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

PUBLIC MEETING MINUTES

FEBRUARY 23 – 24, 2017

Hilton Washington DC/Rockville Hotel & Executive Meeting Center,
1750 Rockville Pike, Rockville, MD 20852

February 23 – 24, 2017
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 Tuesday and Wednesday, February 23 – 24, 2017, at the Hilton Washington DC/Rockville Hotel & Executive Meeting Center in Rockville, 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	Bruce Gates	Ian Robertson
Simon Bare	Ernie Hall	Anthony Rollett
Dawn Bonnell	Sharon Hammes-Schiffer	Frances Ross
Gordon Brown	Marc Kastner	Gary Rubloff
Sylvia Ceyer	Bruce Kay	Maria Santore
Jingguang Chen	Stephen Leone	Esther Takeuchi
Sue Clark	Despina Louca	Douglas Tobias
Helmut Dosch	Monica Olvera de la Cruz	John Tranquada
Persis Drell	Abbas Ourmazd	Stephen Wasserman
Cynthia Friend	Philippe Piot	
Yan Gao	Mark Ratner	

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

Committee Manager:
Katie Runkles, DOE BES

THURSDAY, FEBRUARY 23, 2017

WELCOME AND INTRODUCTION

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) was convened at 8:45 a.m. EST on Thursday, February 23, 2017, at the Hilton Washington D.C. / Rockville 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. Steve Binkley, DOE, Acting Director of the Office of Science (SC), discussed external and internal multi-level transitions impacting SC, as well as transitions in BESAC leadership

SC met with the Presidential transition team on January 20 for a program briefing. SC is awaiting confirmation on Governor Perry's appointment as DOE Secretary. SC has not received further direction from the transition team.

The appointment of Mick Mulvaney as OMB Director is a step in furthering the DOE Fiscal Year (FY) 2018 budget. SC is not yet aware of a schedule for budget submission but anticipates a budget may be due at the end of March.

Binkley reminded BESAC of Pat Dehmer's retirement from SC in 2016. Binkley applauded her role in basic energy science's evolution during her tenure.

Dr. Hemminger's tenure as BESAC Chair is concluding. Binkley shared his appreciation for Hemminger's leadership and the ways that BESAC has helped shape how SC is governed at a headquarters level. Persis Drell will move into the BESAC Chair role.

Discussion

Hemminger asked about the prospect of a continuing resolution. **Binkley** offered that discussion suggests that a CR will continue through the end of the fiscal year. It is believed that the Administration will try to affect changes in programs toward the end of the fiscal year.

NEWS FROM THE OFFICE OF BASIC ENERGY SCIENCES

Dr. Harriet Kung, DOE, Director, BES, shared her appreciation for Pat Dehmer's service and announced her receipt of the DOE Schlesinger Award in August 2016. Binkley will assume the role of Acting Director for SC and was formerly the Associate Director for Advanced Scientific Computing Research (ASCR).

Staffing changes in SC include the addition of Dr. Bruce Garrett as the Division Director for Chemical Sciences, Geosciences and Biosciences. Chuck Peden has joined Catalysis Science.

Kung recognized Dr. Mildred Dresselhaus who served as DOE SC Director in 2000 – 2001.

At the close of FY16, SC launched two solicitations for the Energy Frontier Research Centers (EFRCs). Four new centers were announced on July 18, 2016, and Kung reviewed the focus for each center and their respective partners.

A solicitation for the Computational Materials Science Awards was announced at the end of FY16. This will fill a gap in coding and data to design functional materials for materials sciences, and forge a path to exascale on the software side that complements hardware advances.

More than 15,000 users were hosted by BES facilities in FY16. There was a downtick with the closure of the National Synchrotron Light Source (NSLS). A diverse range of users are served by facilities with the greater numbers coming from life sciences and materials sciences.

A new initiative is the "mission need" approvals for facility upgrades. This is a follow-up to the 2016 BESAC Facility Prioritization Report. The Advanced Light Source Upgrade (ALS-U) and the Linac Coherent Light Source II High Energy (LCLS-II-HE) facilities will receive upgrades. Mission need approval has been gained and BESAC's recognition of these projects enabled the advancement of these initiatives.

Research highlights include work on controlled porous membranes for better batteries. This study features multi-university and industry partnership. The base research has developed membranes for lithium-sulfur batteries made from polymers on intrinsic micro-porosity.

BES has released a report on basic research needs (BRNs) for quantum materials for energy relevant technology. It elaborates on research opportunities in this field.

A report on synthesis science for energy relevant technology BRNs is near completion. It contains priority research areas. Kung asked BESAC to identify any glaring gaps that may exist.

A report on BRNs for innovation and the discovery of transformative experimental tools is forthcoming. It was supported by workshop discussions that proposed ways to couple experiment theory and instrumentation, and adjusting experiment parameters on the fly. This stages opportunity for major breakthroughs.

BES conducted an exascale requirements review with ASCR, looking at research areas for mathematical, software and algorithm developments to leverage exascale computing

architectures. Key scientific themes are identified that look toward advances in algorithms in quantum systems, math and computer science, and workforce development, respectively.

BES Communication produced a 2017 Summary Report that is an update to the 2014 Summary Report. It is an overview of BES and describes how it does business. Conveying how BES is furthering science and supporting the DOE are continuing communication efforts.

An EFRC 2016 booklet describes the first seven years and highlights of the EFRCs.

The EFRC Impact Report was published. It describes scientific thrusts undertaken by each center and their research aims. It features data on scientific publications and the intellectual property produced by the centers.

Kung offered her appreciation for Dr. Hemminger as the BESAC Chair. He is the longest serving Chair and covered the tenure of five SC Directors. His work was aided the construction of the five National User Facilities for Nanoscale Science, and publication of strategic planning documents to include Grand Challenge reports. These have helped BES research programs evolve in ways that could not have previously been envisioned.

Kung shared that BES will celebrate 40 years in 2017. It was formed due to the DOE Organization Act in 1977. A constant has been increasing knowledge of physical phenomena. BES' role in leading the transition to a new era of science is evident in its expanding budget, great community engagement, the maintenance of its portfolio of basic research, development of scientific tools and facilities, and workforce training.

It is anticipated that the budget situation will become more austere and BES is challenged to continue to show its relevance to DOE and leadership in national basic energy science.

Kung announced two solicitations anticipated in Scientific Discovery through Advanced Computing (SciDAC) and Experimental Program to Stimulate Competitive Research (EPSCoR).

There are upcoming workshops that will provide updates to existing focus areas.

Discussion

Hemminger thanked **Kung** for her comments and proposed that BESAC could support the identification of long-term impact examples in alignment with BES' upcoming 40th anniversary.

Dawn Bonnell asked if changes over time in user growth at facilities demonstrates changes in materials science and life sciences. **Kung** noted that capacity at facilities has changed. The life sciences field has become more aware of the value of tools and facilities, and facilities have engaged the field. **Steve Wasserman** added that efficiency has been gained in collaboration between users and facilities that lets people become more productive now versus 15 years ago.

Simon Bare commented that chemical sciences and facilities have new instrumentation for catalytic uses. Any user can now use the facility and this may be reflected in the user data.

Tony Rollett asked what science resonates well with Congressional committees. **Kung** shared that staffers show genuine interest and support, and the overall SC mission resonates well. It is a matter of setting priorities and acting as responsible stewards of precious resources, and showing leaders that these programs reflect wise investments with which SC has been entrusted.

In response to **Bruce Gates'** question about refreshing BRNs and their lifetimes, **Kung** noted that some fields have events that move faster than others. SC has to select which areas to refresh. Solar, for example, is an area that SC has thought about. Thoughts on additional topics are welcome. SC has limited bandwidth to conduct these updates.

Philippe Piot asked about the status of facility upgrades and the 20 cryomodules. **Kung** shared that this is an HD upgrade. The timing of project advancements depends on funding. Key

is preparing them for the opportunity. APS-U is the farthest in the pack and SC is awaiting FY17 appropriations to guide that. The neutron source upgrade at Oak Ridge is being prepared.

Helmut Dosch asked about the BRN list and appreciates the quantum materials list that was developed. He is concerned about conflicting climate change views and climate change research prospects. **Kung** shared that BES' main portfolio is aligned with energy security and offering solutions that indirectly add to climate or energy and national security. BES tries to stay neutral to politically-charged labeling. BES support for core disciplines and principles has not waivered.

Sharon Hammes-Schiffer asked about plans for another call for EFRCs. **Kung** shared that the EFRCs' future is tied up in the FY18 budget. FY17 is focused on sub-surface areas. Details are in Kung's February 2016 talk. The possible resolution in FY17 will help BES' decision. If there is funding available and time to execute it, getting organized will be a challenge.

Esther Takeuchi noted that BES' budget evolution shows a shift in the balance between research and operations funding over time. BESAC should consider this balance and how it should be adjusted over time. **Kung** agreed and pointed out that the FY16 budget reflects a goal to keep research at around 40 percent of total funding.

Gates proposed a request to show the value of the BES portfolio to fossil energy. **Kung** shared that aspects of the portfolio are very relevant to include carbon capture and sequestration. Catalysis work is another example. This speaks to the strong diversity of the BES portfolio and ability to address mission whether it is combating climate change or another aspect.

PRESENTATION ON THE BASIC RESEARCH NEEDS FOR THE ENERGY-WATER NEXUS (EWN) WORKSHOP

Dr. Matt Tirrell described the EWN Workshop held in January 2017. It came from a look on the applied side at fit-for-use water in 2014.

There is a need for new research and discoveries. The workshop assessed basic bottlenecks and gaps. Research directions provoked a look at efficient water use in energy-intensive processes, minimizing use for energy production, and expanding fresh water availability.

There are multiple connection points in the interrelation of energy and water. Water is a topic broadly relevant to basic energy sciences and basic questions that give opportunity for experimental and computational facilities.

Four panels were driven by the need to explore specific actions in their respective topic areas.

Panel one looked at improving water use in industry and electricity generation. Priority areas include modeling and monitoring water for purification and drawing out residual content.

Panel two looked at energy production exclusive to the sub-surface. Hydrocarbon extraction and geothermal interaction provoked a look at man-made chemicals into the sub-surface and the understanding of flow properties and reactivity.

Panel three examined increasing fit-for-purpose water availability and the ability to make water potable for some purposes. Fluid flow through naturally porous media was a focus along with sensing technologies.

Panel four examined material science questions that cross-cut the other panels.

This led to five themes that could become high-priority research areas.

The first is the fundamentals of complex fluids and is not exclusive to water.

Theme two focuses on interfaces and transport in confined environments, defined as natural formations and membranes that could support some separation purpose.

Third is materials and fluids by design, and designing new materials informed by the fluid material environment to improve purifying and moving fluids through the sub-surface.

Theme four consists of water purification and treatment, respectively. Purification applies to making water potable whereas treatment is about making water usable for some application.

The fifth theme covers ways that natural aquifers could enable transport but also be used to purify water in-situ to make waters in reservoirs to interact with waters in different ways.

Tirrell expects that final writing of the report will occur in the next seven days.

Discussion

Rollett suggested that theme one overlaps with the mesoscale report, and **Tirrell** agreed.

Stephen Leone asked about chemical insertion into water that is used for chemical extraction and if the DOE has discussed this. **Tirrell** shared that "fluids by design" in theme three reflects Leone's question. Some aspects of the water can be changed but you do not want to leave it behind in some way. There a chance that polymers or other materials could support absorption.

Tirrell confirmed for **Gates** that climate prediction was not discussed but is relevant.

Dosch asked if the report would refer to water-splitting issues and if it was discussed. **Tirrell** shared that it was not prominently discussed but was addressed in catalysis and other areas.

Monica de la Cruz noted that in theme one, gel could be used to drive greater strength and suggested opportunity in this area. **Tirrell** noted that theme two looked at examples where ion transport is enhanced by confinement. **De la Cruz** shared that this process could be very simple.

Bare asked about any discussion of aging U.S. infrastructure and the delivery of fresh water. **Tirrell** shared that this was not part of the workshop but certainly should be given attention.

Tirrell told **Gordon** that brining was a focus of panel two and there were good ideas. It was agreed that thermodynamic processes in more concentrated media need to be addressed.

Gates noted that there are pretty separation processes but felt that crystallization was missing. **Tirrell** shared that as a separation process, it would fit with panel one's discussion of ways to improve water use for industry and in electricity generation.

Hemminger asked about theme two and hoped that discussion about confined environment included reaction chemistry. **Tirrell** shared that this will be discussed. There is good raw material that will inform the final report.

Maria Santore asked about the potential for living organisms that could be manipulated by materials interactions for purification. **Tirrell** sees this legitimate. There were interesting discussions about fundamental biological research that may be outside BES' scope but there is opportunity for biological research to include biological methods for fit-for-use water.

Rollett asked about discussion of novel characterization and exploiting novel facilities that exist. **Tirrell** shared that this was part of panel four and how BES facilities could fit in.

REPORT ON THE GRAND CHALLENGE SCIENCE REPORTS: A RETROSPECTIVE AND PROSPECTIVE VIEW – PART ONE

Marc Ratner described the report, "Controlling Matter and Energy: Five Challenges for Science and the Imagination."

The overall challenge of the report was to make a leap from observation science to controls science, and to understand how to control materials and processes at the level of electrons.

Ratner reviewed outcomes of the 2007 Grand Challenge report. The report committee looked at research at U.S. institutions defining capabilities to transform basic energy science, how they might help secure our energy future, and produce new applications not yet imagined.

The underlying theory component had to be very strong and examine ways that theory is not formulated to compute anything. A culture for high-risk and high-reward systems was explored, and ways to attract top talent to develop new laws and concepts to control matter with precision.

A challenge was controlling materials process at the level of electrons and making quantum systems work for research and explore things at the core of understanding. A major area therein is to master and control data on the nanoscale level, learn energy and entropy manipulation, and develop and use sophisticated technology. Molecular motors and self-regulation figure into this. Understanding heterogeneities is essential, as is knowing the science of scale, rare events, epidemiology of heterogeneous populations, and degradation and lifetime prediction.

A second challenge was designing and perfecting atom- and energy-efficient synthesis. There are favorable cases at the threshold of directed synthesis of materials with desired properties.

Important was developing new tools to allow for material interrogation at the level of properties of individual molecules.

Facilities and EFRCs were established that helped address themes in the 2007 Grand Challenges report, and DOE has distinguished itself within the Federal government for its ability to construct facilities and instruments.

One challenge is the inability to develop crystal growth facilities.

Keys to advancement are sustained efforts over time, new support and training structures, and interdependent science.

Discussion

Gates asked how these activities have affected international science. **Ratner** shared that efforts have been hugely successful, especially in bringing in scientists from other places. Current challenges are due to funding and identifying good people in other parts of the world.

Hemminger asked if **Dosch** noticed the impact of the report in Europe. **Dosch** shared that reports that DOE has been issuing inform all strategic discussions and are used to spur European investments to stay competitive. The contributions of these reports are broad throughout Europe.

Ratner confirmed for **Despina Louca** that neutron sources are mentioned in the document.

REPORT ON THE GRAND CHALLENGE SCIENCE REPORTS: A RETROSPECTIVE AND PROSPECTIVE VIEW – PART TWO

Hemminger clarified that BESAC reports are run by BESAC and go through a final approval. BRNs originate from workshops run by BESAC. A BESAC report process usually starts with a charge from the SC Director. The processes can drag on due to the desire to get things right. The Grand Challenge report is an example due to lengthy discussion to define the five challenges. The challenges should have a relatively long lifetime.

In 2014, BESAC looked back at the challenges from 2007 to address their relevance. It led to a charge to BESAC to assess and validate the challenges. New discoveries and changes have occurred since 2007. Examples include the use of graphene, new materials, solar cell efficiencies, and x-ray synchrotron development. Changes have occurred since 2015, and yet the underlying themes of the Grand Challenges Report are still drivers even with progress. The reports allowed BES to take advantage of budget opportunities as they have come up.

Since 2007, it is accepted that nanoscience is important but next level complexity should be examined. This led to mesoscale science and push back from some who saw it as an older engineering principle. However, this led to discussion of more complex issues. The impact is seen in proposals to BES and the National Science Foundation Division of Materials Research.

The committee assessed the relevancy of the challenges and important transformational opportunities. Mastering hierarchical architectures and beyond-equilibrium matter is one area.

An understanding of critical roles and heterogeneity, interfaces and disorder present an opportunity. Understanding of this in confined environments is important.

Coherence in light and matter is another opportunity. This takes advantage of natural phenomena. Knowing this is critical to knowing the rules of nature.

Cross-cutting opportunities and challenges include making advances in models, mathematics, algorithms, data and computing. The coupling of theory and experiment is important, and labs and facilities need to get this right. The receipt of data informs what experiment to do next as it is being received. Rapid data analysis requires fundamental theory and applied math to learn how nature works. There is opportunity to optimize how experiments are done. There are groups of computational experimentalists and theorists that are coming to together to enable this.

Imaging capability advances present a cross-cutting opportunity. The coherence of X-ray sources signify big changes in experimental capabilities. Imaging at the atomic scale is critical.

There is value in pushing on synthetic approaches to advance discovery. The development of human capital is also essential and something that BES does.

Hemminger reviewed the tree diagram that explains the challenges and transformational opportunities. John Sarrao was recognized for the completion of the report "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science."

New BRNs are being developed and four BRN workshops are planned for 2017.

Discussion

Cindy Friend recognized that the same questions at the root of challenges remain and asked how the challenges can be effectively communicated without sounding redundant. **Hemminger** shared that reports have positioned BES to capitalize on emerging funding opportunities, and propose things vetted by the community. Not being repetitive is a challenge. Pursuing novel communication requires examining the evolution of what is happening in science and the opportunities that this provides, then coming up with reports to convey opportunities to do what we just accomplished. It is not practical to think of five new challenges every five years.

Hemminger confirmed for **Abbas Ourmazd** that there is more to be learned from existing data. He noted that funding agencies claim to care about data handling and archiving. In the past, archiving was not well handled. One needs to be careful in using older data that was not carefully archived. People need to get on board with how it is archived.

Dosch noted that the European Commission is discussing data handling and open data management among communities. The time difference between experimentation and publication can be pushed out by data standards to as much as three years. We might reconsider how an experiment is defined and a facility's obligation in data marking and analysis. **Dosch** asked if data management should be investigated more deeply. **Hemminger** added that the quality of data archiving is an important facet to management and understanding what data to retain or delete. Efforts cannot be random and a science community plan should be developed.

Ourmazd suggested the way that an experiment should be done be defined by how one will do the analysis. We are trained for tightly-controlled experiments but learn that more random experimentation can provide broader observations. There is opportunity to transform the culture in how we do experiments and better extract data from our work.

Gates noted that there is declining support for science and asked how to make a case for more support. **Hemminger** noted that BES is doing a better job at showing the impact of

research. BESAC could show the long-term, fundamental positive impact of science. One could go to the start of BES and identify breakthroughs that have come from investments. **Gates** asked if there is a way to make a case for advances that could have come from stable or greater funding. **Hemminger** often asks his students to consider how communication advances have changed the world, then to consider changes that could occur in the next 15 years. This type of exercise is worth considering but he questions how accurately breakthroughs could be predicted.

REPORT ON X-RAY LIGHT SOURCES: AN INTERNATIONAL PERSPECTIVE

Dr. Persis Drell and **Dr. Helmut Dosch** shared that BESAC and reports have helped build a range of BES facilities and encouraged a doubling of the basic energy science user community.

The overall desire to probe nature at atomic length and time scales are critical to the domain of the light sources. Goals in this realm to include control are being pursued globally.

With more than 60 facilities worldwide, x-ray light sources are an essential research tool. Five sources are governed by BES. There are ring upgrades internationally, new rings being developed, and new free-electron laser (FEL) investments to include the EU XFEL in Europe.

Strategy is critical to disciplined and coherent approaches, and the community has worked through BESAC to prioritize opportunities. The report in Spring 2016 led to a strategy for light-source upgrades. The APS-U will be replaced and positioned to be globally competitive. The Advanced Light Source-Upgrade (ALS-U) will be upgraded. The LCLS-II will be upgraded to high energy to also maintain competitiveness in the FEL domain. Construction on all three investments is deemed ready to proceed.

The storage ring strategy capitalizes on the strength of the rings and generating high brightness. FELs' strength is short timescales and high peak brightness. Desired parameters for either are different. Harnessing transverse and longitudinal coherence will be more possible through improvements. Longitudinal specifically can be achieved through FEL. The design of improvements focuses on maximizing photon beam brightness. Strategies for achieving desired brightness with storage ring and FELs differs depending on the source.

Accelerator physics and performance at LCLS has advanced past its baseline parameters. LCLS-II is now getting to high energies and transformation advances. Work is underway to study molecular dynamics, among other things. LCLS-II wants to cover both hard and soft x-rays

Helmut Dosch outlined the timeline of advances in Europe, recognizing the current thrust to understand complex matter. This requires coherent x-ray probes and time-resolution. The European strategy to address this challenge is getting the energy needed and a focus on electrons and spins. Understanding comes from a focus on atoms, ions and microstructure. Meeting these challenges requires storage ring sources with soft and hard storage x-rays, and the FELs to generate soft and hard x-rays.

Storage rings are a mature technology and used for the in-situ, operando interrogation of matter. FELs are considered more novel and disruptive, a discovery channel, and pathfinder for new technologies.

There are 12 soft-, medium- and hard energy storage rings, nearly all of which have upgrade plans or are being upgraded. The ESRF and PETRA are the two high-energy facilities.

Many FEL fundamentals are being undertaken. In particular, research is striving to provide a crystallography of local order and non-linear x-ray science advances. There are opportunities in the study of biochemical reactions and applied science, and opportunities for industry.

Conventional x-ray scattering from non-crystalline matter can point to huge advantages over crystalline matter as there is potential for new technologies to emerge. A two-point correlation

function has originated from these types of x-rays. It would not be possible from conventional x-rays. Higher order correlation functions come into play and allow for the elimination of intrinsic spatial and temporal averaging.

The crystallography of non-crystalline matter is a challenge, and the related technical challenges include ultrafast detectors, data storage, and big data petabytes.

Nonlinear x-rays are not often discussed but hold significant potential. The combination of laser with the atom allow for needed disruption. There is no opportunity for x-ray tunneling ionization and new nonlinear physics.

There are seven FELs in Europe. Dosch supports the DESY facility in Hamburg, Germany. It features the co-location of multi-disciplinary facilities.

Photon science is represented by the XFEL, with PETRA IV debuting in 2025, and FLASH in 2020. There are four photon science research centers. Dosch presented the XFEL layout.

The European Commission seeks better facility integration and a more compelling science case. Focus also include long-term sustainability, support to initiatives for greater innovation, creating and advancing communities for integration, and training future lab managers. There is a gap between countries making technological advances and others falling behind.

Dosch established the League of European Accelerator-Based Photon Sources (LEAPS) to respond to the Commission goals and to drive a roadmap for storage ring and FEL facilities, as well as develop useful metrics. The strategies for this concept will take hold in November 2017.

China's strategy is focused on six facilities to include the new High Energy Photon Source (HEPS). Facilities are located in Beijing and Shanghai.

South Korea is making strides with the creation of the PLS-II storage ring and a highly-efficient XFEL, the latter of which is a state-of-the art facility.

Japan has eight facilities to include the Harima Spring-8 and Tsukuba (KEK) facilities.

Leading photon science facilities will have FEL and storage ring strategies, robust long-term funding, and research centers that are exploiting x-rays. Dosch believes that DESY and PSI in Europe will be dominant, and facilities in Pohang, Harima and Shanghai will emerge as leaders.

Exciting breakthroughs are emerging around the globe. Dosch thanked Hemminger for his leadership and shared that the U.S. light source strategy is influential on an international scale.

Discussion

Gao asked what is driving the European strategy. **Dosch** shared that the current language for storage rings is different from the U.S. and new branches of technology. Facilities can give non-expert users lasers in space and time and energy, and provide educated, tailored environments to get needed data. Now the view is that expertise is not needed and European facilities allow for providing information that people need for their technology roadmaps.

Brown asked if there is concern in Germany about the balance between spending on facilities and on research. **Dosch** believes that a nuclear failure in Europe was detrimental to that work. The scientific community should be embraced and show the enormous impact possible. Facilities are pushed to be benchmarks for science and establish the best of the best. Allowing access to the facilities is good for science.

Dosch confirmed for **Brown** that having a leader in Germany who is a scientist.

Gary Rubloff asked about the extent of synthesis work. **Dosch** shared that things are becoming more complex and facilities should define the experimental environment as things become more complex. Facilities are focused on separate areas. X-ray plus alone is not what is needed. The environment is needed to attack all complexity.

NATIONAL SYNCHROTRON LIGHT SOURCE-II OPERATIONS UPDATE

John Hill, Director, NSLS-II, discussed the challenges of standing up the facility.

Several experiments have taken advantage of high coherent flux to include facilitation of the first event speckle and XPCS measurement of charge stripes.

The soft inelastic x-ray (SIX) beamline renormalizes spin excitations and has a low enough resolution to detect excitations. First light was achieved on February 20th.

Accelerator performance has grown from around 25 milliamps to more than 250 and around 96 percent reliability. The accelerator division has been busy with usage, the increase in milliamps, and insertion of new technologies.

There are 19 beamlines which has enabled user support to get up and running. Six more beamlines are planned. The completed beamlines are in operation or in commissioning.

Beam time proposals have grown from 117 in 2015 to 340 in the second quarter of 2017. The number of users in FY17 is 334, with a high of 477 in FY16.

NSLS-II partners with the Center of Functional Nanomaterials. A partnership with Oak Ridge National Laboratory (ORNL) lets a user to write a proposal and use NSLS-II and ORNL.

A current challenge is management of the large amounts of data and data flux. NSLS-II uses its own unique data acquisition system called BlueSky.

A scientific highlight is use of the hard x-ray nanoprobe to understand proteins on the surface of an E.coli molecule. In another study, the nanoprobe was used to image grain boundaries in battery materials. Soft x-rays were used to understand the dynamics of polymer gels applicable in areas such as artificial skin and self-healing gels. Another example is feature collaboration with the nanocenter which used self-assembly of 3D block copolymer morphologies.

Next steps for the NSLS-II are to maintain existing beamlines and accelerator operations, and develop new beamlines. The user community described the beamlines needed and led to the list of six beamlines to be built starting in FY17. The beamlines will give world-leading capabilities and enhance NSLS-II. It is working with BES and others to fund more beamlines.

Discussion

Hemminger asked if there is a machine level understanding about not changing beamline energy in one CSX without impacting energy in another beamline. **Hill** shared that there are things that could be done with masks but the best long-term fix might be moving the beamline.

Hill told **Jingguang Chen** that staffing levels need to be constant to balance the building and use phases. The type of work can change for some depending on the phase of an activity.

Hill responded to **Ernie Hall's** interest in the user program, block allocation and partnership users. Block allocation is for groups sharing a geographic location or common interests. NSLS-II manages time for their work. Partnership users are of two types – those who build an entire beamline and use it, or others who make contributions and partner with NSLS-II to get capability out of what they helped build. **Hall** asked if the partner users were part of the data on users. **Hill** shared that up to 40 percent of the time can go to users. **Wasserman** added that the block allocation operates like that at ORNL. Proposals may feature work on similar or related systems.

PRESENTATION ON BASIC RESEARCH NEEDS WORKSHOPS AND REPORTS: A RETROSPECTIVE AND PROSPECTIVE VIEW

George Crabtree reflected on an initial BRN workshop and the "Basic Research Needs to Assure a Secure Energy Future" report from 2002. World and energy-related events in 2002

were transformative. Oil prices, the emergence of shale oil and gas, electricity from coal, and renewable energy have been transformative. Many predictions were missed as most predictions extrapolate the present. Breakthroughs that occur due to disruptions and new discoveries cannot be predicted. As a result, breakthroughs should be pursued and not passively awaited.

Basic science breakthroughs address showstoppers in current technologies. They can grow the performance, cost and efficiency of current technologies, and are transformative rather than incremental. Examples include controlling matter and energy flow at many levels, working beyond equilibrium, and in-situ observation of chemical reactions as they occur. Transformation can also advance the frontiers of science.

The spectrum of basic to applied science feeds three products: Grand Challenge Reports, BRN Workshops, and DOE and industry roadmaps. BRNs fit in the middle of the spectrum.

The 2002 report led to 17 reports over 14 years and the input of more than 2,000 participants.

Crabtree reviewed the BRN workshop format. Workshop reports are available up to three months following a workshop and can project outward as much as 10 years. The reports can focus the intellectual power of the community on specific problems.

The report on high-energy lithium batteries is an example of a BRN report. Additional examples are reports on metal-organic frameworks for low-energy carbon capture, and the materials project that addressed powerful computing and analysis to discover novel materials.

Since 2016 and over 2017, BRNs will focus on quantum materials for energy relevant technology, synthesis science, transformative experimental tools, the energy-water nexus, next-generation electrical energy storage, catalysis science, and next generation nuclear energy.

The cost of discovery is smaller than development and even more so compared to technology development. Grand challenge and discovery science costs are low but can pay off big. They can indicate what will fail before spending on development and primes the innovation ecosystem.

Discussion

Crabtree described for **Marc Kastner** the evolution of the BRN process and how it has improved over time. It has fed the preparation of talking points to seed discussion, the development of a writing session, and higher-level communication once a report is done. There is also opportunity to track reports back to actual innovations like current car batteries.

Hemminger relayed **Leone's** note that the word "refresh" may not be the best descriptor.

Crabtree told **Rollett** that there is a reference for the data on half of GDP since World War II being due to innovation.

Friend cited examples and how reflection and learning might be applied to basic science examples and finding more disruptive pathways. Crabtree talked about things that come together in the convergence and how science will play a role. Science may not dominate all of the convergence that takes place.

Gates asked how round two workshops might be different from the first one and this new paradigm. **Crabtree** suggested that there could be investigation of what has the most promise and not harping back to the first workshop too much.

Brown shared that a replacement word for refresh could be "evolution."

REPORT ON THE ASCAC LDRD REVIEW

Dawn Bonnell shared the Advanced Scientific Computing Advisory Committee's (ASCAC) Laboratory Directed Research and Development (LDRD) review.

LDRD has been around since 1954 and investigates future direction and program reinvigoration. LDRD's annual budget is around $540M and is from overhead charged by individual labs. They use LDRD to accomplish goals that include undertaking an input process to understand future directions and looking at ways to evolve programs to avoid stagnation.

The committee looked at four labs to understand LDRD program processes and impact. There is a broad span of projects. ASCAC learned about spending, outcomes such as publications, workforce support, labs' goals and successes, and the involvement of researchers at different points in their careers.

One observation is that the LDRD is crucial to national laboratory system vitality. In addition, the committee found that mapping goals to LDRD processes varies from one lab to the next and yet LDRD goals match the overarching strategic framework for laboratories.

The committee expects to have a final report in April or May 2017.

Discussion

Gates asked how researchers seek funding. **Bonnell** noted that it is common to seek seed funding and have individual or joint funding calls to explore ideas. Security labs use smaller amounts for unclassified work and classified work that may help predict what is to come.

Hemminger relayed younger peoples' comment that decision making is not very transparent and asked if the committee heard this. **Bonnell** knows the nature of that comment. At times, leaders might merge ideas. That may not seem clear. Opportunities are communicated to younger researchers around the program and the feedback from that is made clear.

Frances Ross asked why labs do not use the maximum percentage of funding. **Bonnell** answered that this funding is accrued from their overhead. Maximizing this maximizes their overhead rate. National security labs maximize this as they have a challenge in keeping their workforce and want to provide as many opportunities as they can to keep them involved.

Doug Tobias asked about the success rate of LDRD proposals and the variance among labs. **Bonnell** doesn't have the sense that there are large disparities. The greater focus was on the success that came from funded proposals. How often and what impact they will make are useful metrics. In each lab, this evolution to a program can happen on an annual basis.

PRESENTATION ON THE ENERGY FRONTIER RESEARCH CENTERS / INNOVATION HUB COMMITTEE OF VISITORS REPORT

Sylvia Ceyer reported on the EFRC / Innovation Hub Committee of Visitors (COV) activity from November 2016. The COV charge was to assess the efficacy and quality of processes used to solicit, review, recommend and document proposal actions and monitor active projects. And, within boundaries of DOE missions and available funding, to comment on how award process has affected the breadth and depth of portfolio elements, and national and international standing.

The 20-member committee addressed the EFRCs and the Hubs in two groups. This was the second EFRC COV and second for the JCAP Energy Innovation Hub. It was the first COV for the JCESR Energy Innovation Hub.

The EFRCs and Hubs make a compelling case for the role of fundamental research in meeting U.S. energy needs. The EFRC and Hub construct enable this success.

EFRC award processes are rigorous and effective. However, the number of proposals for review can be daunting and could likely result in incomplete documentation for declined awards.

Twenty-five proposals were received for an award call in 2016. In the future, a call will go out every two years to distribute the workload and reduce the award time from five years to four.

The COV recommended that BES explore ways to lower the number of full proposals being reviewed simultaneously. The COV suggests reinstituting a return to a five-year funding model. Four years is not optimal to achieving a maximum scientific impact.

The time between the FOA and due date is often short. This may favor those already engaged with DOE or places that have proposal support and development infrastructures. BES could look for ways to alert the community more broadly about the potential issuance of an announcement.

There were no statistics about women and minorities represented.

EFRC management is effective with effective stewardship of Federal resources. That allows for timely redirection of funds for promising lines of investigation. Management success is seen in the high impact of research. BES and EFRC program directors and researchers have ample communication and yet the multitude of reporting requirements may draw valuable resources.

EFRCs feature an appropriate mix of research and use-inspired topics. The scientific contributions to fundamental science are impressive. The technological impacts are seen in the number of patent applications. There is emphasis on the training of postdocs and students.

The 2015 JCAP renewal was reviewed. A disciplined decision to restrict eligibility included recommendations from the Secretary of Energy Advisory Board. The review was adequate. However, it had six reviewers and the merit review plan only calls for three reviewers. This could be looked at by BES. There was no reviewer who had expertise in CO2 reduction.

The processes used for JCAP renewal were excellent and considered past investment and performance, and that findings be well documented for future renewals.

JCAP management has evolved significantly. The motivation came from on-site reviews. It was unclear if examining milestones to look for modification or adjustment will be continuous.

There should be a final five-year summary of accomplishments that serves as a retroactive measure of transformational impact.

The JCESR procurement processes through to selection were rigorous and well documented. BES' expectations were clear and appropriate guidance was given to the review team and Hub leadership. There were 11 to 13 mail reviews for each proposals. Resulting evaluation scores were spread out and the award was consistent with scoring.

For JCESR, a pre-FOA meeting was held. It is a good practice to ensure understanding of expectations and how this type of program fits into the overall energy strategy.

The JCESR management practices are excellent, and there is synergy between JCESR and BES resulting in new management strategies that are underway at JCESR.

The Energy Innovation Hubs demonstrate world-leading scientists conducting high-risk innovation research that will advance science and understanding from early research to industry.

It could be useful to link JCAP's work in CO2 reduction with other researchers' work. And, it would be useful to see better alignment of Hub research with others.

Funding ends after five years. BES should find ways to continue the investment or reuse what is already in place. DOE should create a process to gauge the Hub's international standing.

It is recommended that the EFRCs and Hubs produce more concise reports and descriptions of accomplishments. It is also important for program managers to travel to facilitate site visits.

Discussion

Gates asked for details about five- versus four-year EFRC funding terms. **Ceyer** noted that EFRC reviewers felt that the time between the award, a team's arrival, hiring, and startup moves quickly. Then two years later, renewal is on their minds. Five years would be more effective.

Ceyer clarified for **Rubloff** that the sunset clause should be maintained but a Hub's goals should be retained. **Hall** added that the investment is significant and after the end of a 10-year period, BES should guide ways to identify alternative funding to make use of the expertise and capabilities that have been developed. **Hemminger** agreed that the Hubs are a big initial investments not to be lost after the 10 years.

Ourmazd suggested that it is hard to find non-conflicted reviewers. **Ceyer** shared that the COV recommends pre-proposals that would not fewer reviewers, could be reviewed more rapidly, and would not exhaust the reviewer pool as quickly. There are disadvantages to this also and other things that may be considered. BES has also used international reviewers.

Hemminger asked for a vote of formal acceptance of the report. The BESAC asked to delay the vote until day two to give time to read the report.

PUBLIC COMMENT

John Galayda relayed that NCLS-II received advice from DESY and a large European contingent when it was started. **Hemminger** suggested that **Dosch** address this off-line.

Claudia Mora noted that discussions comparing U.S. and Europe light source advances brought up the shutdown of the "ANKA" source. It is one of the few sources for actinides. Mora asked how the BESAC feels about the need to study actinides. **Hemminger** noted that the whole issue of actinide chemistry is important to the DOE and should not be allowed to fade away. **Clark** suggested that linking this with other science presents phenomenal opportunities.

ADJOURNMENT

The meeting was adjourned by **Hemminger** at 5:23 p.m.

FRIDAY, FEBRUARY 24, 2017

The BESAC meeting was convened by **Chair John Hemminger** at 8:40 a.m. EST. Hemminger delayed the start of the meeting to allow BESAC members to read the WDTS COV report. A second report on the EFRC / Hub COV report was assigned for reading overnight.

PRESENTATION ON THE UPCOMING BASIC RESEARCH NEEDS – REFRESH PLANNING

Linda Horton and **Bruce Garrett** of BES described the upcoming Basic Research Needs (BRN) Refresh Planning. Horton showed the overlay of DOE BES and BESAC reports with fundamental breakthroughs in chemical and materials sciences, and fields of study.

The BRN for Next-Generation Electrical Energy Storage (BRN-NGEES) workshop will be held on March 27 – 29, 2017. The energy grid and integration of renewable power into the grid are vital technologies. There is a need to address challenges due to greater use of renewables. The widespread use of hybrid and all-electric vehicles are also drivers. Breakout panels will address the growth in the sophistication of basic science around these energy technology issues.

Drivers within BES for the BRN-NGEES include an increase in battery-related research and greater community focus, and the advent of the EFRCs and Hubs. Other factors are the advanced computational tools in battery research are gaining more use, and user facilities' increase of in-situ capabilities, and community advancement.

The BRN for Nuclear Energy will occur on June 11 – 14, 2017. New reactor concepts have brought new challenges to the field. Molten Salt reactor concepts, long lifetime projections

without fuel change-outs, the prospect of new designs with higher temperatures, and emphasis on non-proliferation and safety are driving this BRN.

Planning for the workshop will seek to identify high priority basic research for future nuclear energy systems, with a focus on future generations. Earlier reports will be refreshed, and challenges around performance and lifetimes of fuels will be addressed.

The BRN for Catalysis Science to Transform Energy Technologies will be held on May 8 – 10, 2017. It is driven by changes in the energy landscape and the consequent desire for advanced catalysis. Diverse uses of resources such as shale gas for feedstock have economic impacts. Catalytic techniques exist but need advancement. Changes in energy resources impact carriers and services, and catalysis is needed to support this landscape.

Various technical drivers push the need for the BRN, and include more abundant shale gas and low-cost renewable electricity, respectively. The ongoing need to maximize energy efficiencies is a driver, as well as the need for catalysts that originate from earth-abundant materials. There are also economic drivers such as the expanse of clean-energy jobs.

The BRN will build on a 2007 workshop, a 2009 National Academies of Sciences review of the BES Catalysis Sciences Program, and the Sustainable Ammonia Synthesis Roundtable last year. The design of low T, low P processes is a driver that emerged from the 2016 roundtable.

The BRN will assess basic science bottlenecks and gaps in understanding catalysis issues, and identify research needs for catalytic processes that support resource conversion or use. It will emphasize challenges that present significant impacts. Challenges will be met via four topics.

Discussion

Rollett urged addressing manufacturing issues and that advanced imaging techniques can be applied. **Garrett** thinks that topic three in the Catalysis BRN will see how fundamental science affects industry. **Horton** believes that more can be done in high-temperature environments.

Dosch proposed replacing the word “refresh” with “update.”

Bare suggested that the drive toward more selective processes seems to have been omitted. Separation presents the most costly aspects. **Garrett** agreed that this is important and will be a big driver in the move toward smaller size. He expects it to be part of the Catalysis BRN topics.

Friend suggested the term “new era” rather than “refresh.” **Horton** likes the term “2.0.”

Hall brought up BECAC’s science for technology energy report. There could be something built to address manufacturing technology. In addition, there seem to be topics that were previously addressed that are being woven into the BRNs. That is a positive development.

Chen did not see a reference to more abundant pathways in the Catalysis BRN description. **Garrett** shared that this is one of the drivers and it will be discussed.

Gates asked if catalysis topics one through three provoke the need for new catalysts. **Garrett** responded that this is clear in the drive for new approaches and there can be new efforts. This is an emphasis in the JCAP. For feedstocks, it is a matter of getting to the selectivity issue. That will be part of topic one. Topic three will focus on pressure and temperature. Catalysts today could be running at lower temperatures and there can be different functionality than at present.

PRESENTATION OF THE WORKFORCE DEVELOPMENT FOR TEACHERS AND STUDENTS (WDTS) OVERVIEW

Jim Glownia, Director, SC Office of Workforce Development for Teachers and Students (WDTS), told BESAC that the WDTS is a workforce development effort and supports the DOE mission at the highest level. Bringing in young researchers is an emphasis and ties clearly to SC.

The DOE labs have 30,000 scientists and engineers. Meeting workforce needs allows for mapping across the DOE. There are experience-based learning opportunities in a unique environment. Around 70 percent of the overall budget goes to labs but was once just 25 percent.

WDTS programs are all lab-based. The largest program based on funding is the Science Undergraduate Laboratory Internships (SULI). Participants are at labs working directly with staff. They are encouraged to pursue science careers based on awareness of pathways. Students come from undergraduate institutions and community colleges, and all receive mentor support.

Undergraduates can be sophomores through seniors. For older students, SULI can be a bridge to graduate school. Deliverables include a structured research report, oral or poster presentation, engagement in a peer review activity, and the creation of a general audience abstract. WDTS manages SULI applications but host labs themselves make their selection of participants.

Community college participants can participate in the spring, summer or fall.

The Office of Science Graduate Student Research Program (SCGSR) lets graduate students conduct thesis work at a DOE lab with a collaborating PI. Students can apply their skills with specific capabilities at a lab. Students receive a supplemental award, housing and travel stipend, and are qualified Ph.D. candidates. They develop a collaboration with a scientist at a DOE lab. Glownia described the application review and selection process.

The visiting Faculty Program seeks to grow the competitiveness of faculty members who work at historically-underrepresented institutions. Faculty can work directly with DOE lab staff on projects. Faculty can bring along up to two students. A joint research proposal is required.

WDTS programs are now at 16 of 17 DOE laboratories and at two user facilities.

The WDTS Application and Review System (WARS) is an online system that seamlessly collects data and keeps people in swim lanes regarding their role within WDTS. WARS and evaluation have been transformative to the growth of WDTS.

Longitudinal surveys of participants are a next step.

Discussion

Glownia confirmed for **Drell** that labs get together to share lessons learned and collaborate. Program reviews convene the labs. Each has extensive expertise in conducting these programs. WDTS' goal is to conduct programs uniformly. There are core requirements and a set of model practices, fulfilled by each lab's implementation plan. They consider each lab's unique setting. A recent peer review will refuel collaboration and drive toward a shared fate. **Drell** suggested that the rising talent does not always look like the talent in place. **Glownia** acknowledged that the most appropriate students for this experience are not always the ones involved.

Ratner asked about feedback on SULI. **Glownia** shared that anecdotally there is data about long-term impacts but that is a challenge in STEM. It is hard to find alumni and SULI has been going on since the 1970s.

PRESENTATION ON THE WDTS COMMITTEE OF VISITORS REPORT

Gordon Brown reviewed the 2016 WDTS Committee of Visitors (COV) report. WDTS started in 1990 with an emphasis on getting more students into STEM education. It is meant to counter retirements in the labs and train the future workforce in ways that affect changes in the laboratories and that reflect changes in the ethnic composition of the workforce.

The COV reviewed the WDTS SULI, community college program (CCI), Visiting Faculty Program (VFP), and the SCGSR. The COV charge included looking at changes since the 2010 COV review, and WDTS' new directions and new operational baselines for the four programs.

Most recommendations from the 2010 COV have been implemented. These include the elimination of some programs and shift of funds to new ones, the start of the SCGSR, expanding WDTS leadership, a closer relationship to Laboratory Education Directors (LEDs), the creation of WARS, and alignment of WDTS reviews with SC program reviews.

A town hall meeting with LEDs generated positive feedback about WDTS. Highlights included appreciation for WARS and WDTS leadership, and increasing coordination among the laboratories. Five of the six participating labs have more capacity to accept more participants.

The COV presented 15 recommendations. Notable is urging WDTS to evaluate the impact of SULI on student career selection, and increasing the number of SULI internships. The CCI program should seek additional funding to encourage involvement in the lab workforce, and engage more local community colleges to obtain a diverse participant pool. Outreach associated with the VFP should be more active, increase in breadth and impact, and ask VFP participants to be mentors and career advisors. The COV recommended that the SCGSR match the Ph.D. timescale, assess the impact of multi-year awards, and evaluate the potential interest of and impact of M.S. students. The SCGSR could be restructured to standardize mentor identification, and mentors could give more detail on students' activities following SCGSR participation.

Brown reviewed WDTS' new direction and that WDTS has been reviewed in different ways two other times since 2012. The 2012 site visit identified the value of core requirements. A peer review in 2015 – 2016 focused on specific programs and the need for high-impact experiences.

The COV recommended engaging high school students, and that WDTS work with SC, NSF and other STEM agencies to build a diverse future workforce. It was also recommended that the WDTS Equipment Donation Program be better advertised at laboratories.

Discussion

Bare asked about adding a graduate-level SULI program and how this is different from the SCGSR. **Brown** explained that the SCGSR is really thesis research, and SULI is for students in programs. There is a way to get M.S. and Ph.D. students involved early to guide their careers.

Brown told **Drell** that there was little access to demographic data about participants especially as this COV looked at process and was not a program evaluation. There is little information about long-term STEM career impacts. **Glownia** confirmed that there is data and it can be made available to labs in a compliant manner. **Hemminger** reminded BESAC that this is always an issue related to privacy rules.

Ross asked about the success rate for students' entry into a lab. **Glownia** pointed out that about one in three are accepted for summer programs. The semester rates are less competitive and there are fewer students.

Maria Sartore pointed out that there are many students not ready to get a Ph.D. and the need to help them develop skills to do this. This is a community problem and there are few internships for master's students. **Brown** explained that the problem is that students must have a 3.0 GPA and ultimately the mentors are the ones who interact with students. There really is no evaluation of the success of these programs. The CCI program does address this but consists of only around 100 students. **Sartore** pointed out that this is only in certain fields. **Brown** shared that the labs emphasize specific and applicable fields. **Glownia** added that an M.S. is often a terminal degree especially in a field like computer science.

Takeuchi asked if there could be information at the next BESAC meeting that describes the WDTS diversity range.

Brown added that **Pat Dehmer** is really the one who salvaged the WDTS program and brought it forward from the 2010 COV. A major takeaway from this COV was lab directors' happiness with WDTS and Glownia.

Hall suggested that one of the greatest needs are support staff who maintain equipment and the like. **Brown** shared that CCI does this but only reaches about 100 students per year.

Hemminger applauded the review.

Bare moved to accept the WDTS COV report, **Drell** seconded, and the BESAC voted and accepted the report.

BESAC BUSINESS

Hemminger confirmed that the members had read the EFRC and Hubs report from day one. **Ratner** suggested that EFRCs are well known but little is known about the future. **Kung** shared that SC is still awaiting for information about the budget. The BESAC moved to accept the EFRC and Hubs report.

UPDATE ON THE CHEMICAL SCIENCES, GEOSCIENCES AND BIOSCIENCES STRATEGIC PLANNING AND COMMITTEE OF VISITORS PLANNING

Bruce Garrett described the Chemical Sciences, Geosciences and Biosciences (CSGB) strategic planning process as a way to align activities in the portfolio in order to work on the most important things. The mission and vision for CSGB proposes balancing discovery and use-inspired research while also conducting innovative management of the portfolios.

Fundamental interactions, photochemistry and biochemistry, and chemical transformations are the three areas of emphasis in CSGB. There are additional division-wide themes that impact the Division's work. These define problems that should be looked at in the future.

The photochemistry and biochemistry team is an activity that is integrating the vision across programs. The scientific programs interact with and are aligned to specific scientific processes.

The planning activity has been assessed at the level of core research areas (CRA), looking at current programs, capabilities and opportunities. The next step is to analyze CRA level findings, set direction and define objectives to advance the portfolios. An action plan will account for budget, organization, operations and communication. The latter is critical to CSGB success.

The Condensed Phase and Interfacial Molecular Science (CPIMS) is an example of how a program goal can be aligned with team and division focus, and shows how the planning activity can be effectively executed. CPIMS addresses surface-types studies, ways to understand water, and learning more about transitioning from molecular-scale chemistry to collective phenomena in complex systems. Garrett discussed areas of reduced and increased emphasis within CPIMS. The program will address the mesoscale challenge and has relied on BESAC reports since 2007.

Dosch pointed out that in the area of reducing emphasis, there are capabilities at SLAC that allow for understanding the dynamics of single molecules with extreme spatial and temporal resolution on model systems, and exploring these in a new timescale.

Dosch wondered about how this will increase the emphasis of future work. **Garrett** explained that this is true in the overall portfolio and that it may impact other SC programs. Work is moving away from focus on a single molecule. This is just one of 15 core research areas that SC has so this is just an idea about where things are going now. This is not necessarily true of the overall portfolio.

Garrett acknowledged **Hemminger's** comment that the BES science community is very interested in this strategic planning process and that the chemistry community through program

managers and PIs has been engaged. PI meetings are an opportunity and program managers are asked to share plans for the future and get feedback on those. This is a snapshot of today. Molecular imaging is something that can grow from other investments. There are investments in other places in SC that can inform.

Ourmazd found it to be helpful to attend community meetings to know where the field stands and to build new partnerships. He added to **Dosch's** earlier question about reduction, commenting that the amount of relevance of a single molecule may not be relevant in a large scale if one wants to know about catalysis with is often at high pressure and high temperature. **Garrett** responded to thoughts about PI meetings. They help build the community, inform state of the field understanding, and give input on future direction. In terms of earlier comments about areas being reduced, SC is not entirely going away from that. CPIMS is really about more complex interfaces and process. There could be a role for more single molecule studies in those. We need to find ways to understand what others are doing and identify the big goals.

Hemminger recommended that BESAC stay closely connect with the CPIMS planning process as it moves forward.

Friend described the use of the model systems to understand complex interfacial and solution systems as important to understanding complexity. These should be taken into account. **Garrett** shared that this a core system and some things have to be given up to get there.

Gates talked about maintaining the balance and health of university programs, noting that there are trends to do better science, software and facilities, yet budgets go down. **Gates** asked how health can be assessed, what conditions are being used to make assessment about big issues, and when science programs get too big to be sustained. **Garrett** agreed that these are important considerations. SC reviews individual projects and review the portfolio internally. SC is open to suggestions on looking at things more holistically.

Garrett continued with an overview of the CSGB COV to be held on March 28 – 30, 2017. He reviewed the charge and commented on how the Portfolio Analysis and Management System (PAMS) has enabled reviews. The collection of demographic data is becoming popular but at this time is too incomplete to present in this COV.

Specific recommendations from COVs in 2011 and 2014 have been initiated and continued. The 2017 COV will review actions taken by CSGB in FY14 – FY16.

The COV will examine each of the CSGB's three topic areas. Garrett described the agenda for the review and the materials that PAMS will provide.

Discussion

Hall commented that having a COV in a hotel in his prior COV activity was more efficient than getting people into and around a DOE facility.

Kay predicts that a recommendation for this COV will be identifying more travel funds to allow programs managers to travel to meetings to hear about the research they are funding. **Kung** shared that the funding is tied to program director funding. In recent years there has been a trend that the overall size of the federal staff. Funding has been constrained and will likely continue to be constrained. Last year, SC had a travel moratorium and many trips were cancelled. This has not stopped SC from making this critical recommendation and the need will not go away.

PUBLIC COMMENT

Ken White thanked the BESAC for the WDTS COV. He thanked Pat Dehmer and Julie Carruthers for transforming the WDTS program over many years. It is rewarding to bring young

people into the DOE and use facilities and tools to do so. By the end of the program, students know that they can work in a lab and fit in. WDTS is an important piece. WARS is exciting and gets closer to a complex-wide assessment system. The model practices and core requirements aspect of WDTS' implementation was invaluable to one of White's colleagues and helped her fall into her role, get her up to speed, and set standards for implementing the program. These programs are more than what you see on the surface. They set a baseline for labs to work in this area and bring young people into the facilities. White can go to other agencies and venues, and partners with other people based on his strong program. The WDTS platform creates many more opportunities. Anecdotally, one of his lab's directors was a student in a laboratory, and White has the benefit of a colleague who is now working within his facility to bring people in to use the synchrotron.

ADJOURNMENT

This is the final meeting for **Hemminger** as the Chair. He thanked BESAC members and the SC for their collaboration. **Hemminger** adjourned the meeting at 11:10 a.m. EST.

The minutes of the Basic Energy Science Advisory Committee meeting held on February 23 – 24, 2017 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)