lights on.

At what point or how close do you think we are—and this might be a question for everyone. At what point do think we are that we can store something that comes from an 1,100-acre field out in the Mojave Desert that is producing a huge amount of energy but we are burning that—or we are using that energy very quickly, instan-

taneously?

Mr. HALLINAN. Sure. So that's a—it's a challenging problem, and I think there are a number of constraints that we face. So one is we don't want to be spending large amounts of money to make these batteries just to store this energy for a short period of time, right? So we have this cost constraint, but then we also want these batteries to last a long time. We don't want to have to be replacing them regularly. We also need them to charge and discharge at a rate commensurate with either the production or the consumption of the energy.

And so when you look at batteries, there's a very wide array of different types of—we call them battery chemistries. Lithium-ion are very good for portable electronic devices, and they are now being used in electric vehicles. Nickel metal hydride are used in hy-

brid vehicles, so there are many different chemistries.

I think what Dr. Scherson mentioned earlier about these redox flow batteries, they seem to be the most promising for what I would call stationary storage. So we're—if we don't need to move battery around, we really don't care how much it weighs or how large it is to some limit. We care mainly about cost and satisfying the other needs of storage.

And so for—I think for grid storage, really these flow batteries—and the reason they're so interesting is once you've designed the electrodes, then if you need to scale them up, you just make a bigger tank of your liquid that you're going to flow to the battery. Now, I would say, you know, they're still at the research stage, but

they seem the most promising from what I've seen.

Mr. KNIGHT. So I'm going to—if the Chair will allow me just to ask one more question. I'm going to put this back to Dr. Lewis because I think he understands this. What we go through in California, what we go through in Texas, what we go through in some of the states is the issue is not—well, the land is an issue, but we have a lot of land that we can put these thousand-acre fields out there. And it does become an issue more politically than for the science community, but that will become a problem.

If we cannot store this energy, if we cannot use this energy at a later time, then we might be on the wrong technology. And I say that just personally. We might want to look at something else because if we cannot store this, we are going to be using so much of

our land that I think that it might be a problem.

And the second question—I'll give this to you, too—is we've got car companies coming out and they're doing cars that can do about 225 miles on a charge and exactly what Dr. Hallinan said, we would change out the batteries at changing stations instead of filling up your gas tank with gasoline, and that could be a problem because now we're producing all of these batteries. We're going to have a huge amount of batteries if we've got 50 million cars on the road and we have to have 100 million batteries out there just

changing stations. I think that that's a problem with this technology. But it could just be me.

Dr. Lewis. I'll at least try to address the first question. Storage is in my view—I agree with you—the number one problem to think about actually at scale deploying intermittent renewable sources. We have technologies that are reasonable at solar and wind, but if we can't store, we can't have power after 4:00. It's pretty simple.

We should do this broadly. You should think about ramping up and down nuclear power plants fast in certain designs, about natural gas-fired power plants, about demand management, about making fuel directly from the sun, about batteries. There are probably lots of ways to think about this.

Storage of electricity has been realized as a gap since Thomas Edison noticed it in 1931, and we have to solve this problem. This is where, I think, a broad program not just in batteries but in all sorts of technology options that can help us meet load in the face of a dynamically changing energy market are critically important.

With respect to the battery recycling, that solves one problem and introduces another. It solves a problem in that there won't be a rapid recharge of a battery by electricity for a very long time because all batteries have what's called an internal resistance that prevents them from shorting. If you try to charge them up, you dissipate so much heat through that resistor that you would boil all the liquid in your car if you tried to do that in five minutes.

So instead, you swap a battery out with a previously charged battery, and the problem of course is now you have at least twice as many batteries on your hand you have to move around. This again points to what would be a dream solution of if instead you could make liquid fuel and store the energy that way, then you could convert that electricity into stored fuel and we know how to handle that.

So there are lots of things we should be thinking about. These are incredibly important problems and we need to do a lot more research in order to try to make them into reality.

Mr. KNIGHT. Thank you very much. Thank you, Mr. Chair, for the indulgence.

Chairman Weber. Thank you for yielding back.

The gentleman from—is it Illinois—Mr. Lipinski is going to be recognized for five minutes as soon as he's ready.

recognized for five minutes as soon as he's ready.

Mr. Lipinski. Thank you very much, Mr. Chairman. Thank you

very much for stalling there for a second. I was at another hearing. I just finished my questioning there, so I thank the witnesses for being here today.

And this may be a little bit of a repeat and that's what we're trying to avoid here, but I wanted to make sure that I directly had you address some of these things. Dr. Hallinan, the Basic Energy Sciences Advisory Committee, BESAC, recently released a report detailing which BES upgrade proposals should be prioritized, and I was pleased that BESAC recommended beginning construction on the Advanced Photon Source at Argonne National Lab, which is located in my district.

It's my understanding that your research has relied on APS, so could you talk a bit about your work that uses the APS and how

upgrading it would advance both your research in the field of high-

energy light source research in general?

Mr. Hallinan. Sure. So the electron beam at APS is—and actually at all of our synchrotron light sources is actually this long, wide beam—sorry, not the electron beam, the light—the x-rays themselves. And so if we want to do some of these advanced experiments, some measuring dynamics, we're essentially taking movies, very rapid movies, and we need to have a point source. And so what they do now is they just block off the vast majority of the light that's generated by these light sources. Well, what the upgrades will enable is actually in—so this is not—the actual upgrades is not my area of expertise, so I can't actually tell you a lot about the technical details of the science. But my—but as I understand it, they're able to shrink that x-ray down to a point without having to block lots of it, and so they're increasing the—what we call the brightness by 10 to 100, maybe even more times what it is now.

And that's what enables us then to—with this brighter beam we can basically take faster frames of the movie, of the dynamics of these structured materials whether—and it doesn't only need to be applied to polymers. I don't want to give you that impression. That's—my research uses polymers. And the theory predicts that there are these segmental motions that are on very small length scales and are very rapid that we want to be able to look at experimentally to verify that the theory is predicting correctly. And then if we understand the fundamentals from this theoretical and experimental standpoint, then we may be able to design faster or better transporting polymer electrolytes.

I think the impact is going to be much broader than just polymer electrolytes for batteries. I mean, there are people doing research in biological systems looking at DNA, looking at ribosomes. There have been Nobel Prize—the Nobel Prize in chemistry in 2009 ap-

parently was awarded for work at the APS.

And—but—so what is it—essentially what it's going to allow us to do is look at faster and smaller with all the different capabilities. So I think I answered your question.

Mr. LIPINSKI. Yes. What about the—in general the impact on international competitiveness for the U.S. to do this upgrading?

Mr. Hallinan. I think it's essential. I mean, this is a new breakthrough in synchrotron science, and it's really going to push the limits of what we can do—of the research questions that—the scientific questions that we can answer. Any scientific questions, I think, are important for several of our technological challenges of the country. And we don't—you know, I mentioned earlier that the personnel, the people behind the science, it's like if you gave a vehicle to a monkey, he wouldn't really make much of it, and so these beam line scientists are also crucial, and so if we don't upgrade, we're going to start losing some of our really great talent to these other countries would be my concern.

Mr. LIPINSKI. Thank you. One other question I want to throw out there, I know you talked already about energy storage. JCESR is also centered at Argonne. Is the Energy Innovation Hub model the best way to pursue this type of research and other research? I just

want to get a reaction to that if that's the best way to do this and to continue on with other research challenges that we face?

Dr. Scherson. Well, I'm fairly well-acquainted with JCESR. I belong to their advisory board. And this is some sort of a large-scale experiment in trying to do the basic science and then migrate all the basic science through all the steps that are required to put the final product out the door of commercial companies that may want to take that technology and bring it to the marketplace.

It is a remarkable thing that's working very well from what I can tell. It encompasses activities from the chemical engineering but it goes into the design of the system to the very basic teaching so far what one particle can do when the electrode gets charged and discharged. So it's the entire spectrum of activity that is concentrated into one organization under one head.

Mr. LIPINSKI. My time is expired so I will yield back. Thank you.

Chairman Weber. Thank you, Mr. Lipinski.

The Chair now recognizes Mark Takano from California.

Mr. Takano. Well, I'd like to thank the Chairman of the Energy Subcommittee for allowing me to be here today due to my specific interest in this sector, so I really appreciate that, Mr. Chairman.

I am co-Chair of the Battery Energy Storage Caucus and have a particular interest in energy storage and what we can do as policymakers to support and spur innovation in this industry.

California is making large investments in energy storage, and in my district at the University of California Riverside at the Center for Environmental Research and Technology they are working on the local—they're working with the local utility to integrate battery

storage, as well as combining it with electric transportation.

We have heard from scientists and policymakers alike that there's often a false boundary between basic and applied science. To some, supporting basic research is an important role of government, while applied research should be left to the private sector. Yet this idea that there is a line that neatly divides the two separate levels of research is not realistic, and it goes against our general understanding of scientific discovery and innovation. Would you agree with this characterization, this last characterization? And I want to ask that question first and if you can briefly just address that, each one of you.

Dr. Lewis. Certainly. To efficiently utilize our researches and our capital, our intellectual capital, we have to focus on the seamless transition of end use. We don't want to be wasting our time making discoveries of materials that end up when they're combined into a battery are explosive and unsafe. We don't want to be doing that

with solar fuels generators either.

And the only way you can do that is if you actually build a system and then understand from the system-level what the constraints are on the materials that go into that system, whether it's a solar fuels generator or a battery or a flywheel or any other type of consumer or industrial product.

So to the extent that the use-inspired fundamental research has an outlet into practical implementation, there should be no boundary. On the other hand, there is a discussion about whether or not taking it further than a demonstration and constraining it is the role best served by the government or is that for all best handed off to private industry? And I think that boundary is something that is beyond where the technical expertise—that's more a policy.

Mr. TAKANO. Okay. Great. Dr. Scherson?

Dr. Scherson. Yes. I will just simply complement the answer given by Nate. I just learned that about ten percent of the cost of an actual battery goes into materials, 90 percent into manufacturing. So, you know, we have to be able to bridge the gap between what we regard as fundamental research and applied research. I'm afraid that companies may not want to take the risk of trying to take something from the laboratory and try to produce something under their cost into a final product. So in my view, JCESR has managed to be able to bridge this gap in trying to make these boundaries disappear.

Mr. TAKANO. Great. Dr. Broholm?

Dr. Broholm. I think the—we—it is important to focus on the key role that the government has in supporting discovery-driven research, and let me give an example, which is that in the pursuit of superconducting material that might in fact solve some of these storage and transmission problems that we have been talking about, there comes a time when perhaps one does need to look at a material which superconducts at 100 millikelvin. And this material may in fact provide the intellectual breakthrough that allows you to then compose a material that will become a practical superconductor.

So I would—so on the other hand I think that the cross-fertilization of the motivation from discovery-driven research to use-inspired research is very important such that those who are working in the discovery realm need to have the ability to view some of the challenges that exist in the real world as well. So this artificial barrier is in fact very unfortunate if it exists. On the other hand, we have to really remember to also support the discovery-driven part of it, not to have it cast aside for not being practical.

Mr. Takano. Yes.

Mr. HALLINAN. So, yes, and I'd like to just emphasize that with a quick example, that there needs to be a balance between supporting these for-profit entities and basic science. And so I think a great example is the discovery of the MRI, which is widely used in the medical industry now, was originally completely driven only by a fundamental science question. There was no perceived application of that research.

And so I think, you know, I just want to—I would like to moderate the responses with the statement that I think it shouldn't—while taking things to market is extremely important, it shouldn't be at the expense of basic science.

Mr. TAKANO. Might I ask just a follow-up?

Chairman Weber. Yes.

Mr. TAKANO. Thank you, Mr. Chairman.

The work supported through the Basic Energy Sciences program, would you agree that it's a major example of how there is really no clear boundary between basic and applied science even if basic is in its title?

Dr. Lewis. I think that's a fair characterization in the sense that we don't know what the applications will be of many of the materials made or fundamental concepts that are supported by basic energy sciences will end up specifically into an energy system in a consumer or in a generator's kind of infrastructure. So that's foundational research, and its outcome and where it goes should be unconstrained.

There are separate parts that are use-inspired that I think should be properly constrained into things that could be implemented and are devoted to, say, using elements that are not so expensive or so rare that you could never actually use them at scale for energy applications. There are still fundamental research questions, but it's constrained into don't give me an answer on a material that I can't possibly think about ever using. Give me an answer that's relevant to ones that I could think of using. And I think they're both important to founder.

Mr. Takano. Dr. Scherson?

Dr. Scherson. If I could address the importance of theoretical research. Nowadays, we have the ability of throwing at a computer all the elements in the periodic table and begin to ask questions. And we said what kinds of materials could possibly be designed in the computer that are going to end up giving us the ideal material for an actual application? And, you know, I have been many times and I'm sure that my colleagues are the same that the computer produces something that we never thought of. And there is a case at the moment of the material discovered by the computer that is very good in terms of allowing magnesium two plus to migrate through the cathode.

And so people at JCESR are contacting one laboratory in the world which happens to have that capability, and then you can then validate what the computer predicted and then do the experiment to find out whether that is a good one or not. So this interchange between theory and experiment is becoming to be crucial in order to discover new and more efficient materials for all sorts of

applications.

Mr. TAKANO. Fascinating. Dr. Broholm?

Dr. Broholm. Yes, I—let me return to a topic that I opened with, which was the nature of AT&T Bell Labs or Bell Laboratories, which was a very interesting institution where you have this connection between truly fundamental science and very specific applications. And so I think I actually worked at a time and I think there was a tremendous inspiration in fact even though we were working on topics that were truly discovery-driven science, we had the opportunity to talk to individuals who are working in a very applied end of it. And this actually—it can become a motivating factor.

And so I think basic energy sciences has the opportunity to be the place where these strands of research actually connect to each other, both the fundamental and the applied side.

Mr. Takano. Dr. Hallinan? Mr. Hallinan. Yes, I would agree. I think that the questions that we need to answer are well-defined by the applied side, and then we can approach them from a fundamental perspective. So, for example, as an engineer, the reason that I'm interested in studying polymer electrolytes is that I recognize the massive energy efficiency gains we can achieve by transitioning to electric vehicles from conventional internal combustion vehicles, for example.

But my research does not cover trying to put these batteries into a car. That's for someone else to do.

So I think that I agree with you that there is not really a clear line between basic and applied, and that we get the important questions from the applied side and then we figure out how to answer them, I think, from the basic side.

Mr. TAKANO. Thank you, Mr. Chairman. I appreciate the extra time.

Chairman Weber. You're welcome. Doctor—the Chair recognizes

himself for five minutes for a couple more questions.

Dr. Broholm, could you give us a general sense of how far we are from being able to—I know I'm asking you to predict the future now. How far are we from being able to really develop useful quantum computing systems and explain the materials challenges?

Dr. Broholm. So there are many different forms of quantum computing that are now being pursued, and I think that already shows you that we don't know now which approach is actually going to become the one that functions or which approach is—the general challenge that one is facing there is that it is necessary in the quantum computer to allow a physical quantity such as a nucleus in or a photon or a patch of a superconducting material to respond quantum mechanically to specific conditions that are imposed.

And it's important that the wave mechanics associated with quantum physics can unfold without loss of coherence until the quantum computation has actually been completed. And so having a quantum material that can respond quantum mechanically for a sufficient period of time is actually a first step towards quantum—

to having a quantum computer.

And as I said, there are a number of different materials, platforms that are now being explored, and I would say that I'm optimistic because of the excitement that surrounds the topic and the talent that's being applied to it at this time. But I think the timescale is—one would be—it's a folly to try to really pin down a timescale on that, and I think we should be thinking of that as a vision that needs a sustained level of research of the type that I think predominantly the government will be able to support.

Chairman Weber. I think you just said you don't know.

Dr. Broholm. I'll take that.

Chairman Weber. Okay. Thank you, Doctor. And I want to follow up with that. What role can the DOE research program in BES and even in the ASCR program within the Office of Science play

in advancing this research?

Dr. Broholm. As you pointed out, this is really early stages, and it's very important to take that approach. And so I think we're talking about the development of new classes of materials, quantum materials that sustain quantum coherence for sufficient timescales to allow quantum computing. And so one of the key approaches that we need to take is to combine the theory of materials with the synthesis of materials and the ability to measure those materials in order to examine the viability of different class of materials to function in a quantum computing system.

And if I may, I would say that one of the key roles that I see of Department of Energy in basic energy sciences is the provision of world-class facilities that can actually probe the structure and the dynamics of quantum materials to determine their viability in

these purposes.

And in my own research I'm using the technique of neutron scattering to actually visualize the quantum mechanical electronic wave function of these—some of these materials, and in fact it's in many cases the only method that we have to inquire the quantum physics of these materials at the appropriate length scale. So I think that the provision of world-class facilities for this kind of research is one of the important roles of the Department of Energy.

Chairman WEBER. Thank you. In your exchange with Congressman Takano, you mentioned looking for a superconductor fabric of

100 million—

Dr. Broholm. MilliK.

Chairman Weber. MilliK.

Dr. Broholm. That's a very low temperature, 0.1 above the absolute zero. And my point was that that is something that we do in the lab, and it teaches us about the fundamental behavior of electronic systems. But we can then take that knowledge and develop materials that are practical at higher temperature based on the same principle. And the connection there is trying to make to storage and transmission of energy. I did-while there was a discussion, I didn't quite have the opportunity to make that, but superconducting—a practical superconducting material is a potential component in a large-scale energy storage system where you could in fact take the energy being generated by a photovoltaic station and put it into a current in a superconducting solenoid system that will hold the energy for a long period of time without loss and can then disperse energy when it is required. So this is another example of there being a range of different potential technologies that we have to be pursuing.

Chairman WEBER. Is that because it's so low temp, number one; and number two, when it releases that energy, doesn't it generate

heat?

Dr. Broholm. No. In fact, it doesn't have to be low temp. And so this is what we're pursuing as to materials that will allow superconductivity to persist at very high temperatures. And once you have superconductivity, you have absolutely zero resistance. And so imagine you can simply put the current into the superconducting ring and then just close the ring and the current will persist—

Chairman WEBER. Well, then when you charge it, it doesn't

produce heat, zero resistance.

Dr. Broholm. Zero resistance. It just sits there. So as long as it is in the superconducting state and then you—when you want to release that energy for use, that can then be done as well. So it's a really quite interesting potential way of storing energy particularly for these intermittent distributed energy—renewable energy resources.

Chairman Weber. Okay. And one last question and then I'm going to yield to my good friend from Florida. Dr. Lewis, are you seeing discussions—I think in your earlier comments you said most of the comments were coming from Japan, China in your publication, about half of them. I didn't hear you mention Russia in there.

Russia is noticeably absent. But are you seeing these kinds of discussions in your publication?

Dr. LEWIS. We don't see much from Russia.

Chairman WEBER. Not Russia specifically but the quantum part that Dr. Broholm is discussing.

Dr. LEWIS. Not particularly much. Most of the discussions are focused toward solar, wind storage—

Chairman Weber. Right.

Dr. LEWIS. —and more use-inspired things that would be true to the energy and environmental science—

Chairman Weber. Absolutely.

Dr. Lewis. —is vital.

Chairman Weber. So, Dr. Broholm, do you know of publications that are discussing the superconductivity that you're discussing in a quantum fashion? Are there—is that discussion being held worldwide?

Dr. Broholm. Yes, it's a very—countries around the world are putting in effort to try to discover a practical superconductor, and there are advances being made, and we're very optimistic that we'll be successful.

Chairman Weber. Okay. And then, Dr. Hallinan, and lastly for you since I come from the district that has a lot of what we call petrotech chemical industry, petroleum and other chemical industries, when you're talking about polymers of course you're talking about something that kind of gets my attention. Are you also hearing that discussion on a worldwide basis?

Mr. HALLINAN. Regarding polymer—

Chairman Weber. Yes.

Mr. HALLINAN. —electrolytes and—yes, absolutely. And we have been for decades because they can fill many different roles. They can fill hydrogen fuel-cell roles. They can fill artificial photosynthesis role. They're batteries, water purification, and so there are definitely publications from all around the world. Yes. So I——

Chairman Weber. Okay. Who would you—what country is our runner-up if you will, is doing the most—you're hearing the most

from?

Mr. HALLINAN. I would say probably Italy actually is the runnerup to the United States in terms of polymers and for membranes, all kinds of polymer membrane applications.

Chairman Weber. Okay. Thank you. And I yield to my good friend from Florida.

Mr. Grayson. Thanks. A few questions for Dr. Broholm regarding superconductivity. Doctor, join me in our time machine. We're jumping back to 1986 and the discovery of the possibility that you could have much higher temperature superconductivity that anybody had ever realized before. People thought that anything above 30 K, 30 kelvin was impossible, and now suddenly 70, 80, 90 is possible. And nobody knows exactly how high you can go, maybe as far as even room temperature. Nobody knew 30 years ago. Well, here we are 30 years later and we still don't know. What should we have done 30 years ago to try to pin down the possibilities and get that science done?

Dr. Broholm. I think the point here is that these are extremely difficult problems. Despite the supercomputers, despite the ad-

vances in theory of electronic systems, really no one would have predicted that materials such as iron and selenium, those two elements joined together can actually be a superconductor in that case at relatively low temperatures. No one would either have been able to predict that when you place a single atomic layer of iron and selenium onto strontium titanate you actually can greatly enhance the superconducting transition temperature to 50 kelvin in that system. And again, it's something that even the smartest theorists at this point are not able to really predict as an issue, kind of as

a basic prediction.
So I think that the statement is that these are simply extremely complicated problems because they involve the interaction of a very large number of electrons amongst each other. On the other hand, there also very, very rich sets of materials that give the ones of us who are working in them a sense of amazement and a sense of optimism in terms of the kinds of properties that we will be able to extract from these materials as we advance our understanding. So I think we have to take the long view as we look at these properties. It's as true today as it was in '86 that there is potential for us to create superconducting—practical superconducting materials, not necessarily at room temperature but practical for our use in energy and information.

Mr. Grayson. So what should we do right now to bring the future forward and make that scientific discovery happen sooner?

Dr. Broholm. I think a lot of things are being done. I think perhaps what I would advocate—we talked about a little earlier is the close interaction amongst scientists that have different perspectives on materials, different techniques and different ways of thinking about materials. This tends to be a very fruitful exercise. So what appears to be a brick wall for a Knudsen, a physicist, a chemist may have a different way of thinking about the material that allows you to really tunnel through that challenge.

And so I think bringing together people who are experts in synthesis, people who are experts in theory of materials, and people who have innovative new methods to probe materials, that this is the way that we can best make progress on these very complicated but very promising areas of materials development.

Mr. Ğrayson. Thanks. I yield back. Chairman Weber. Well, I thank the witnesses for their valuable testimony and the Members for their questions. The record will remain open for two weeks for additional comments and written questions from the Members.

This hearing is adjourned.

[Whereupon, at 11:49 a.m., the Subcommittee was adjourned.]

## Appendix II

ADDITIONAL MATERIAL FOR THE RECORD

## STATEMENT SUBMITTED BY RANKING MEMBER EDDIE BERNICE JOHNSON

## OPENING STATEMENT Ranking Member Eddie Bernice Johnson (D-TX)

House Committee on Science, Space, and Technology
Subcommittee on Energy
"Innovation in Solar Fuels, Electricity Storage, and Advanced Materials"
June 15, 2016

Thank you Chairman Weber for calling this hearing, and thank you to our excellent panel of witnesses for being here today.

The purpose of today's hearing is to discuss some of the research activities supported by the Department of Energy Office of Science's Basic Energy Sciences program. This program supports critical fundamental research to better understand matter and energy at the electronic, atomic, and molecular levels. Such knowledge is vital for improving the efficiency and cost competitiveness of new energy technologies, and will undoubtedly lead to a cleaner and more sustainable energy future.

More than 14,000 scientists and 170 research institutions, as well as hundreds of private industry researchers across the United States, rely on the Basic Energy Sciences program each year for its state-of-the-art user facilities as well as its competitive research grants. Yet, as in many other research areas, our leadership position in energy innovation is now being aggressively challenged by other members of the international community.

I would like to call attention to the Basic Energy Sciences Advisory Committee's (BESAC) report released on June 9th which details many priorities for upgrading the major user facilities under this program's purview. The BESAC report finds five project upgrades to be "absolutely central to contribute to world leading science." The report also notes that "increased international competition provides both a challenge and an opportunity for the U.S."

I hope that one area on which many of my friends on the other side of the aisle and I can agree upon is the need to support and strengthen American leadership in energy innovation, and I look forward to working with my colleagues to ensure that the Basic Energy Sciences program and other important programs in this area are as robust and effective as they can possibly be.

I want to thank our witnesses again for being here, and I look forward to your testimony.

Thank you Mr. Chairman. I yield back.

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