BASIC ENERGY SCIENCES ADVISORY COMMITTEE
to the
U.S. DEPARTMENT OF ENERGY

PUBLIC MEETING MINUTES

JUNE 9 - 10, 2016

Bethesda North Marriott Hotel and Conference Center
5701 Marinelli Road, North Bethesda, MD 20852

June 9 - 10, 2016
DOE BASIC ENERGY SCIENCES ADVISORY COMMITTEE
SUMMARY OF MEETING

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) was convened on Thursday and Friday, June 9 - 10, 2016, at the North Bethesda Marriot Hotel and Conference Center in North Bethesda, MD, by BESAC Chair John Hemminger. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act. Attendees can visit http://science.energy.gov/bes/besac/ to learn about BESAC.

Committee members present:

John Hemminger, Chair
Simon Bare
Dawn Bonnell
Gordon Brown
Beatriz Roldan Cuenya
Sylvia Ceyer
Persis Drell
Bruce Gates
Ernie Hall
Stephen Leone
Monica Olvera de la Cruz
Philippe Piot
Mark Ratner
Anthony Rollett
Frances Ross
Gary Rubloff
Maria Santore
Esther Takeuchi
Douglas Tobias
John Tranquada

BESAC Designated Federal Officer:
Harriet Kung, DOE Associate Director of Science for Basic Energy Sciences (BES)

Committee Manager:
Katie Runkles, DOE BES

THURSDAY, JUNE 9, 2016

WELCOME AND INTRODUCTION

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) was convened at 8:30 a.m. EST on Thursday, June 9, 2016, at the Bethesda North Marriott Hotel and Conference Center by BESAC Chair **Dr. John Hemminger**. Committee members introduced themselves and Hemminger reviewed the agenda.

NEWS FROM THE DOE OFFICE OF SCIENCE

Dr. Cherry Murray, DOE, Director of the Office of Science (SC), reviewed the six SC programs and budgets for each. The Fiscal Year (FY) 2016 budget of $5.35B is being executed and SC is awaiting conferencing on House and Senate marks for FY17. The FY18 budget may be delayed due to the Administration change. Flat or slight increases in budgets are expected based on discussion with Congressional staff members.

The SC FY17 budget request is $5.67B, six percent increase over FY16. Mission Innovation, mostly linked to Basic Energy Sciences (BES), is part of the overall budget and is funded at $1.8B.

House and Senate Appropriations marks for SC are up by three percent over FY16 but there are differences between the two. Differences in appropriations for BES are very small.

Balancing support for research with scientific user facility construction and operation is a top priority. BES has a history of achieving balance, more so than other offices in SC. Murray is looking forward to BESAC's response to the recent charge on future facilities upgrades.

BES's investment profile demonstrates a planned continuation of construction activities with new projects starting as others roll off. This allows for balanced support for projects with research. Murray shared that some facilities are becoming large enough that they need to be international projects.

The balance of discovery research with science for clean energy and departmental crosscuts is a priority. Mission Innovation is a key driver for the budget for the latter activities. The FY17 request for Mission Innovation includes about 30% of the SC budget. It will allow for a funding balance for areas that Murray wants to support.

The exascale computing project is another priority. SC is collaborating with DOE National Nuclear Security Administration (NNSA), the National Science Foundation (NSF), the Department of Defense (DOD), and industry partners to overcome the end of semiconductor technology and identify new computing technologies that include new materials and designs. New hardware, software and algorithms are among the things that will be required. An inundation of data is provoking advances in machine learning, and associated computing advances are part of the exascale initiative.

International partnerships are another priority. Murray shared an update on ITER noting that some in Congress is not in favor of the project. The FY19 budget request will include a decision on ITER. A new director general has been established, and hope for a revamped project baseline and culture. There are still issues and risks associated with ITER, to include the status of European Commission support.

The Long Baseline Neutrino Facility (LBNF) is progressing well. Around 30 percent of in-kind contributions are anticipated. A challenge is the growing number of international collaboration agreements. There are over 20 agreements at present for LBNF.

SC manages 10 national laboratories and supports around 60 percent of the research at the labs, each of which have a broad mission. SC's lab stewardship is important and includes developing young researchers and bridging universities and industry. Multiple agencies fund the laboratories and they should be viewed as a network.

DOE has been working on two streamlining contract initiatives since last year. The results from the Evolutionary Working Group will be incorporated at Fermi National Accelerator Laboratory (Fermilab) and the results from the Revolutionary Working Group are being considered for the SLAC National Accelerator Laboratory. DOE is conducting laboratory reviews of science and energy together. This process could lead to more coordination between the two areas.

Discussion

Murray clarified for **John Hemminger** that the Evolutionary Working Group was charged by the Secretary of Energy Advisory Board to look at DOE Orders and requirements to identify things that could be pulled out. Nine orders were pulled out and some were streamlined. The concurrence process for this group took time and the Secretary approved it. The Revolutionary Working Group was started within the Department to start with a blank sheet of paper and identify what needs to go into a contract. This was less revolutionary than envisioned. The group worked hard to identify the appropriate contract type. The M&O (management and operating) contract is best for SLAC. Contract clauses were paired down to essentials and a compliance plan identified how the lab and site office would comply with each regulation. The approach is in concurrence and the Office of General Counsel will determine if this meets the FAR (Federal Acquisition Regulations) and other guidelines.

Anthony Rollett asked about international collaborations, asking if a framework for collaboration is needed at policy levels, and if this should originate with Congress or at a grass roots level. **Murray** shared that the State Department manages bilateral agreements and DOE Protocols fall under these. If bilateral agreements do not exist, DOE, State and the Office of Science and Technology Policy (OSTP) strive to get agreements in place and achieve consistency. Bilateral agreements are a convenient way to meet framework needs. ITER is challenging as it is a multilateral agreement. DOE seeks to use the CERN model that honors bilateral provisions with individual countries while maintaining multinational partnering.

Simon Bare asked if Mission Innovation is a positive step. **Murray** sees it as positive as clean energy goals need to be met and global innovation is needed. Something could be imposed at a policy level for reduction in carbon but that is difficult internationally. LED prices have decreased by 90% in 10 years and other innovations can cause the adoption of energy saving technologies. Mission Innovation involves 20 countries and the European Commission who have pledged to double their investments in energy technology innovation over the next 5 years.

NEWS FROM THE OFFICE OF BASIC ENERGY SCIENCES

Dr. Harriet Kung, DOE, Director of BES, shared a staffing update for BES and noted that applicants for the Division Director position for Chemical Sciences, Geosciences and Biosciences are being reviewed. Kung pointed out new arrivals and vacancies.

The Energy Frontier Research Centers (EFRCs) include more than 100 participating institutions. At the end of the American Recovery and Reinvestment Act, the number of EFRCs were reduced. EFRC demography shows large graduate student representation and a nearly 25 percent representation for undergraduate students. EFRC annual reports indicated positive health and production. Accomplishments include a growth in publications and in intellectual property from year one through seven, and ongoing contributions to the private sector.

The development of transparent solar technology that has now been privatized as Ubiquitous Energy and is one EFRC technical accomplishment. Another is the development of the world’s first 3D electronics printer that allows for printing customized electronics and on-the-fly laser assisted direct writing with conductive ink. This led to the creation of ink for printing thermo-elastics.

A core research highlight is the development of light-driven N_2 reduction by a CdS:MoFe protein hybrid. This research illustrates the power of different modalities. Discovery research coupled with use-inspired research is a strength of the BES research portfolio.

Mid-term reviews for the 32 EFRCs were conducted in 2016. Guidance letters were sent to the EFRCs in May that proposed actions, recommendations, and funding adjustments for some.

A funding opportunity announcement for EFRCs on environmental management research is underway with an award announcement expected in July.

Kung reviewed case studies in catalysis. This fits the tradition of sharing BES themes that are of interest to the BESAC. Catalysis may be BES’ most visible program. Catalysis for fossil conversion, biologically derived feedstocks, and photo- and electro-driven conversion of carbon dioxide and water are three areas of focus. Chemical production is a growing trend in energy consumption. Ammonia is at the top of this list. There have been some reductions in energy use but this remains a challenge. This is a fertile area for game-changing approaches.

Kung explained catalysis research activities being supported by BES, specifically research in understanding catalytic mechanisms and novel synthesis routes. Examples of the pay-off are advances in fuel cell development and biomass conversion.

The National Synchrotron Light Source-II (NSLS-II) achieved CD-4 in March 2015 and the first full year of operations is underway. Top-off operations are running. The storage of 400 mA in the storage ring was achieved in April 2016. Preventing rust corrosion is a scientific achievement possible through NSLS-II research. Defining the crystal structure of nanoprecipitates that cause embrittlement and degradation of steel in nuclear reactor pressure vehicles is another example.

The FY17 BES budget request is $1,937M, an increase of $87.7M over FY16. Most of the increases are in research and consist of new EFRCs for subsurface research, exascale computing, and Mission Innovation core research. There are modest increases for scientific user facilities.

The House marks for the BES budget recommend an $11M increase over the FY16 budget, with language reducing the EFRCs and increasing the Experimental Program to Stimulate Competitive Research (EPSCoR). Computational chemical sciences is funded. User facilities and construction are fully supported.

Senate marks propose $64M above the budget, to include full support for the exascale crosscut. Increases are recommended for EPSCoR. The Senate included funding that would allow all BES facilities to operate at optimal levels.

Both the House and Senate strongly support Major Items of Equipment and Construction investments, but also suggest reductions in core research.

Basic Research Need workshops have been conducted since 2002. These inform BES planning and thinking about its research portfolio. In 2016, a workshop was conducted on environmental management.

BES is building on the report “Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science” and the guidance that it provides. Workshops on three key areas highlighted in the report were held in 2016.

Discussion

Kung clarified the EFRCs’ philosophy for **Bruce Gates**. The first EFRCs had five-year charters while newer Centers have four-year charters. This current term of length is driven by a goal of more frequent turnover in a two-year solicitation cycle. In the renewal phase, some Centers wanted to investigate different areas. The bar for renewing the EFRC portfolio is set very high. Centers must make strategic decisions about what they pursue, supported by world-leading research.

Beatriz Roldan Cuenya commented that within the scientific discovery process, some experiments are trial-and-error and show a lack of connection between theory and process. She asked about efforts to advance the theory for electrified liquid-solid interfaces. **Kung** shared that these activities are not trial-and-error, as most BES research shows strong links with theory collaborators.

Dawn Bonnell noted emphasis on use-inspired research and that in the age of flat budgets, increases for this puts pressure on discovery research. **Kung** added that the seed corn of long-term basic research is vital.

Bare pointed out that Senate mark language supports the development of co-located facilities. **Kung** shared with **Bare** that this may relate to the nanoscale science research centers which are co-located with light source and neutron facilities.

Rollett asked if Senate mark language shows favor toward simultaneous support of multiple construction projects. **Kung** noted that the marks honor BES' request and show favorable support for the Linac Coherent Light Source-II and Advanced Photon Source-Upgrade.

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

Colin Broholm reviewed the Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology held in February 2016. The investigation of quantum materials looks into quantum mechanics beyond the atom to include superconductivity and magnetism. A newer field is the use of quantum transport behaviors.

The workshop was based on intellectual curiosity around quantum materials. Attendees were excited about the fundamental properties of quantum materials and advances possible.

The discovery of iron superconductivity and electronic interactions has driven interest, as has the topic of topological materials. Knowledge of topological content grows understanding of materials. Work in quantum materials is elaborated via connections between synthesis, theory and experimentation.

The number of university and government labs, amount of private funds, and number of proposals worldwide in this field all seem to be growing.

Greater understanding of the behaviors of electron systems was prioritized at the workshop as an essential area for future research. Superconductivity and magnetism are focus areas.

Knowledge of the quantum materials topology was also identified as a research priority. Topology can play a role in transport properties. This area drives the promise of groundbreaking functionalities supported by topologically protected transport and fractional quasi-particles. A method to probe and manipulate the topology of materials is needed.

The ability to drive and manipulate quantum behavior is an area needing additional research. Work at the nanoscale level could point out new capabilities, and connect fundamental research with application in meaningful ways.

Tools for synthesis, characterization, and modeling of quantum materials was the final area described as important for this field. There is potential for looking at materials in new ways and learning about materials when exposed to different levels of stress.

The progression in the use of materials highlights the need to reach the atomic scale. The science of transforming the understanding of matter can present strong opportunities for application opportunities.

Discussion

Broholm defined quantum material for **Mark Ratner** describing it as quantum physics that transcends the atomic scale. Usually there is a transition in the longer length scale beyond the classical scale. Research is looking at materials that extend the coherence length to 10s and maybe 100s of atoms.

Rollett asked about current abilities in theory and math to describe these interactions and phenomena. **Broholm** shared that the underlying framework exists. What differs now is that strongly correlated collective states exist so individual electron is not what we need to look at. This development challenges theoretical description. Progress is being advanced by quantum discoveries. The second influence is topology due to work in the past ten years and recognition of its importance in materials.

REPORT ON THE BES FACILITY UPGRADE PRIORITIZATION SUBCOMMITTEE REPORT

John Hemminger, BESAC Chair, shared the subcommittee report. Facilities have evolved, and five upgrades are proposed by BES. The BES omnibus appropriation bill asked BESAC to evaluate the upgrades. A guideline is facilities' ability to push the frontiers of discovery science.

BESAC examined and ranked the ability of upgrades to contribute to world-leading science and the readiness of each upgrade to proceed to construction. Lab and facility directors presented details to BESAC at its meeting in February. The subcommittee held further discussions in April.

Hemminger described the evolutionary and revolutionary pace of technological development, and how this process is undertaken and executed at research laboratories and facilities. Underlying support systems and the synergy of interacting systems can advance progress.

There are three facilities proposed for x-ray light source upgrades. One is the Advanced Photon Source-Upgrade (APS-U). Storage ring advances (multi-bend achromat lattice) are one feature of improving light source technology proposed for APS-U. An outcome of the upgrade is growth in brightness by several orders of magnitude and the ability to do experiments previously unconceived. The APS-U is seen as essential to world-leading science and ready to proceed with construction. A coupling of simulation and theory to experiments is recommended for APS and all of the facilities.

The Advanced Light Source-Upgrade (ALS-U) would provide orders of magnitude more coherent flux. The upgrade design is based on the multi-bend achromat lattice. All of the storage rings have a large number of beamlines associated with them with multiple end stations. ALS is beginning to upgrade existing beamlines to ensure compatibility with the upgrade. They are working with the user community and what it could mean for their research. ALS-U is seen as essential to world-leading science and ready to proceed with construction. Dark time would be about one year. The coupling of simulation and theory to experiments is robust.

The Linac Coherent Light Source-II High Energy (LCLS-II-HE) upgrade could build on the success of LCLS. The upgrade would enable a high repetition rate pulse at high energy (beyond 5 keV). European competitors are challenging this capability with the launch of EuXFEL in 2016 or 2017 with a different pulse rate. The LCLS-II-HE upgrade would support studies of dynamics near the Fourier transform limit. The upgrade is seen as essential to world-leading science and ready to proceed with construction. There would be no dark time beyond the normal maintenance period.

There are two neutron facilities proposed for upgrade.The Spallation Neutron Source (SNS) has been a major success and is the most powerful pulsed neutron source in the world. It operates at 1.4 MW at 60 Hz and would grow to 2.8 MW under the Proton Power Upgrade (PPU) project. The European Spallation Source is likely to go live in 2019 and offers the ability to do new types of experiments. The SNS-PPU would increase the power of the proton accelerator. The SNS Second Target Station (STS) would direct one of every six pulses to a second target station. The subcommittee wondered about the selection of this pulse ratio. It was recommended that SNS get a handle on the target lifetime of the first station and make it fully robust to take full advantage of the power upgrade. The subcommittee sees the value of having a second target station to remain competitive and continue to expand the ability to work with neutrons. The SNS-PPU and SNS-STS are both essential to world-leading science. The subcommittee recommended that a review panel be formed to examine the proposal for the second target station and consider options for repetition rate and pulse length, Significant scientific and technical challenges need to be resolved. Coupling of simulation and theory to experiment was seen as vitally important to neutron work.

Discussion

Hemminger clarified for **Gates** that construction readiness meant that there are no technological roadblocks.

Esther Takeuchi commented that extended dark times could significantly impact the user community. She asked about staging the dark time with other light sources coming online. **Hemminger** shared that the NSLS transition gave lessons learned. APS and ALS should not be shut down simultaneously. Along with the budget, the dark periods need to be managed.

Cuenya suggested that a strong scientific case was not clear from the report. She asked if facilities described the new science that could be done with upgrades, if a prioritization of new science informed subcommittee decisions, and what criteria might have been used to do this prioritization. **Hemminger** described the scientific case put forth by all facilities as strong. Looking at the brightness curves, all facilities would have second-class status without upgrades. If there is no exciting science to go along with it, then the investment is not worthwhile.

Rollett moved that the report be accepted and **Ernie Hall** seconded the motion.

Hall shared concern about denoting everything as ready for construction. There is potential for Congress to discern a desire to shut things down as quickly as possible. He suggested adding a sentence that the dark period staging is important with continued support for users. **Hemminger** was open to amending the report to emphasize the need to minimize the impact on users.

Rollett modified his motion to include **Hall's** suggestion.

Hemminger was asked by **Gates** to project a timeline for all the upgrades. APS-U is already moving ahead. An Argonne representative proposed that a shutdown could occur in mid-2022. Both ALS and LCLS-II-HE would be ready to follow that. LCLS-II-HE does not require a shut down and could be fit into this period. **Hemminger** would like ALS to determine what it will do with its beamlines to readily move into shut down once APS-U is complete.

John Tranquada suggested that the SNS review committee may determine that a long-pulse approach is not competitive with the European Spallation Source. **Hemminger** added that thought needs to be given to what the short pulse rate might look like.

Rollett re-read the motion language that the BESAC will accept the subcommittee report with an amendment that addresses the timing of upgrade shutdowns. Those BESAC members not recused from voting voted to accept the subcommittee report.

REPORT ON THE BASIC RESEARCH NEEDS FOR SYNTHESIS SCIENCE FOR ENERGY RELEVANT TECHNOLOGY WORKSHOP

Jim DeYoreo of Pacific Northwest National Laboratory (PNNL) reported on the Basic Research Needs for Synthesis Science for Energy Relevant Technology Workshop. The workshop was stimulated by the "Challenges at the Frontiers of Matter and Energy" and the "Directing Matter and Energy" reports.

Many new materials and technologies show the value of synthesis. The Materials Genome Initiative, as an example, highlights the value of advancing synthesis. A focus now is knowing how to get atoms to move to assimilate desired structures.

Five workshop panels and two cross-cutting panels accepted the BES charge to examine basic research needs and priority research directions for synthesis science with a focus on new and emerging areas to develop new energy technologies.

The elucidation of fundamental pathways for materials formation was identified by one panel as a significant challenge.

A second panel identified three challenges: enabling programmable assembly through the synthesis of information-encoded building blocks, navigating energy landscapes to achieve hierarchical assemblies, and developing strategies based on sustainable energy relevant materials and processes.

Panel three focused on interface-defined matter. Many materials feature interfaces but what had not yet been appreciated was the ability to produce materials through interfaces that otherwise could not be developed.

Crystalline matter was addressed by panel four, with a desire to master the science of crystal synthesis and hierarchies of crystalline complexity.

Panel five looked at emerging approaches to synthesis at all length scales.

The identification and control of synthetic pathways, and enabling the prediction of pathways and ensemble outcomes of synthesis that can direct processes on the fly were challenges identified by the two cross-cutting panels.

Three themes emerged from the workshop. One is understanding mechanisms, pathways and intermediates as a key to achieving control. An emphasis on developing hierarchical materials was second theme. The third is that even with advances in theory, simulation and tools, synthesis will always be part of the voyage to new discoveries. This is underlined by ongoing knowledge growth among scientists and researchers that have led to the creation of new materials.

Discussion

Gates asked about the prospects for synthesis of amorphous materials and how that would differ. He asked if catalysis was discussed. **DeYoreo** shared that amorphous materials did not emerge as a priority but was part of the discussion. Relative to catalysis, the idea of using interfaces to promote synthesis is a way of catalyzing synthesis. It was not a main point in discussions. **Hemminger** suggested that **Gates** could provide some input for the report.

DeYoreo shared with **Gordon Brown** that biomaterialization was well represented and discussed in the workshop. One panel felt that the macromolecular solid was a bigger challenge.

DeYoreo shared with **Rollett** that the in-situ panel discussed the value of multi-model tools. That will be called out in the report. **Hemminger** added that there are always new methods of synthesis. There may be new elements of technology that may further synthesis. **DeYoreo** noted that members highlighted what they would like to see developed. **Hemminger** suggested that these sound like characterization methods. **DeYoreo** shared that there was really no discussion on instrumentation that had to be developed for synthetic processing. Recent discoveries such as nanoparticle robots are enabling chemists and scientists to explore phase space rapidly.

DeYoreo told BESAC that the report will be complete in September.

Gates noted that the Grand Challenges report described looking at atom-by-atom synthesis of materials, and asked how far things are from that goal. **DeYoreo** shared that there are good examples. One is small cluster of atoms and a question of the preciseness of assembly. In the molecular world, assembly is achieved through the design of the molecules. In terms of other materials, like interface defined matter, atomic layer deposition can be thought of as assembly atom-by-atom.

REPORT ON THE BASIC RESEARCH NEEDS FOR INNOVATION AND DISCOVERY OF TRANSFORMATIVE EXPERIMENTAL TOOLS WORKSHOP

Ali Belkacem of Lawrence Berkeley National Laboratory (LBNL) reported on the Basic Research Needs for Innovation and Discovery of Transformative Experimental Tools Workshop held on June 1-3, 2016.

Belkacem shared that an examination of basic energy research thrusts provokes the need for enabling tools for innovation and discovery. Advances in tools can lead to the paradigm shift required to advance basic energy research. The field is very broad due to the diversity of tools that are used, and it is very easy to get lost in the broad range.

The "Challenges at the Frontiers of Matter and Energy" report was a guide to the role of tools and ways to get information from functional systems. The workshop charge was to look at instrumentation science to provide ways to advance grand challenge energy research. Four panels addressed this challenge within a range of sub-topics.

Belkacem reflected on an earlier question about synthesis and materials, chemistry and biology. There is an extremely strong connection between these three in materials science.

Chemical reactions and transformation was one panel at the workshop. Attendees considered the design, creation and probing of local functionality at high resolution, and imagining the value of tools that would allow for characterizing functional complex systems while running experiments, doing detection, and observing data.

A second panel looked at imaging materials far from the equilibrium. The challenge here is doing this in complex systems and the move from 3D to 4D. Attendees proposed advancing imaging and spectroscopy across time scales, and length scales while preserving high resolution to watch chemistry as it is happening.

Heterogeneity as a challenge across multiple length and time scales was a third panel. Panelists examined instrument and capability development to characterize and correlate different aspects of functional complex systems. This would propose focusing many eyes on one sample at the same time and correlating those observations.

The fourth panel looked at the integration of experimental tools with theory and computation. The attendees explored the value of developing tools at the conception of an experiment. This integration at the outset could accelerate discovery science.

Discussion

Gates asked about modalities and limitations, and about achieving these things step-by-step. **Belkacem** shared that a challenge is funding people to synthesize materials or look at synthesis or a catalyst. Often they need to develop a tool and that is the end product. Development as an end point itself needs to be emphasized. Science cannot be separated from instrumentation.

Gates asked about getting input from users of different modalities and how they approach these challenges. **Belkacem** suggested developing an approach in the U.S. that fits how work is done at universities and national labs.

Hemminger noted that BESAC has highlighted the importance of forming a methodology to develop experimental scientists. Graduate students could be given the chance to spend part of their career on instrumentation development. **Belkacem** shared that workforce development was discussed and that actions are needed.

Philippe Piot asked for an example of a multi-modal instrument. **Belkacem** described that in catalysis, we can look at the surface to understand the intermediates, otherwise we only get the reaction rate and averages. Simultaneously, one could look at the oxidation state and the product with infrared spectroscopy, while also looking at the intermediates with a time sensitive probe. Current efforts are being done piecemeal. **Belkacem** highlighted a talk given by **Frances Ross** and work being done by IBM.

Persis Drell noted earlier references to the linkage between theory and simulation with experiments. The community has had to make compromises rather than get coherence across laboratory and individual experiments. Leadership is needed before funding, and the community needs to be ready to lead the charge. **Belkacem** added that leadership is required, and scientists seem ready to accept that change. The integration of theory, simulation, and experiment during the conceptual design phase is important.

Rollett asked about whether the committee consider facility upgrades and specific improvements such as higher fluxes. **Belkacem** noted that facility-specific upgrades were not heavily discussed. The workshop focused on higher level themes.

PRESENTATION OF THE AMMONIA SYNTHESIS ROUNDTABLE REPORT

Jens Norskov of Stanford University and the SLAC National Accelerator Laboratory presented a report from the Ammonia Synthesis Roundtable.

Ammonia synthesis is a complex process. The discovery of this reaction has had an incredible impact. Increased production has been linked to growth in the human population. More than one percent of all energy used in the world goes into this reaction.

Ammonia is an energy dense fuel. New ways to produce and safely store ammonia are needed. Currently, production is a forced process.

The rate (turnover per second) is a function of the N_2 transition-state energy and the N_2 absorption energy. Optimal catalysis is done at a lower transition-state energy. A challenge is that 250,000 materials have been investigated. All are less than optimal.

Fertilizer production via ammonia is valuable but most of the nitrogen used has detrimental environment impact. Less than 50% of nitrogen applied in the field ends up in the crop. The rest washes into our rivers and oceans.

A goal is to devise an electrochemical cell that splits water, and makes protons and electrons using solar and wind power. This just-in-time fertilizer would be produced only when the sun is shining and water is available.

Work has been done to develop the Schrock catalyst to produce N_2, but it is not yet sufficiently long lived.

The workshop concluded that there is no catalyst today in any form that is active, selective, scalable and long lived. It is a big challenge to fundamental chemistry to identify relatively low pressure and low temperature thermal processes to produce ammonia.

The workshop examined potential solutions to include developing hydrogen in a sustainable manner. The distribution and infrastructure that are part of the optimization are very expensive, when looking at this from a systemic view. This could be accomplished in small units rather than a big factory. A catalyst is needed to operate at low pressure. There is incredible potential in finding approaches that work at higher levels of the two variables.

Development of electrochemical and photochemical routes for N_2 reduction based on proton and electron transfer is another challenge and opportunity.

An option discussed was the combination of biological and chemical systems. Biochemical routes to N_2 reduction hold strong possibilities.

Implementing these solutions could occur not at one temperature but in a looping process. Step catalysis or chemical looping has been used for water splitting and could be used for nitrogen splitting as well.

Another challenge is using this reaction to examine what is important for catalysis. Finding descriptors and ways to use other motifs to do this could be useful. Combining theory and experiment could draw on machine learning to expand our knowledge of all materials that could enable catalysis.

Integrating different forms of catalysis into one frame of thinking presents another challenge with the notion that this simple form of interaction could yield benefit.

In-situ and in-operando techniques are essential.

The significant scientific challenges presented have not been solved and have an impact on energy, the environment, and the food supply. This may be a chance to consider new chemistry and ways to drive sustainable, distributed production.

The fossil fuel industry is generally focused on central production facilities. If production is distributed, more sustainable chemical production is possible and the rationale for large facilities is no longer valid. The argument for larger facilities is generally economy of scale, yet efficacy of scale can be balanced with mass production.

Discussion

Norskov confirmed for **Rollett** that efforts to measure the rate of reaction in a spatially resolved way have been tried. Different strategies could resolve the inherent challenges that have not yet yielded results.

Gates asked about pushing energy in ways that are different from the way nature does it. **Norskov** sees that energy rich electrons is how nature does it. Lessons have not been learned yet, however, and there has not been much activity in this field for many years.

Cuenya noted that BESAC was surprised that this topic originated with Congress and that they felt it was a good topic to revisit. She asked who else is trying to work on these topics, including Europe, and what the U.S. can do. **Norskov** shared that there are activities elsewhere, especially in Japan and several places in Europe. There is more interest in the U.S., and **Norskov** is getting calls from the private sector. This is a problem that was perceived as very hard but new techniques and theory and experiment make this desirable to get into again.

Gates asked for perspective on how the technology of the Haber Bosch process has been improved. **Norskov** shared that it has been driven by good chemical engineering with greater energy efficiency by integrating steam reforming with ammonia synthesis.

PRESENTATION ON THE BES CHEMICAL SCIENCES, GEOSCIENCES AND BIOSCIENCES DIVISION: TEAM PRESENTATIONS AND STRATEGIC PLANNING

Gail McLean, Raul Miranda and **Jeff Krause** of the BES Chemical Sciences, Geosciences and Biosciences (CSGB) Division presented an update on division activities. The team reviewed the CSGB mission and its goals.

Catalysis science is the largest component of CSGB. Strategic planning is informed by BESAC, roundtables, council workshops, community and scientific societies, and proposals and review processes.

The CSGB Council serves to identify emerging research opportunities and conduct a workshop that publishes its findings. In 2015, CSGB merged its “Chemistry and Biochemistry” and “Earth Sciences” councils into one body. McLean reviewed recent and upcoming workshops conducted by the CSGB Council.

Strategic discussions are consistently held. Three in 2016 focused on the lab review timeline.

Krause gave background on the Fundamental Interactions (FI) Team. Consisting of four programs, FI seeks to understand reactive chemistry at full quantum detail. Its mission emphasizes structure and dynamical studies of atoms, molecules and nanostructures, and the description of their interaction in full quantum detail. This aligns with the BES and SC missions.

FI is integrated with the Division, giving cross-cutting relevance and synergy. Most work on FI is discovery type research but there is also opportunity for use-inspired science opportunities.

The Atomic, Molecular, and Optical Sciences (AMOS) program is one highlight of FI, focused on intense field and ultrafast x-ray science. There are also investments in correlated dynamics and nanoscience. About 50 percent of AMOS funding goes to labs, and university research funding supports 61 PIs.

The Gas Phase Chemical Physics group in FI supports fundamental research into fully predictive models for combustion.

Condensed Phase and Interfacial Molecular Science (CPIMS) focuses on the study of reactions and dynamics at well-characterized metal and metal-oxide surface and clusters. CPIMS interacts with many other programs. It provides university and lab support with co-funded projects in multiple areas.

The Computational and Theoretical Chemistry (CTC) Program has evolved into eight focus areas since its origination in 2009.

McLean described the Photochemistry and Biochemistry Team (PBC) and its four program areas. PBC addresses a general theme of energy capture, conversion and storage, through its four programs in photosynthetic systems, physical biosciences, solar photochemistry and the Fuels from Sunlight Hub: Joint Center for Artificial Photosynthesis (JCAP).

The PBC mission looks at fundamental studies of the molecular mechanisms involved in capture of light energy and its conversion into chemical and electrical energy through biological and chemical pathways. As with FI, PBC has a lot of interactions intra-team and across the division. Interactions within PBC range from biochemical through chemical transformation and are demonstrated by interaction between the teams and with areas that include Catalysis, AMOS, CTC and CPIMS.

The Physical Biosciences Team focuses on redox biochemistry. The program provides basic knowledge to develop catalysts, enhance biochemical pathways for biofuels and chemicals, and next generation energy conversion / storage technologies.

The Photosynthetic Systems program is driven by the natural photosynthesis systems found in nature. This program gives insight to develop bio-inspired and bio-hybrid energy systems, while also improving biological photosynthesis for biofuels and biochemicals.

The Solar Photochemistry Program has been in place since 1977 and has been enhanced by chemists’ ability to build on original model photosynthesis systems and the synthesis of new variants. The program has supported the creation of semiconductive photovoltaic cells and photoelectrochemical conversion processes.

The Fuels from Sunlight Hub established in 2010 and lead by California Institute of Technology strives to develop efficient and scalable technology to convert carbon dioxide, water and sunlight into transportation fuels.

Miranda described the Chemical Transformations (CT) team and its four programs. CT is currently funded at around $85M with an average of 50 percent going to national labs. CT strives to understand and control the stabilization, transport, and chemical conversion of matter. It ultimately seeks to transform chemical and geochemical technologies.

Miranda described ways that CT integrates across the division and with specific programs in other BES divisions. CT also works with offices in other parts of SC.

The Catalysis Science (CS) program has a long history but is evolving and working to extend catalysis science to include the examination of alternative energy sources and feedstocks. There are efforts to improve atom and energy efficiency, the cleanliness of chemical conversions, and understanding of interacting dynamic systems to reduce the number of reaction steps.

The Geosciences Program works within geochemistry and select areas of geophysics, and is funded at around $20M. Miranda described evolving opportunities in Geosciences.

The Heavy Element Chemistry Program investigates spectroscopy, bonding reactivity, and the separation of actinides and fission products. The program is uniquely defined by the chemical elements with which it works, and underpins work at applied nuclear programs to include the discovery of new elements now part of the seventh row of the periodic table of elements.

The Separations and Analysis Program has the larger vision to identify analytical methods relevant to energy processes and the purification of critical materials. There are many evolving opportunities within the program, and opportunity to impact the efficiency aspects of Mission Innovation.

Next steps for the Division include conducting more program discussions, identifying best management practices, and solidifying ways to communicate the science that it is funding. McLean reviewed the body of questions that CSGB uses to plan its strategies and investments, and described its future direction.

Discussion

Drell asked about CSGB's guidance questions, and if questions are asked about how CSGB would best achieve its goals. **McLean** confirmed that there are activities such as review discussions that drive the analysis of needed changes and look at timelines for changes.

Steve Leone asked about mechanisms within strategic planning to identify new direction and areas that should be part of the portfolio. **McLean** shared that discussion about new direction and input are ongoing, factoring in how best to use funding. Scientific meeting attendance, proposal review, community interaction, advisory committees and Councils give indicators to bring in new concepts, high-risk and high-reward investments and other direction. **Kung** added that CSGB exists in a BES environment that examines ways to engage the community, factors in workshop reports, and examines quadrennial reports. There are both top down and bottom up initiatives that go into the budget request. More mature areas are phased out for new priorities.

Krause identified for **Hemminger** studies in CPIMS that feature the aqueous aspect of the overall CPIMS mission, including solvation and dynamical processes in solution.

Hall was surprised by the information about the amount of energy that goes into separation processes. **Miranda** clarified for **Hall** the scope of overall research being done and that some is funded by other agencies. Most separations are performed by thermal separation, which is expensive. The solution is to work in non-thermal separation such as membranes but it's difficult for products like oil.

Bare highlighted the focus on using new feedstock and materials, and suggested that there are many opportunities to work in hydrocarbon catalysis. The reality is that petroleum use is not going away. **Miranda** described some supported research such as nanostructured catalysts for hydrocarbons. C-H activation is the number one topic supported by CSGB and C-O activation is growing.

Gates shared thoughts on seeking out new directions for the CSGB. The implication is that there are some things that will stop. **McLean** shared that there are many factors that influence where to disengage. One is to view investment by other agencies and achieving balance with their work. One can look at where impacts are happening and understand this through the review process. This poses the idea of incremental investment or larger levels of investment to discern the greatest needs and the potentially greatest impacts. This requires a very thoughtful decision and taking an educated chance. **Hemminger** added that input can be gained through the Committee of Visitors (COV) processes. **McLean** shared that there will be a COV held in 2017.

PUBLIC COMMENT

None

ADJOURNMENT

The meeting was adjourned by **Hemminger** at 5:00 p.m.

FRIDAY, JUNE 10, 2016

The BESAC meeting was convened by **Chair John Hemminger** at 8:35 a.m. EST.

PRESENTATION ON THE SCIENTIFIC USER FACILITIES COMMITTEE OF VISITORS

John Tranquada reported on the Scientific User Facilities Committee of Visitors (COV) held on April 12–14, 2016. The charge was to examine the efficacy and quality of the processes used for proposal actions, the monitoring of active projects and programs, and to evaluate how the process has affected portfolio elements.

The COV covered FY13–15 and during that time, the Scientific User Facilities Division consisted of six x-ray-light sources, three neutron scattering facilities, five Nanoscale Science Research Centers, and three Electron-Beam Micro-characterization Centers.

The COV also looked at ongoing, completed and terminated projects, and those on hold.

Tranquada reported on the COV's main conclusions. The COV found that the implementation of previous COV findings was appropriate and the COV process was effective.

The new method of reviewing each facility's budget was effective. Facility directors and the COV communicated by guidance letters. Letters should contain more detail as it relates to budgets and the impact on facility activities.

The COV recommended finding ways to use budget reviews in triennial facility reviews, providing review findings to facilities within six months of the review, support for program manager travel to project sites, and partnering with the National User Facility Organization.

Tranquada shared reviews of the light source and accelerator and detector R&D programs, emphasizing a focus on beamline staffing levels, the use of benchmarking against international facilities in triennial reviews, an evaluation of a review process against the staff time given to the activity, and keeping records of facility director teleconferences.

Recommendations for included a focus on beamline staff development, career paths, and workload. The facility triennial review process should be evaluated on the balance between a rigorous review and the time needed to support the review. Questions, answers and action items should be recorded for the monthly teleconferences with facility directors.

It was recommended that the Nanoscale Science Research Centers (NSRC) be given greater visibility, that its capital budget be increased, and that the NSRC portal be further developed.

The Neutron Scattering Facilities should join other agencies in expanding the role of neutron science in the U.S., understand how terminating support for user programs can impact the community and productivity, and work to recover the experimental capabilities lost due to the end of BES funding for the Lujan Center.

Discussion

Tranquada described the National User Facility Organization for **Rollett**. It is a representative body of facilities that work to lobby for general user facility issues that including uniform training requirements across labs. They help advertise user facilities in Washington DC.

Tranquada told **Brown** that the BESAC User Facility Upgrade Prioritization Subcommittee Report would not have an impact on the COV. The COV examined the processes, not the decisions.

Gates asked for a summary of points that have come up in earlier COVs. **Tranquada** shared that there were not many. There was a suggestion to look at neutron needs in the U.S. That does have some overlap with the BESAC prioritization activity.

Drell asked about the health and success of the facilities, and the appropriateness of facilities taking a long-term view. **Tranquada** shared that the COV did not address this. Each facility does have a plan for its own goals and future. The COV looked at whether facilities have done that. It is believed that a process is in place, and the next COV could look at that. **Drell** added that validating that this process is in place is a good thing.

Doug Tobias asked where the capabilities that were at Lujan could be placed. **Tranquada** shared that one instrument that was lost was the total scattering instrument which had a large detector bank for diffraction and elastic scattering. He is unaware of plans to replace it. It is hard to move these things. There have been unique capabilities for high-pressure sampling, and some capabilities are being developed at SNS.

Takeuchi noted that the COV expressed concern about the staffing levels associated with beamline and synchrotron facilities, and that the model for the Nanoscale Science Research Centers is different. **Tranquada** clarified that the comment was from the light sources panel and focused on light sources staff. The nanoscience panel was concerned that the nanocenters found guidance to them to be challenging as they do need to replace equipment. There are no separate funds for this, and decisions can impact the staffing.

Bare described the decline in industrial users as a perennial and ongoing problem that needs to be taken seriously. Even with partnership opportunities and placement of this topic on meeting agendas, nothing seems to change.

Tranquada clarified for **Hemminger** that the integration of theory and computation with facilities was not discussed. It is an appropriate question to address to the facilities.

Brown moved to accept the report and **Rollett** seconded the motion. The report was accepted by BESAC.

PRESENTATION ON PREPARARTION FOR THE ENERGY FRONTIER RESEARCH CENTERS / HUB COMMITTEE OF VISITORS

Andy Schwartz shared plans for the Energy Frontier Research Centers (EFRC) and Energy Innovation Hubs COV to be held on November 15–17, 2016. The hubs are the Joint Center for Artificial Photosynthesis (JCAP) and the Joint Center for Energy Storage Research (JCESR).

This is the second EFRC and Hub COV. The previous one was held in May 2013.

The 2016 COV will follow a format similar to the one used in 2013. Schwartz reviewed findings from the 2013 COV and described the major recommendations.

The DOE Secretary of Energy Advisory Boards (SEAB) 2014 Hubs+ Task Force provided EFRC recommendations that also inform perspective for the 2016 COV. Schwartz reviewed DOE's response to the SEAB.

A formal charge to the COV has not been received but Schwartz believes that it will look similar to the charge presented in 2013.

Ceyer will chair the COV. **Jim McCusker** and **Rick Osgood** will chair the EFRC panel and **Hall** will lead the Hubs panel.

Discussion

Rollett suggested that the COV might define which broader impacts or interests are relevant. **Schwartz** shared that DOE tracks as much information as possible. EFRCs are asked annually for information on things such as patent applications. While this is not the primary measure of success for the EFRCs, it is part of their mission and is part of the evaluation process.

Drell noted that issues around diversity came up last time and should be part of this COV.

Hall encouraged BESAC to tweak the charge as this COV would not necessarily look at a broad portfolio that is part of the standard charge. The charge helps to keep panels focused.

Takeuchi shared that management and mid-term reviews were helpful. **Schwartz** added that it would be useful for the COV to look at the management and mid-term review processes.

UPDATE ON THE JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

Harry Atwater provided an update on the Joint Center for Artificial Photosynthesis (JCAP). The Center is a partnership among multiple institutions. The research team consists of research staff, scientists and engineers; graduate students; and postdoctoral scholars.

JCAP has active engagement with industry partners, and actively uses user facilities.

Broadly, there are many advances in materials discovery, measurement and mechanisms, and integration and demonstration of devices.

JCAP's mission is to demonstrate a scalably manufacturable solar fuel generator that produces fuel ten times more efficiently than current crops. A key outcome is the development of catalyst benchmarking that is being embraced by a broader community. Device advances include demonstrating robust water splitting capabilities.

Passive corrosive protection and catalytically active surface protection have been advanced through JCAP work in protection schemes and operations at extreme pH.

Work in stable oxide-based photoanodes highlight JCAP's integration of theory and simulation into experiment. This example focuses on ternary oxides, and is a process that began with theory-initiated screening of candidates. The effort identified a high number of oxide conductors and new materials with a range of ternary photoanodes that met the criteria established for this work. The previous list of materials thought possible for the capability was doubled.

Atwater reviewed findings from comprehensive catalyst benchmarking. This research has pointed out a large number of potential materials to be used in experiments.

Materials discovery work linked with theory have brought about a portfolio of water-splitting prototypes. These use III-V semiconductor stacks and membranes for full product separation.

The status of solar fuel generators has broadened since 1975 and JCAP has narrowed this list to identify those that meet its criteria.

In its renewal, JCAP has taken on the challenge to find a catalyst that can reduce carbon dioxide with high efficiency and selectivity.

JCAP goals are advanced by four research thrusts: electrocatalysis; photocatalysis and light capture; materials integration into components; and modeling, test-bed prototyping, and benchmarking.

The evolution of JCAP's work from phase one to two has moved to examining selective CO_2 reduction catalysts. Work on water-splitting in year six will cede to a more divergent research base that will elicit catalyst choices toward more convergent activities that harvest outcomes of the catalyst discovery and integrate catalysts into photoelectrodes and evaluate them. There will be more focus on the choices that were pursued in the first few years of renewal.

Future work will focus on use-inspired and applied research to develop device level prototypes to test materials in an integrated fashion. Challenges to address include identifying higher density fuels, associated differences in use challenges, identifying routes to fuels from CO_2, and working through methods to selectively drive catalysis toward a specific fuel type. JCAP will work toward an end use goal of usable solar fuels with an efficiency rate better thand current solar to fuel conversion of around 5.7 to 10 percent, depending on the fuel type.

Atwater reviewed surface structure experiments, and highlighted the influence of theory on experiments being conducted at JCAP. In the latter, JCAP can draw on theoretical predictions that impact the measureable parameters used in experiments. Theory has illuminated approaches to enable catalysis research on different surfaces. Theory has also pointed out surface over-layers that go beyond copper to include other candidates for electrocatalysis. Candidates include nickel-gallium.

Earlier outcomes of JCAP work have pointed out a strategy for selective CO_2 reduction that involves control over more complex environments, developing multi-functional catalysts, and forming strategies for breaking the scale between CO binding and other intermediates.

JCAP publishes about 10 papers per month and has had numerous intellectual property disclosures. More than 20 alumni of JCAP have gone on to tenure-track research positions.

Discussion

Bonnell noted the value of combining theory with high-throughput screening. Understanding mechanisms can take decades. **Atwater** shared that there is not a time lag in mechanistic studies before using high throughput screening as these are being conducted simultaneously. Discovery is not preceding experimentation. While developing high throughput rapid screens, it is important to think about mechanisms to avoid getting stuck in configuration space and missing the best approach for selectivity.

Ceyer asked the hydrogen conversion catalysts, noting that some have higher efficiencies than the ones Atwater shared. **Atwater** explained that the focus in the first five years was on the solar fuels generator. To advance this, stability is important. In phase one, energy return on investment was explored and the two outcomes were energy efficiency and durability. This package is JCAP's objective. Most important is understanding how to bring those together into a solar fuel generator.

Ceyer asked about hitting a wall on catalyst development. **Atwater** shared that JCAP continues to work on this for oxygen evolution and that is a materials discovery challenge. When integrated into an electrode, a catalyst's characteristics can change. There is more complexity when integrating components.

Gates asked about doing catalyst discovery without testing for lifetime. The possibility of changes in activity could lead to things that do not meet JCAP's usefulness criteria. **Atwater** noted that for hydrogen and oxygen evolution catalysts, that was a key insight that drove thinking about benchmarking. Appropriate compromises were built into testing. There are components of long-term testing to inform the understanding of long-term efficiency. JCAP has focused on the discovery end of the initial stability due to its mandate. Soon, there will be efforts on the applied side that focus more on durability.

Ceunya pointed out that ethylene as an end product was not in the slides. **Atwater** shared that JCAP's initial thinking was informed by fuel conversion data. That led to thinking about methanol. In terms of bridging theory and experiment, JCAP identified ways to bring those together to understand the kinetic energy possible. **Cuenya** shared that funding on this topic in Europe is considered climate change research and that influences focus. **Atwater** noted that the focus is on producing a renewable fuel path for liquid fuels. The focus is similar but JCAP also has to focus on scalable industrial processes.

Rollett asked if similar methods used in JCAP have been used in ammonia research. **Gates** confirmed that this is being done.

UPDATE ON THE JOINT CENTER FOR ENERGY STORAGE RESEARCH

George Crabtree shared an update on the Joint Center for Energy Storage Research (JCESR) describing the vision for JCESR. Currently, energy storage technology focuses on consumer electronics. There are big opportunities in energy and transportation, and grid-scale electricity storage. The cost of energy production and storage are ongoing drivers.

JCESR works beyond lithium-ion batteries for cars and the grid to drive toward high performance, low cost energy storage. Its legacy will consist of a library of fundamental science, prototypes for the car and the grid, and a new paradigm for battery R&D.

Battery R&D focuses beyond lithium ion. It is driven by computer-based simulations, an electrochemical discovery lab, and building and testing a battery in a virtual space. Work is conducted through sprints that seek to develop a prototype in a finite timeframe.

JCESR has 20 institutional partners from among academia and the private sector.

There are four concepts for JCESR's beyond lithium ion batteries. In January 2016, prototype targets were selected with an end goal of materials components integration to produce proof-of-concept prototypes.

Multivalent intercalation is one concept being pursued. Progress has been slow as there are many materials candidates but few that are a good fit. Two multi-valent cathodes have been identified -- calcium and magnesium. Mobility becomes a bigger challenge that affects the ability to quickly charge and re-charge. The design rule that emerged states that barriers needs to be low.

Full cell cycling has been done at JCESR. Magnesium and Ti_2S_4 have been used to make the battery work. Zn has also shown positive results.

Work in ion pairing in electrolytes has enabled rational design for stability, and stripping and plating. This pairing has the ability to shift the electrochemical stability window. This understanding along with knowledge of the decomposition pathway can lead to a rational design.

Multivalent data and applications have been released to the public by JCESR in order to enable community research.

Crabtree shared research on lithium-sulfur batteries. Low cycling life is one of the biggest challenges associated with these batteries. Prototypes have been constructed and tested that push the state-of-the-art in this area of work. JCESR seeks to use less than 100 percent of excess lithium and increase energy density, and is on target to continue its development beyond current industry standards. Breakthrough concepts promise low-cost.

In lean electrolyte / sparing solvation, JCESR is focused on a small portion of unexplored space presenting unique opportunities for research. Graphene oxide protective membranes are being used to achieve a coherent interface. The functionalized membrane will be integrated with the sparingly solvated electrolyte.

JCESR is working on an air-breathing aqueous sulfur flow battery. The materials cost for this type of battery is very low. The challenge is to determine if solar energy can be stored in the summer and used in the winter at a cost of less than $1 per kilowatt hour. Four teams are addressing specific research opportunities in this area.

The concept of macromolecular-based redox electrolytes is one opportunity for working in the grid. Polymers can be cross-linked into a colloid, and energy density will increase. It presents the chance to develop an inexpensive and recyclable design. This work would open up a new area for flow batteries. The target for current research is to achieve a better cost target. A new class of redox flow molecules have been discovered based on macromolecules.

JCESR has 44 invention disclosures and 26 patent applications.

Discussion

Olvera asked if JCESR should study a polymer gel electrolyte. **Crabtree** shared that the problem is the motion of the lithium. A solid state electrolyte would be great to make. The methods being used are not gels but methods that could be used in two types of batteries.

Takeuchi shared interest in the use of a acetonitrile and if it could be stabilized for lithium. Achieving divalent batteries is difficult. **Takeuchi** asked how it compares in energy density with others. **Crabtree** shared that lithium batteries are typically low voltage and instability problems are not big. That lessens the stability challenge associated with acetonitrile. **Takeuchi** noted that the problem is other types of stability. **Crabtree** commented that the 15-person sprint will look at this issue. **Crabtree** responded to **Takeuchi's** other question about new cathodes sharing that these are about 30 percent better than the best results presented back in 2006. JCESR's candidate for the future is Cr_2O_4.

Rollett asked about the formation for lithium metal and putting lithium onto something that would reduce stress. **Crabtree** explained that the lithium has to go through that membrane. The insight or hope here is that by having a coherent contact that latches on the lithium and maintains it, the smoothness will work. Melt infusing lithium seems to be accomplishing this.

Hemminger expressed confusion about the graphene oxide films. **Crabtree** shared that before cycling, the layer looks perfect. The layer after cycling that JCESR is losing is the top layer which is smooth and looks homogeneous compared with the lower layers.

PUBLIC COMMENT

None

ADJOURNMENT

Hemminger adjourned the meeting at 11:15 a.m EST.

NEXT MEETING

The minutes of the Basic Energy Science Advisory Committee meeting held on June 9–10, 2016 are certified to be an accurate representation of what occurred.

Signed by John Hemminger, Chair of the Basic Energy Science Advisory Committee on (date).

(Insert electronic signature)